On boundary value problems for Willmore surfaces and Hartree-Fock theory of pseudo-relativistic atoms

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Zusammenfassung

Die vorliegende kumulative Habilitationsschrift befasst sich zum einen mit Willmoreflächen, die vorgegebene Randbedingungen erfüllen, zum anderen mit dem Hartree-Fock Atommodell für pseudorelativistische Atome. In beiden Fällen untersuchen wir dazu ein Minimierungsproblem und die qualitativen Eigenschaften der Lösung. Im ersten Teil dieser Habilitationsschrift, der aus den folgenden Artikeln besteht, werden die Resultate zu Randwertproblemen für Willmoreflächen vorgestellt.

[1] A. Dall'Acqua, K. Deckelnick, H.-Ch. Grunau, Classical solutions to the Dirichlet problem for Willmore surfaces of revolution, *Adv. Calc. Var.* **1** (2008) 379–397.

[2] A. Dall'Acqua, S. Fröhlich, H.-Ch. Grunau, F. Schieweck, Symmetric Willmore surfaces of revolution satisfying arbitrary Dirichlet boundary data, *Adv. Calc. Var.* **4** (2011) 1–81.

[3] M. Bergner, A. Dall'Acqua, S. Fröhlich, Symmetric Willmore surfaces of revolution satisfying natural boundary conditions, *Calc. Var. PDE* **39** (2010) 361–378.

[4] M. Bergner, A. Dall'Acqua, S. Fröhlich, Willmore surfaces of revolution bounding two prescribed circles, Preprint Nr. 13/2010, Universität Magdeburg, eingereicht.

[5] A. Dall'Acqua, Uniqueness for the homogeneous Dirichlet Willmore boundary value problem, Preprint Nr. 06/2011, Universität Magdeburg, eingereicht.

Gegenstand des zweiten Teils dieser Habilitationsschrift ist die Hartree-Fock-Theorie pseudorelativistischer Atome, welche in den folgenden Artikeln behandelt wird.

[6] A. Dall'Acqua, T. Østergaard Sørensen, E. Stockmeyer, Hartree-Fock theory for pseudorelativistic atoms, *Ann. Henri Poincaré* **9** (2008), no. 4, 711–742.

[7] A. Dall'Acqua, S. Fournais, T. Østergaard Sørensen, E. Stockmeyer, Real Analyticity away from the nucleus of pseudorelativistic Hartree-Fock orbitals, Preprint Nr. 9/2011, Universität Magdeburg, eingereicht.

[8] A. Dall'Acqua, J.P. Solovej, Excess charge for pseudo-relativistic atoms in Hartree-Fock theory, *Doc. Math.* **15** (2010) 285–345.

Randwertprobleme für Willmoreflächen Eine Willmorefläche ist ein kritischer Punkt des Willmorefunktionals, welches jeder hinreichend glatten zweidimensionalen Fläche das Integral der quadrierten mittleren Krümmung über die Fläche zuordnet. Dieses Funktional modelliert die elastische Energie dünner Zellen oder Biomembranen. Die Willmoregleichung (d.h. die zum Willmorefunktional gehörende Euler-Lagrangegleichung) ist eine nichtlineare Gleichung von vierter Ordnung. Ihr Studium ist anspruchsvoll, da viele der für elliptische Differentialgleichungen zweiter Ordnung entwickelten Methoden nicht funktionieren. Während viele Fortschritte zur Existenz und

Regularität geschlossener Willmoreflächen erzielt wurden, ist viel weniger bekannt über Flächen mit Rand, welche Gegenstand dieser Habilitationsschrift sind. In diesem Fall müssen zur Willmoregleichung noch geeignete Randbedingungen hinzugefügt werden. Wir betrachten zwei Arten von Randbedingungen: Dirichletsche Randbedingungen und natürliche Randbedingungen. Unter Dirichletschen Randbedingungen verstehen wir, dass sowohl der Rand als auch die Tangentialräume der Fläche am Rand vorgeschrieben sind. Im Falle natürlicher Randbedingungen wird die Position des Randes festgeschrieben sowie die Tatsache, dass die mittlere Krümmung am Rand null sein muss.

Um ein Verständnis zu gewinnen für die Art der Phänomene, welche auftreten können oder welche Art von Resultaten erwartet werden können, untersuchen wir das Willmorerandwertproblem in der Klasse der Rotationsflächen. In [1] und [2] beginnen wir mit der Untersuchung des Dirichletschen Randwertproblems für Rotationsflächen, die vom Graphen einer symmetrischen positiven Funktion auf dem Intervall $[-1,1]$ erzeugt werden. Der Rand dieser Flächen besteht aus zwei Kreislinien, die in zur y,z-Ebene parallelen Ebenen liegen und Mittelpunkte $(-1,0,0)$ bzw. $(1,0,0)$ besitzen. In diesem Fall werden die Randwerte durch die Höhe des Graphen am Rand (d.h. durch die Radien der beiden Kreislinien welche den Rand beschreiben) mittels eines Parameters $\alpha > 0$, und der Wert der Ableitung der Funktion am Rand mittels eines Parameters $\beta \in \mathbb{R}$ vorgeschrieben. Das Hauptresultat besagt, dass es zu jeder Wahl von Parametern $\alpha > 0$ und $\beta \in \mathbb{R}$ glatte Rotationsflächen gibt, welche die Willmoregleichung und die Randbedingungen erfüllen. Hierbei wird der Fall $\beta = 0$ in [1] gelöst, während andere Werte für β in [2] untersucht werden. Die Existenz einer Lösung wird durch die Lösung eines Minimierungsproblems mithilfe der direkten Methode der Variationsrechnung gezeigt. Beginnend mit einer Minimalfolge wird diese modifiziert um eine neue Folge zu erhalten, welche den Schranken genügt die benötigt werden, um ein Kompaktheitsargument anzuwenden. Dies wird durch sehr explizite geometrische Konstruktionen erreicht, die nicht nur die Existenz eines Minimierers zeigen, sondern auch viele qualitative Informationen über ihn liefern. In der Konstruktion wird der Graph in geeignete Teilstücke unterteilt und mit Stücken expliziter Graphen glatt ($C^{1,1}$) verklebt, die nicht nur eine bessere, sondern sogar optimale Willmoreenergie besitzen. Diese Graphen sind zum einen die, welche Minimalrotationsflächen erzeugen (die Katenoiden), zum anderen Bogenstücke von Kreislinien mit Mittelpunkt auf der x-Achse. Hierbei wird benutzt, dass für den Fall von Dirichlet-Randbedingungen, die Minimierung des Willmorefunktionals für Rotationsflächen auf das Gleiche wie die Minimierung des elastischen Funktionals in der hyperbolischen Halbebene hinausläuft. Desweiteren wird gezeigt, dass die Minimierer C^∞-glatt sind. Für das asymptotische Verhalten der Lösung mit festem $\beta \in \mathbb{R}$ und gegen null strebendem α wird gezeigt, dass die Lösungen gegen die Oberfläche der Einheitskugel mit Mittelpunkt im Ursprung konvergieren.

In [3] und [4] wird das Problem mit natürlichen Randwertbedingungen für Rotationsflächen untersucht. Dabei wird in [3] eine Verallgemeinerung des Willmorefunktionals betrachtet, in der das mit einem Parameter $\gamma \in [0,1]$ multiplizierte totale Integral der Gaußkrümmung vom Willmorefunktional abgezogen wird. Die kritischen Punkte dieses verallgemeinerten Willmorefunktionals erfüllen immer noch die Willmoregleichung, da das Integral über die Gaußkrümmung nur Beiträge zu den Randtermen liefert. In [3] beschränken wir uns auf Rotationsflächen, die von symmetrischen Graphen erzeugt werden. Als Randbedingungen schreiben wir den Radius $\alpha > 0$ der den Rand beschreibenden Kreislinien vor sowie die Forderung, dass die mittlere Krümmung am Rand gleich dem Parameter γ multipliziert mit der Normalkrümmung am Rand ist. Diese zweite Randbedingung tritt natürlich auf, wenn das verallgemeinerte Willmorefunktional über Flächen minimiert wird, für die nur die Position des Randes festgelegt ist. Es wird zu jedem $\alpha > 0$ und $\gamma \in [0,1]$ die Existenz einer Willmorerotationsfläche, welche die vorgeschriebenen Randbedingungen erfüllt, gezeigt. Die Beweisidee ist es, dass falls ein Minimierer des Randwertproblems mit den natürlichen Randbedingungen ein Graph ist, dass dieser dann auch die Dirichletschen Randwertbedingungen für einen gewissen Wert der Ableitung am Rand erfüllt, so dass wir zum Dirichletschen Randwertproblem zurückgeführt werden. Der Beweis, dass der Minimierer tatsächlich ein Graph ist, gelingt durch Betrachtungen von Stetigkeits- und Monotonieeigenschaften der Energie. In [4] werden wieder natürliche Randbedingungen betrachtet, allerdings für das Willmorefunktional, nicht das verallgemeinerte. Die Randwertbedingungen sind in diesem Fall durch das Vorschreiben zweier Kreislinien, welche die Ränder der Fläche bilden, und der Tatsache, dass die mittlere Krümmung am Rand null sein muss, gegeben. Im Vergleich zum in [3] betrachteten Problem brauchen hier die beiden Kreislinien nicht den gleichen Radius zu haben. Desweiteren beschränken wir uns weder auf Graphen noch auf symmetrische Kurven. Für alle positiven Werte der die Ränder beschreibenden Kreisradien zeigen wir die Existenz eines Minimierers. Dazu wird zunächst ein Minimierungsproblem mit Zwangsbedingungen gelöst und danach gezeigt, dass es einen Minimierer im Inneren der Menge gibt, über die minimiert wird. In diesem Fall ist das Minimum der Energie über Rotationsflächen, die von Kurven erzeugt werden, gleich dem Minimum der Energie über Rotationsflächen, die von Graphen erzeugt werden. Wir zeigen weiterhin, dass die Lösungen gegen die Einheitskugel mit Mittelpunkt im Ursprung konvergieren, wenn die Radiien der beiden Randkreislinien gegen null streben.

In [5] wird eine zweidimensionale Fläche betrachtet, welche eine Parametrisierung als Graph über ein striktes sternförmiges Gebiet erlaubt. Als Randbedingung betrachten wird das folgende Dirichletsche Randwertproblem: der Rand wird durch den Rand des Gebietes, über den die Fläche als Graph definiert ist, festgelegt, und die Tangentialebene ist in jedem Punkt des Randes gleich der Ebene, die das sternförmige Gebiet enthält. Dann wird ein Eindeutigkeitsresultat bewiesen, in dem gezeigt wird, dass die einzige glatte Willmorefläche, welche diesem Randwertproblem genügt, ein Stück der Ebene ist. Im ersten Teil des Beweises wird gezeigt, dass die mittlere Krümmung am Rand identisch null sein muss. Der Beweis ist inspiriert von der Beweisidee der Identität von Pohozaev, unter Benutzung der konformen Invarianz des Problems. Die Schlussfolgerung, dass die Fläche ein Teilstück der Ebene sein muss, folgt dann aus dem Klassifikationssatz für Willmoreflächen von Bryant.

Hartree-Fock-Theorie für pseudorelativistische Atome Ein Model für ein pseudorelativistisches Atom mit N Elektronen und einem Atomkern der festen Ladung Z (im Ursprung) ist in der Schrödingertheorie durch den Hamiltonoperator

$$H = \sum_{j=1}^{N} \big(T_j - \frac{Z}{|\mathbf{x}_j|}\big) + \sum_{1 \le i < j \le N} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|}$$

gegeben. Hierbei ist die kinetische Energie T_j des j-ten Elektrons gegeben durch $T_j = T$, $j = 1, \ldots, N$, wobei $T = \sqrt{-\alpha^{-2}\Delta + \alpha^{-4}} - \alpha^{-2}$ und α die Sommerfeldsche Feinstrukturkonstante ist, welche physikalisch den Wert $\alpha \simeq 1/137.036$ hat. Der Operator $Z/|\mathbf{x}_j|$ beschreibt die Anziehung, die das j-te Elektron vom Atomkern erfährt, wohingegen die Operatoren $1/|\mathbf{x}_i - \mathbf{x}_j|$ die gegenseitige Abstoßung der Elektronen beschreiben. Die Wahl der kinetischen Energie als Pseudodifferentialoperator der Ordnung eins gewährleistet die Einbeziehung einiger relativistischer Effekte, weshalb auch von pseudorelativistischen Atomen gesprochen wird. Um Beschränktheit von unten des Hamiltonoperators zu gewährleisten, muss man sich auf Atomkernladungen Z beschränken, welche $Z\alpha \le 2/\pi$ erfüllen. Die Elektronen werden durch "Wellenfunktionen" $\Psi \in \wedge_{i=1}^{N} L^2(\mathbb{R}^3)$ beschrieben, wobei $|\Psi|^2$ als Wahrscheinlichkeitsdichte zu verstehen ist, d.h. das Integral von $|\Psi|^2$ über eine Menge im $\mathbb{R}^{3N}$ ergibt die Wahrscheinlichkeit, die N Elektronen in dieser Menge zu finden. Die Antisymmetrie wird wegen dem pauli'schen Ausschlussprinzip benötigt. Die *(Quanten) Grundzustandsenergie* ist das Infimum des Spektrums von H, wenn H als Operator auf dem Raum der Wellenfunktionen betrachtet wird:

$$E^{\mathrm{QM}}(N, Z) := \inf \sigma_{\mathcal{H}_F}(H) = \inf\{\, \langle \Psi, H\Psi \rangle \,|\, \Psi \in \wedge_{i=1}^{N} L^2(\mathbb{R}^3), \langle \Psi, \Psi \rangle = 1\} \,.$$

Hierbei bezeichnet $\langle\cdot,\cdot\rangle$ das Skalarprodukt im $L^2(\mathbb{R}^{3N})$. Ein Ziel der Quantenmechanik ist das Studium der Grundzustandsenergie und, wenn sie existiert, der Wellenfunktion welche die Energie minimiert. Wegen der hohen Dimensionalität des Problems werden viele Approximationen betrachtet. Eine der bekanntesten ist die Hartree-Fock-Approximation. Hierbei beschränkt man sich im Minimierungsproblem auf die Minimierung über die einfachsten antisymmetrischen Funktionen. Dies sind die reinen Wedgeprodukte (auch Slaterdeterminanten genannt), d.h. Wellenfunktionen Ψ welche eine Darstellung der Form $\Psi(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N)=\frac{1}{\sqrt{N!}}\det(u_i(\mathbf{x}_j))_{i,j=1}^N$ mit $\{u_i\}_{i=1}^N$ orthonormal in $L^2(\mathbb{R}^3)$ erlauben.

In [6] zeigen wir die Existenz eines Hartree-Fock-Minimierers für das oben beschriebene Model eines pseudorelativistischen Atoms, unter der Bedingung, dass die ganzzahlige Anzahl N der Elektronen der Bedingung $N < Z+1$ genügt. Diese Schranke an die Anzahl der Elektronen ist die gleiche wie im klassischen nichtrelativistischen Fall, in dem die kinetische Energie durch $-\frac{1}{2}\Delta$ gegeben ist. Das Minimierungsproblem wird dadurch gelöst, indem man die Menge über die minimiert wird erweitert, um sie zunächst konvex zu machen und dann sogar noch weiter erweitert um einen möglichen Kompaktheitsverlust, der eine Reduktion der Teilchenzahlen bewirken könnte, zu berücksichtigen. Die Hauptschwierigkeit besteht darin, dass das Potenzial des Atomkerns nicht relativ kompakt bezüglich der kinetischen Energie ist. Wir zeigen weiterhin die Regularität der Orbitale. Genauer wird gezeigt, dass sie C^∞ außerhalb einer beliebigen Umgebung des Ursprungs sind, und dass sie exponentiell abfallen. Die Schwierigkeit kommt von der Nichtlokalität der kinetischen Energie, durch welche die Singularität des Atomkernpotenzials überall Einfluss hat. In [7] untersuchen wir die Regularität der Orbitale weiter und zeigen, dass sie außerhalb einer beliebigen Umgebungen des Ursprungs reell-analytisch sind. Abgesehen vom mathematischen Interesse an dieser Fragestellung erwarten wir Anwendungen dieses Ergebnisses für die Theorie von Atommodellen. Im Falle der nichtrelativistischen Energie ist die reelle Analytizität der Orbitale entscheidend, um zu zeigen, dass der reale quantenmechanische Grundzustand niemals ein Hartree-Fock-Grundzustand sein kann.

In [6] wurde die Existenz eines Hartree-Fock-Minimierers unter der Bedingung $N < Z+1$ bewiesen. Das heißt, in der Hartree-Fock-Theorie kann man Atome beschreiben, deren totale Ladung fast bei -1 liegt. Ein lange offenstehendes Problem ist die Charakterisierung der maximalen Anzahl N an Elektronen, die ein Atomkern der Ladung Z binden kann. Dies ist bekannt als die Ionisierungsvermutung und kann wie folgt formuliert werden: Betrachtet man Atome mit beliebig großer Atomkernladung, kann dann die maximale Anzahl an Elektronen, die ein Atomkern binden kann, durch die Atomkernladung plus einer universellen Konstante beschränkt werden? Die Antwort auf diese Frage hängt natürlich vom betrachteten Modell ab. Im Jahr 2003 hat Solovej die Ionisierungsvermutung für nichtrelativistische Atome im Hartree-Fock-Modell bewiesen. In [8] erweitern wir Solovejs Resultat auf den Fall von pseudorelativistischen Atomen. Dies geschieht durch Vergleich des Hartree-Fock-Minimierers mit dem Minimierer eines anderen Atommodells, nämlich dem Thomas-Fermi-Minimierer. Das Ergebnis wird erzielt, indem man iterativ zeigt, dass bis auf einen Abstand der Ordnung $1 = Z^0$ verschiedene Thomas-Fermi-Modelle gefunden werden können, welche den Hartree-Fock-Minimierer gut approximieren. In jedem Schritt berücksichtigt das neue Modell die Tatsache, dass Elektronen in einem gewissen Abstand vom Atomkern eine Ladung spüren, die durch die am Atomkern näheren Elektronen abgeschirmt ist. Die Beweismethode liefert ebenso eine Abschätzung für die Ionisierungsenergie als auch für den Hartree-Fock Atomradius.

Hiermit erkläre ich, dass ich bei allen zu dieser Habilitationsschrift gehörenden Arbeiten maßgeblich beteiligt war sowie alle Koautoren und alle benutzen Hilfsmittel vollständig angegeben habe. Die Habilitationsschrift als Ganzes habe ich selbständig verfasst.

Magdeburg, den 30. März 2011

(Dr. Anna Dall'Acqua)

Summary

This dissertation is a cumulative one concerned on the one hand with Willmore surfaces satisfying prescribed boundary conditions and on the other hand with the Hartree-Fock atomic model for pseudo-relativistic atoms. In both cases we study some minimisation problem and the qualitative properties of the solutions. In the first part of this dissertation, which consists of the following papers, we present the results concerning boundary value problems for Willmore surfaces.

[1] A. Dall'Acqua, K. Deckelnick, H.-Ch. Grunau, Classical solutions to the Dirichlet problem for Willmore surfaces of revolution, *Adv. Calc. Var.* **1** (2008) 379–397.

[2] A. Dall'Acqua, S. Fröhlich, H.-Ch. Grunau, F. Schieweck, Symmetric Willmore surfaces of revolution satisfying arbitrary Dirichlet boundary data, *Adv. Calc. Var.* **4** (2011) 1–81.

[3] M. Bergner, A. Dall'Acqua, S. Fröhlich, Symmetric Willmore surfaces of revolution satisfying natural boundary conditions, *Calc. Var. PDE* **39** (2010) 361–378.

[4] M. Bergner, A. Dall'Acqua, S. Fröhlich, Willmore surfaces of revolution bounding two prescribed circles, Preprint Nr. 13/2010, Universität Magdeburg, submitted.

[5] A. Dall'Acqua, Uniqueness for the homogeneous Dirichlet Willmore boundary value problem, Preprint Nr. 06/2011, Universität Magdeburg, submitted.

The Hartree-Fock theory of pseudo-relativistic atoms is the subject of the second part of this dissertation and is treated in the following papers.

[6] A. Dall'Acqua, T. Østergaard Sørensen, E. Stockmeyer, Hartree-Fock theory for pseudorelativistic atoms, *Ann. Henri Poincaré* **9** (2008), no. 4, 711–742.

[7] A. Dall'Acqua, S. Fournais, T. Østergaard Sørensen, E. Stockmeyer, Real Analyticity away from the nucleus of pseudorelativistic Hartree-Fock orbitals, Preprint Nr. 09/2011, Universität Magdeburg, submitted.

[8] A. Dall'Acqua, J.P. Solovej, Excess charge for pseudo-relativistic atoms in Hartree-Fock theory, *Doc. Math.* **15** (2010) 285–345.

Boundary value problems for Willmore surfaces A Willmore surface is a critical point for the Willmore functional which associates to a sufficiently smooth two-dimensional surface the integral over the surface of its mean curvature squared. This functional models the elastic energy of thin cells or biological membranes. The Willmore equation (i.e. the Euler-Lagrange equation corresponding to the Willmore functional) is a fourth order nonlinear equation and its study is challenging since many methods developed for the study of nonlinear elliptic equations of second order fail. While much progress has been achieved concerning existence and regularity of closed Willmore surfaces, much less is known concerning surfaces with boundary which is the subject of

this dissertation. In this case appropriate boundary conditions have to be added to the Willmore equation. We consider two kinds of boundary conditions: Dirichlet and natural. By Dirichlet boundary conditions we mean that the boundary of the surface and its tangential spaces at the boundary are prescribed. In the case of natural boundary conditions the position of the boundary is fixed and the mean curvature has to be zero at the boundary.

In order to have an understanding of which kind of phenomena may occur or of which kind of results one may expect, we investigate the Willmore boundary value problem in the class of surfaces of revolution. In [1] and [2] we start by studying the Dirichlet boundary value problem for surfaces of revolution generated by graphs of positive symmetric functions defined on the interval $[-1,1]$. The boundary of such surfaces consists of two circles on planes parallel to the y,z-plane and centered at $(-1,0,0)$ and $(1,0,0)$, respectively. In this case, the boundary conditions are given prescribing the height of the graph at the boundary (i.e. the radii of the circles constituting the boundary) via a parameter $\alpha > 0$ and the value of the derivative of the function at the boundary via a parameter $\beta \in \mathbb{R}$. The main result states that for any choice of the parameters $\alpha > 0$ and $\beta \in \mathbb{R}$ there exists a smooth surface of revolution solution of the Willmore equation and satisfying the boundary conditions. The case $\beta = 0$ is solved in [1] while the other values of β are studied in [2]. The existence is achieved solving a minimisation problem via the direct method in the calculus of variations. Starting from a minimising sequence we modify it to get to a new sequence satisfying the bounds needed for the compactness argument. This is achieved by very explicit geometric constructions yielding not only the existence of a minimiser but many qualitative informations on it. In the construction, we suitably cut the graph and smoothly ($C^{1,1}$) glue to it pieces of explicit graphs with not only better but optimal Willmore energy. These graphs are, on one hand the ones generating minimal surfaces of revolution (the catenoids) and on the other hand arcs of circles with center in the x-axis. Here one uses that, in the case of Dirichlet boundary conditions, minimising the Willmore functional for surfaces of revolution is the same as minimising the elastic functional in the hyperbolic half-plane. Further, the minimisers are shown to be C^∞-smooth. Concerning the asymptotic behavior of the solutions for $\beta \in \mathbb{R}$ fixed and α going to zero, convergence to the unit sphere centered at the origin is proven.

In [3] and [4] the natural boundary value problem for surfaces of revolution is studied. In [3] a generalisation of the Willmore functional is considered. In this case from the Willmore functional we subtract the total integral of the Gauss-curvature multiplied by a parameter $\gamma \in [0,1]$. Critical points of this generalised Willmore functional still satisfy the Willmore equation since the integral over the Gauss curvature only contributes to the boundary terms. In [3] we restrict to the case of surfaces of revolution generated by symmetric graphs. As boundary conditions we prescribe the radius $\alpha > 0$ of the circles constituting the boundary and that the mean curvature at the boundary has to be equal to the parameter γ times the normal curvature of the boundary. This second boundary condition is the one that naturally appears when minimising this generalised Willmore functional among surfaces where only the position of the boundary is fixed. For any $\alpha > 0$ and $\gamma \in [0,1]$ existence of a Willmore surface of revolution satisfying the boundary value problem is proven. The idea of the proof is that if a minimiser for this natural value problem is a proper graph, it solves the Dirichlet boundary value problem for some value of the derivative at the boundary, and so we are lead back to the Dirichlet boundary value problem. The proof that the minimiser is a graph is achieved by studying continuity and monotonicity properties of the energy. In [4] we consider again natural boundary conditions but simply for the Willmore functional, not the generalised one. The boundary conditions are in this case given by prescribing the two circles that constitute the boundary and that the mean curvature has to be equal to zero at the boundary. Comparing the problem to the one studied in [3] here the two circles do not need to have the same radius. Moreover, we do not restrict to graphs, neither to symmetric curves. For all positive values of the radii of the circles constituting the boundary we have existence of a minimiser. First a constrained minimisation problem is solved and then it is proven that a minimiser is in the interior of the set over which we minimise. In this case the minimum of the energy over surfaces of revolution generated by curves is equal to the minimum of the energy over surfaces of revolution generated by graphs. We further prove that the solutions converge to the unit sphere centered at the origin when the radii of the two circles constituting the boundary go to zero.

In [5] a two-dimensional surface that admits a parametrisation as a graph over a strict star-shaped two-dimensional domain is considered. As boundary condition we study the following Dirichlet boundary value problem: the boundary is given by the boundary of the domain over which the surface is given as a graph, and the tangent planes along the boundary are given by the plane containing the star-shaped domain. What we prove is a uniqueness result. That is, the only smooth Willmore surface satisfying this boundary value problem is a piece of the plane. In the first part of the proof it is shown that the mean curvature has to be equal to zero at the boundary. This is done in the spirit of the proof of Pohozaev's identity using the conformal invariance of the problem. The conclusion that the surface is a piece of a plane is then obtained using the classification theorem for Willmore surfaces of Bryant.

Hartree-Fock theory for pseudo-relativistic atoms A model for a pseudo-relativistic atom with N electrons and a nucleus of charge Z fixed (at the origin) is in Schrödinger theory given by the Hamiltonian (operator)

$$H = \sum_{j=1}^{N} \big(T_j - \frac{Z}{|\mathbf{x}_j|}\big) + \sum_{1\le i<j\le N} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|}\,,$$

where the kinetic energy T_j of the j-th electron is given by $T_j = T$, $j = 1, \dots, N$, with $T = \sqrt{-\alpha^{-2}\Delta + \alpha^{-4}} - \alpha^{-2}$ with α Sommerfeld's fine structure constant; physically, $\alpha \simeq 1/137.036$. The operator $Z/|\mathbf{x}_j|$ gives the attraction that the j-th electron feels from the nucleus while the operators $1/|\mathbf{x}_i - \mathbf{x}_j|$ describe the mutual repulsion of the electrons. The choice of the kinetic energy as a pseudo-differential operator of order one is done to take into account some relativistic effects. This is the reason for speaking of pseudo-relativistic atoms. In order to have boundedness from below of the Hamiltonian one needs to restrict to values of the nuclear charge Z satisfying $Z\alpha \le 2/\pi$. The electrons are described by a "wavefunction" $\Psi \in \wedge_{i=1}^{N} L^2(\mathbb{R}^3)$, where $|\Psi|^2$ has to be understood as a probability density. That is, its integral over a region in $\mathbb{R}^{3N}$ gives us the probability of finding the N electrons in that region of space. The antisymmetry is needed because of Pauli's exclusion principle. The *(quantum) ground state energy* is the infimum of the spectrum of H considered as an operator acting on the space of wavefunctions:

$$E^{\mathrm{QM}}(N, Z) := \inf \sigma_{\mathcal{H}_F}(H) = \inf\{\, \langle \Psi, H\Psi\rangle \,|\, \Psi \in \wedge_{i=1}^{N} L^2(\mathbb{R}^3), \langle \Psi, \Psi\rangle = 1\}\,,$$

where $\langle \cdot, \cdot\rangle$ denotes the scalar product in $L^2(\mathbb{R}^{3N})$. One of the aims of quantum mechanics is the study of the ground state energy and, if it exists, of the wavefunction minimising it. Due to the high dimension of the problem, many approximations are studied. One of the most famous is the Hartree-Fock approximation. In this approximation, one restricts the minimisation problem minimising only over the simplest antisymmetric wavefunctions. These are pure wedge products (also called Slater determinants), i.e. wavefunctions Ψ that admit a representation as $\Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) = \frac{1}{\sqrt{N!}} \det(u_i(\mathbf{x}_j))_{i,j=1}^{N}$ with $\{u_i\}_{i=1}^{N}$ orthonormal in $L^2(\mathbb{R}^3)$.

In [6] we prove the existence of a Hartree-Fock minimiser for the model of a pseudo-relativistic atom given above, under the condition that the number N of electrons is an integer satisfying $N < Z + 1$. This bound on the number of electrons is the same as the one in the classical non-relativistic case where the kinetic energy is given by $-\frac{1}{2}\Delta$. The minimisation problem is solved by extending the set over which we minimise making it convex and then extending it even further in order to take into account some possible loss of compactness that could cause a reduction of the number of particles. The main difficulty is due to the fact that the nuclear potential is not relatively compact with respect to the kinetic energy. We further prove regularity of the orbitals. These are shown to be C^∞ outside of the origin and exponentially decreasing. The challenge here is due to the non-locality of the kinetic energy through which the singularity of the nuclear potential can be felt everywhere. In [7] we study further the regularity of the orbitals proving that these are real analytic away from the origin. Apart from the mathematical interest, we expect that this information may have applications in the theory of atomic models. In the case of non-relativistic kinetic energy, the real-analyticity of the orbitals is crucial to show that the real quantum mechanical ground state is never a Hartree-Fock ground state.

In [6] the existence of a Hartree-Fock minimiser under the condition $N < Z + 1$ was proved. That is, in the Hartree-Fock theory one can describe atoms with total charge almost equal to minus one. A long standing open problem is the characterisation of the maximal number of electrons N that a nucleus of charge Z can bind. This is known as the ionization conjecture that can be formulated as follows. Consider atoms with arbitrarily large nuclear charge, is it true that the maximal number of electrons that a nucleus can bind is bounded by the charge of the nucleus plus a universal constant? The answer to this question depends of course on the model one considers. In 2003 Solovej proved the ionization conjecture in the Hartree-Fock theory for non-relativistic atoms. In [8] we extend Solovej's result to the case of pseudo-relativistic atoms. The result is achieved comparing the Hartree-Fock minimiser with the minimiser for another atomic model: the Thomas-Fermi minimiser. The result follows showing, iteratively, that up to a distance of order $1 = Z^0$, we can find several Thomas-Fermi models that are a good approximation of the Hartree-Fock minimiser. At each step, the model we consider takes into account that electrons at a certain distance from the nucleus feel a charge that is screened by the electrons nearer to the nucleus. The method of proof yields also an estimate on the ionization energy and on the Hartree-Fock atomic radius.

Hereby I declare that I have significantly contributed to each paper constituting this dissertation. All my coauthors as well as all the sources I have used are listed. I have produced this dissertation as a whole entirely myself.

Magdeburg, 30th of March 2011

(Dr. Anna Dall'Acqua)

Introduction

This dissertation is a cumulative one concerned on the one hand with Willmore surfaces satisfying prescribed boundary conditions and on the other hand with the Hartree-Fock atomic model for pseudo-relativistic atoms. In the following introduction we shall describe the two topics separately. For both the main tools of the underlying mathematical theory are variational methods and regularity theory for partial differential equations. Here we give a short introduction to the subjects and an overview of the results. The results concerning boundary value problems for Willmore surfaces are proved in the papers [3, 4, 7, 8, 10], which constitute the first part of this dissertation. The ones on the Hartree-Fock theory of pseudo-relativistic atoms, which form the second part of this dissertation, are in [9, 11, 12]. For a more thorough discussion of the results and of their proofs we refer to the papers themselves.

1 Boundary value problems for Willmore surfaces

The *Willmore functional* associates to a sufficiently smooth two-dimensional immersed surface Γ the value

$$\mathcal{W}(\Gamma) := \int_\Sigma H^2 \, dS \,,$$

with $H = (\kappa_1 + \kappa_2)/2$ the mean curvature (κ_1, κ_2 denote the principal curvatures of Γ) and dS the area form induced on Γ by the canonical metric in $\mathbb{R}^3$. This functional models the elastic energy of thin cells or biological membranes (see e.g. [17, 33, 56, 57]) and it appeared already in the 19th century in the first studies in elasticity of Germain and Poisson (see e.g. [29, 59]). It was forgotten during the first half of the twentieth century and it was Willmore's work [76] which popularised again its investigation. In more recent years other applications of the Willmore functional in image processing (for problems of surface restoration and image in-painting), and even in string theory have been discovered (see e.g. [35, 40]). In these applications one is usually concerned with minima, or more generally with critical points of the Willmore functional. Such a critical point $\Gamma \subset \mathbb{R}^3$ has to satisfy the *Willmore equation*

$$\Delta_g H + 2H(H^2 - K) = 0 \qquad \text{on } \Gamma, \tag{1.1}$$

where Δ_g denotes the Laplace–Beltrami operator on Γ with respect to the induced metric g and $K = \kappa_1\kappa_2$ is the Gauss curvature (see [76, Sec. 7.4]). This equation is highly non-linear since Δ_g depends on the unknown surface. Moreover, the equation is of fourth order. A solution of the differential equation (1.1) is called a *Willmore surface*. Classical examples of Willmore surfaces include spheres, minimal surfaces and stereographic projections of the Clifford Torus in $\mathbb{R}^3$. This is a circular torus in $\mathbb{R}^3$ with the ratio of the radii given by $1/\sqrt{2}$. Spheres are the absolute minima of the Willmore functional among all compact surfaces (see [76, Sec. 7.2]). The famous *Willmore* *conjecture* states that the stereographic projection of the Clifford Torus is the minimum of the Willmore functional among compact surfaces of genus 1.

An important characteristic of the Willmore functional is its conformal invariance. Indeed, it is trivially invariant under Euclidean transformations as well as under scaling. If I is an inversion in $\mathbb{R}^3$ with center at a point not in the surface ($p \notin \Gamma$) then $\mathcal{W}(I \circ f) = \mathcal{W}(f)$ (see [76, Sec. 7.3] or Weiner [75]). In fact, the Willmore functional appears also in conformal differential geometry as the simplest conformally invariant variational problem (see [74]). In this field Willmore surfaces are known as conformal minimal surfaces.

Various existence and regularity results for *closed* Willmore surfaces of prescribed genus are extensively discussed in the literature. In [67] Simon proves that the minimum of the Willmore functional among compact surfaces of arbitrary prescribed genus is attained when the genus is equal to one or, for higher genus, a certain condition is satisfied. Bauer and Kuwert in [1] prove that this condition is indeed always satisfied. We also wish to mention the works of Kuwert and Schätzle [42, 43] and of Leschke, Pedit and Pinkall [46] for existence of constrained closed Willmore surfaces of fixed conformal class and Bryant [5] for a classification theorem. The best regularity result on solutions to (1.1) is that proved by Rivière in [61] stating that a suitably defined weak solution of (1.1) is the image of a real-analytic immersion. This extends a previous regularity result of Kuwert and Schätzle [41]. In all these works the conformal invariance of the Willmore functional plays a key role. Results on local and global existence of the L^2-gradient flow associated with the Willmore functional (the *Willmore flow*) as well as numerical algorithms and numerical analysis on Willmore surfaces and Willmore flow are available in the literature. We refer to [10] for a short discussion and some references.

In the present dissertation we are interested in surfaces *with boundaries.* Then, appropriate boundary conditions should be added to (1.1). Since this equation is of fourth order one requires two sets of conditions. A discussion of possible choices can be found in Nitsche's survey article [56]. We are interested mainly in two kinds of boundary conditions: Dirichlet and natural. By Dirichlet boundary conditions we mean that the boundary $\partial\Gamma$ of the surface and the tangential spaces of Γ at $\partial\Gamma$ are prescribed. In the case of natural boundary conditions the position of the boundary $\partial\Gamma$ is fixed and the mean curvature H must be zero at the boundary. This kind of boundary condition is the natural one when considering critical points of the Willmore functional when only the position at the boundary is fixed.

Nitsche's work [56] contains some existence results for several kinds of boundary conditions. These are based on perturbation arguments and hence require smallness conditions on the data. The question arises whether it is possible to specify more general conditions on the boundary data that will guarantee the existence of a solution to (1.1). Such a task seems to be quite difficult since the problem is highly nonlinear and of fourth order and so, lacking any form of a general maximum or comparison principle. Most of the well established techniques from second order problems seem to break down completely in higher order problems. A first result without any smallness condition is the one of Palmer in [58] where he proves that a Willmore surface of disk type which has its boundary on a circle and which intersects the plane of the circle at a constant angle is a spherical cap or a flat disk. In [14] Deckelnick and Grunau prove existence of solutions to the one-dimensional Willmore problem for arbitrary Dirichlet boundary conditions and without assumptions on symmetry. (The Navier one-dimensional boundary value problem is studied in [14, 15].) Schätzle [62], using methods from geometric measure theory, proved an important general result concerning existence and regularity of branched Willmore immersions in $\mathbb{S}^n$ with boundary which satisfy Dirichlet boundary conditions. By working in $\mathbb{S}^n$, some compactness problems could be overcome. Assuming the boundary data to obey some explicit geometrically motivated smallness condition Schätzle's solutions can even be shown to be connected and embedded.

In order to start working on a theory of classical bounded smooth solutions for the Willmore boundary value problem it seems to be a good and appropriate strategy to investigate situations enjoying symmetry. A natural class to start with is the class of surfaces of revolution. Although there, one has an underlying ordinary differential equation, understanding solvability of the corresponding boundary value problems is by no means straightforward. In [3, 4, 8, 10] existence and qualitative properties of Willmore surfaces of revolution with Dirichlet and natural boundary conditions are studied. These studies indicate which phenomena and results concerning compact embedded solutions in $\mathbb{R}^3$ of boundary value problems for the Willmore equation might be expected. The obtained results are in some cases surprising and indicate some unexpected behavior. In [7] a Willmore surface given by a graph over a strictly star-shaped two-dimensional domain and satisfying homogeneous Dirichlet boundary conditions is shown to be necessarily a piece of a plane.

1.1 Willmore surfaces of revolution

For $a_1, a_2 \in \mathbb{R}$, $a_1 < a_2$, let $c : [a_1, a_2] \to \mathbb{R} \times \mathbb{R}_+$, $c(t) = \big(x(t), y(t)\big)$, be some smooth regular curve. Here and in the following $\mathbb{R}_+ := (0, +\infty)$. Rotating the curve c about the x-axis generates a *surface of revolution* $\Gamma \subset \mathbb{R}^3$ which can be parametrised by

$$\Gamma : f(t, \varphi) = \big(x(t), y(t)\cos(\varphi), y(t)\sin(\varphi)\big) \in \mathbb{R}^3,\ t \in [a_1, a_2]\ ,\ \varphi \in [0, 2\pi)\,. \tag{1.2}$$

The term surface always refers to the mapping f as well as to the set Γ. The condition on the second component of the curve $c^2 = y > 0$ implies that f is embedded.

The boundary of Γ consists of two circles on planes parallel to the y, z-plane and centered at $\big(x(a_1), 0, 0\big)$ and $\big(x(a_2), 0, 0\big)$ respectively. In this case, Dirichlet boundary conditions means that we prescribe the two circles that give the boundary of Γ and the values of the derivatives (x', y') at the boundary. In the case of natural boundary conditions, only the two circles constituting the boundary are prescribed.

The principal curvatures of Γ are respectively

$$\kappa_1 = \frac{x''y' - x'y''}{(x'^2 + y'^2)^{\frac{3}{2}}} \quad \text{and} \quad \kappa_2 = \frac{x'}{y\sqrt{x'^2 + y'^2}}\,. \tag{1.3}$$

Notice that κ_1 is the (Euclidean) curvature of the plane curve c. The Willmore energy of Γ is given by

$$\mathcal{W}(c) = \frac{\pi}{2}\int_{a_1}^{a_2} \Big(\frac{x'y'' - x''y'}{(x'^2 + y'^2)^{3/2}} - \frac{x'}{y(x'^2 + y'^2)^{1/2}}\Big)^2 y(x'^2 + y'^2)^{1/2}\, dt\,. \tag{1.4}$$

From this formula we see that $\mathcal{W}(c) \in [0, \infty)$ if c is a $W^{2,2}$-curve (i.e. $c = (x, y)$ with $x, y \in W^{2,2}(a_1, a_2)$) with $c^2 = y > 0$ in $[a_1, a_2]$. If the curve c is in fact a graph over the x-axis, i.e. $c(t) = (t, u(t))$ for some smooth function $u : [a_1, a_2] \to \mathbb{R}_+$, then we obtain

$$\mathcal{W}(c) = \frac{\pi}{2}\int_{a_1}^{a_2} \Big(\frac{u''}{(1 + u'^2)^{3/2}} - \frac{1}{u(1 + u'^2)^{1/2}}\Big)^2 u\sqrt{1 + u'^2}\, dx =: \mathcal{W}(u)\,. \tag{1.5}$$

A natural approach to prove existence of Willmore surfaces of revolution satisfying prescribed boundary conditions is the variational one. That is, we find a solution to (1.1) with the prescribed boundary conditions by proving the existence of a minimiser for the Willmore functional in an appropriate class, via the direct method in the calculus of variation. It is convenient now to restrict the discussion to the case of surfaces of revolution generated by graphs. Indeed, these are the surfaces we consider in [3, 8, 10]. In [4] we consider the case of natural boundary conditions and start by considering surfaces of revolution generated by curves, but we prove that, in the minimisation problem, one may restrict oneself to the study of graphs.

For fixed $\alpha > 0$ let us consider the following minimisation problem

$$M_\alpha := \inf\{\mathcal{W}(u) \,:\, u \in W^{2,2}(a_1,a_2),\, u > 0 \text{ in } (a_1,a_2) \text{ and } u(a_1) = u(a_2) = \alpha\}\,.$$

Let $(u_k)_{k\in\mathbb{N}}$ be a minimising sequence, that is, a sequence of positive functions in $W^{2,2}(a_1,a_2)$ such that $\lim_{k\to\infty}\mathcal{W}(u_k) = M_\alpha$ and $u_k(a_1) = u_k(a_2) = \alpha$ for all k. From formula (1.5) it is clear that the uniform bound for the Willmore energy $\mathcal{W}(u_k)$ of the elements of the sequence does not give a bound for their $W^{2,2}$-norm. From the same formula one may see that uniform estimates from below and from above for the functions u_k (i.e. of the form $0 < C_1 \le u_k \le C_2$ in $[-1,1]$) and from above for $|u_k'|$ (i.e. $|u_k'| \le C_3$) would yield a uniform bound in $W^{2,2}$-norm. The existence of a $W^{2,2}$-minimiser would then follow by standard arguments. Therefore, the crucial point is to prove that we can restrict to minimising sequences satisfying the needed a priori estimates. We do this by very explicit geometric constructions substituting, when necessary, the elements of the minimising sequences by others with a very precise qualitative behavior. As a consequence, we do not only get existence of a minimiser but also qualitative informations on it.

A key observation for the geometric constructions yielding an a priori bounded minimising sequence is the correspondence between the Willmore functional on surfaces of revolution and a curvature functional (which we call the *hyperbolic Willmore functional*) on curves in the hyperbolic half plane. This observation goes back to Bryant and Griffiths [6] and Langer and Singer [45]. It is convenient at this point to present the transformation in some details. The hyperbolic half plane $\mathbb{R}^2_+ := \{(x,y) \,:\, y > 0\}$ is equipped with the metric $ds_h^2 = (dx^2+dy^2)/y^2$. A graph $[a_1,a_2] \ni x \mapsto (x,u(x)) \in \mathbb{R}^2_+$ has (hyperbolic) curvature (see [8, Sec.2.2])

$$\kappa_h(x) = -\frac{u(x)^2}{u'(x)}\frac{d}{dx}\left(\frac{1}{u(x)\sqrt{1+u'(x)^2}}\right) = \frac{u(x)u''(x)}{(1+u'(x)^2)^{3/2}} + \frac{1}{\sqrt{1+u'(x)^2}}. \tag{1.6}$$

Geodesics are circular arcs centered on the x-axis and lines parallel to the y-axis; the first (together with minimal surfaces) will play a crucial role in choosing suitable minimising sequences for the Willmore functional. Notice that the two terms on the right hand side of (1.6) differ from those inside the brackets in the integral in (1.5) by a factor u and in (1.6) these are summed while in (1.5) the two terms are subtracted. With this in mind, concerning the elastic energy in this metric, that we call *hyperbolic Willmore energy* and denote with $\mathcal{W}_h(u)$, we find

$$\begin{aligned}\mathcal{W}_h(u) \;&:=\; \int_{a_1}^{a_2}\kappa_h(x)^2\,ds_h(x) = \int_{a_1}^{a_2}\kappa_h(x)^2\frac{\sqrt{1+u'^2}}{u}\,dx\\ &=\; \frac{2}{\pi}\mathcal{W}(u) + 4\int_{a_1}^{a_2}\frac{u''}{(1+u'^2)^{\frac{3}{2}}}\,dx = \frac{2}{\pi}\mathcal{W}(u) + 4\left[\frac{u'}{\sqrt{1+u'^2}}\right]_{a_1}^{a_2}. \end{aligned}\tag{1.7}$$

This shows that the Willmore energy $\mathcal{W}(u)$ and the hyperbolic Willmore energy $\mathcal{W}_h(u)$ differ only by a boundary term. One can see this also via the Theorem of Gauss-Bonnet since

$$\int_{a_1}^{a_2}\frac{u''}{(1+u'^2)^{\frac{3}{2}}}\,dx = -\int_{a_1}^{a_2}\kappa_1\kappa_2 u\sqrt{1+u'^2}\,dx = \frac{1}{2\pi}\int_\Sigma K\,dA\,,$$

with κ_1,κ_2 given by (1.3) (for $(x(t),y(t)) = (t,u(t))$), $K = \kappa_1\kappa_2$ the Gauss curvature of Γ and $\Sigma = (a_1,a_2)\times(0,2\pi)$. The same transformation and similar formulas hold in the more general case of surfaces of revolution generated by curves. It is interesting to notice that the parametrisation given in (1.2) is conformal if the curve c is parametrised by the hyperbolic arc-length.

As described above, the strategy to prove the needed a priori estimates is to substitute, when necessary, the elements of the minimising sequence with elements satisfying the same boundary conditions, with better energy and with quite a precise qualitative behavior. This is achieved by suitably cutting the graph and smoothly gluing to it pieces of explicit graphs with not only better but optimal Willmore energy. First of all, since the problem is of fourth order, for the gluing it is not sufficient to have continuity but continuity also of the first derivative is needed. Also because of this, we consider the minimisation problem in $C^{1,1}([a_1, a_2]) \subset W^{2,2}(a_1, a_2)$. Secondly, one needs to find which are the graphs with optimal Willmore energy. Since the Willmore energy is equal to the total integral over the mean curvature squared, it is natural to look for axially symmetric surfaces with mean curvature identically equal to zero. These are the so called *catenoids*: a two-parameter family of surfaces generated by rotating the graph of the function $x \mapsto \frac{1}{b}\cosh(bx+a)$ (for $b \in \mathbb{R}_+$ and $a \in \mathbb{R}$) around the x-axis. These are the only minimal surfaces of revolution. The second family of optimal graphs is to be found looking at the hyperbolic Willmore functional given in (1.7). Indeed, for the gluing the values of the function and its first derivative need to be preserved and are therefore given at the end-points. Formula (1.7) shows then that minimising the Willmore functional is equivalent to minimising the hyperbolic Willmore functional in this case. Therefore, the other family of optimal graphs are the (pieces of) spheres with arbitrary radius and center on the x-axis, since these are the geodesics of the hyperbolic half-plane which are also graphs. There are constructions where one cannot use the gluing just described. However, also in this situation the understanding of the graphs with optimal Willmore energy is crucial.

The conformal invariance is a key feature of the Willmore functional of which we make frequent use in the geometric constructions. Rotation and translation are frequently employed, and scale invariance is very important. On the other hand, inversions are not addressed since in most cases they do not preserve the particular shape of surfaces of revolution generated by graphs.

The critical points of the hyperbolic Willmore functional parametrised by arc-length satisfy the ordinary differential equation

$$\frac{d^2}{ds^2}\kappa_h(s) - \kappa_h(s) + \frac{1}{2}\kappa_h(s)^3 = 0\,. \tag{1.8}$$

This equation is discussed in detail in [44, 45] where a classification of possible curvature functions in terms of elliptic functions is given. However, we did not see any possibility to solve directly and explicitly the Willmore boundary value problem based upon this classification.

1.1.1 Symmetric Dirichlet boundary conditions

In this paragraph we present the results proved in [8, 10]. In these works surfaces of revolution generated by graphs with prescribed symmetric Dirichlet boundary conditions are considered. Due to the scaling and rotational invariance of the problem it is sufficient to consider positive functions u defined on $[-1, 1]$. In this case, the boundary conditions are given prescribing the height of the graph at the boundary (i.e. the radii of the circles constituting the boundary) and the value of the derivative at the boundary. So, we may consider two parameters: a positive parameter α for the height at the boundary and a parameter $\beta \in \mathbb{R}$ for the value of the derivative at the boundary. Then the boundary value problem we wish to solve is

$$\begin{cases} \Delta_g H + 2H(H^2 - K) = 0 \quad \text{in } (-1,1), \\ u(-1) = u(+1) = \alpha, \qquad u'(-1) = -u'(+1) = \beta, \end{cases} \tag{1.9}$$

with Δ_g the Laplace-Beltrami operator on the surface of revolution generated by the graph of u. Formula (1.7) gives that for all smooth $u : [-1, 1] \to \mathbb{R}_+$ satisfying the boundary condition in (1.9),

$$\mathcal{W}(u) = \frac{\pi}{2}\,\mathcal{W}_h(u) + 4\pi\frac{\beta}{\sqrt{1+\beta^2}}\,. \tag{1.10}$$

This equality shows that in the case of Dirichlet boundary conditions for the study of the minimisation problem we may switch between the Willmore functional and the hyperbolic Willmore functional choosing in each situation that which is more convenient.

For $\alpha > 0$ and $\beta \in \mathbb{R}$ we introduce the function space

$$N_{\alpha,\beta} := \Big\{v \in C^{1,1}([-1,1],\mathbb{R}_+), v \text{ is even, positive, } v(-1)=\alpha,\ v'(-1)=\beta \text{ and,} \\ \text{if } 0>\beta>-\alpha \text{ and } \alpha\,\mathrm{arsinh}(-\beta)\geq\sqrt{1+\beta^2}, \\ v \text{ satisfies the extra condition } u'(x)\leq\alpha \text{ in } [0,1]\Big\}. \tag{1.11}$$

This is the space where we study the minimisation problem. The main result concerning the existence of solutions to (1.9) is the following theorem.

Theorem 1.1 (Cf. Theorem 4 in [8] and Theorem 1.1 in [10])**.** *For each $\alpha > 0$ and each $\beta \in \mathbb{R}$, there exists a positive even function $u \in H^2\big((-1,1)\big)\cap C^1([-1,1])$ satisfying $u(-1)=\alpha$, $u'(-1)=\beta$ such that*

$$\mathcal{W}_h(u) = M_{\alpha,\beta} \overset{def}{=} \inf\{\mathcal{W}_h(v) : v \in N_{\alpha,\beta}\}.$$

This minimum is such that the corresponding surface of revolution $\Gamma \subset \mathbb{R}^3$ is a weak solution of the Dirichlet problem (1.9)*. Moreover, u is smooth, i.e. $u \in C^\infty([-1,1])$.*

The solution has the following additional properties:

1. *If $\alpha\beta > 1$, then $u' < 0$ in $(0,1]$ and $|u'(x)| \leq \beta$ for all $x \in [-1,1]$.*
2. *If $\alpha\beta \leq 1$ and $\beta \geq 0$, then $u' < 0$ in $(0,1)$ and $|u'(x)| \leq \frac{1}{\alpha}$ for all $x \in [-1,1]$.*
3. *If $\beta < 0$ and $\alpha\,\mathrm{arsinh}(-\beta) \geq \sqrt{1+\beta^2}$, then $u' > 0$ in $(0,1]$.*
4. *If $\beta < 0$ and $\alpha\,\mathrm{arsinh}(-\beta) < \sqrt{1+\beta^2}$, then u has at most one critical point in $(0,1)$.*

In the previous theorem, the case $\alpha > 0$ and $\beta = 0$ is proven in [8] while all the other cases are proven in [10].

The reader familiar with the theory of minimal surfaces might be surprised that in the theorem above existence of axially symmetric solutions to (1.9) for all values of $\alpha > 0$ and $\beta \in \mathbb{R}$ is stated. Axially symmetric critical points of the area functional are the catenoids. The ones symmetric with respect to zero are obtained for any $b \in (0,\infty)$ by rotating the curve $x \mapsto \frac{1}{b}\cosh(bx)$ around the x-axis. One may see that catenoids satisfying $u(\pm 1) = \alpha$ exist only for $\alpha \geq \alpha^*$ where

$$\alpha^* := \inf\{\frac{\cosh(b)}{b} : b \in \mathbb{R}_+\} = 1.5088795\ldots \tag{1.12}$$

Not only do these catenoids cease to exist for boundary data $\alpha \in (0,\alpha^*)$, but there is no connected minimal surface solution at all for $\alpha < 1$.

To prove Theorem 1.1 we consider positive symmetric functions in $C^{1,1}([-1,1])$ satisfying the given boundary conditions and study the minimisation problem in this class. As described above the idea is to pass from arbitrary to suitable minimising sequences satisfying strong a priori bounds. These bounds are obtained by explicit geometric constructions which lower the Willmore energy. We describe here the main ideas of the constructions.

As can be seen from the statement of Theorem 1.1, the behaviour of those solutions of the Willmore equation constructed there depends not only on whether $\beta \geq 0$ or $\beta < 0$. In both cases we have to make further distinctions. The switch between the different cases occurs at the values of the parameters for which spheres or catenoids are solutions. These solutions mark the values of the parameters where the qualitative behaviour of solutions changes.

In the case $\beta \geq 0$ it is convenient to study the reformulation of the minimisation problem in the hyperbolic half plane. If $\alpha\beta = 1$ then a solution is given by an arc of the circle with center at the origin and passing through the point $(1, \alpha)$ which we denote by S_α. This is a geodesic in the hyperbolic half plane. The corresponding surface of revolution is part of a sphere which is the simplest possible closed Willmore surface. It is then convenient to distinguish the cases $\alpha\beta > 1$ and $\alpha\beta < 1$. In the case $\alpha\beta > 1$ a graph satisfying the boundary conditions starts above S_α. By gluing pieces of spheres and using the conformal invariance of the Willmore functional we prove that one can restrict to minimising sequences for which the functions are increasing on $(-1, 0)$ and the maximum of the derivative is attained at the boundary. Further, S_α is a strong barrier from below for the modified minimising sequence. This property follows from the following result.

Lemma 1.2 (Cf. Lemma 3.9 in [10])**.** *Let α and β be strictly positive and such that $\alpha\beta > 1$. For each positive even function $u \in C^{1,1}([-1, 1])$ with $u(-1) = \alpha$ and $u'(-1) = \beta$ there exists a positive even function $v \in C^{1,1}([-1, 1])$ with Willmore energy smaller than or equal to the Willmore energy of u, satisfying the same boundary conditions as u and such that*

$$x + v(x)v'(x) \leq 0 \text{ in } [0, 1]\,. \tag{1.13}$$

We give the idea of the proof of this lemma since its proof requires only one geometric construction and it gives the opportunity to give an example of the gluing procedure described above. Let φ be defined by $\varphi(x) := x + u(x)u'(x)$ for $x \in [0, 1]$ and u as in the lemma. The function φ gives the x-coordinate of the center of the semicircle with center in the x-axis and tangent to the graph of u in $(x, u(x))$. Since $\alpha\beta > 1$, $\varphi(1) < 0$ and by the symmetry of u, $\varphi(0) = 0$. If there exists $x_0 \in (0, 1)$ with $\varphi(x_0) = 0$, a new symmetric function with smaller Willmore energy than u is constructed as follows. On $[0, x_0]$ we take the arc of the semicircle with center at the origin and tangent to the graph of u in $(x_0, u(x_0))$, while on $[x_0, 1]$ we take u. Extending by symmetry the function to $[-1, 1]$ we get a $C^{1,1}$-even positive function satisfying the same boundary conditions as u. Moreover, the Willmore energy of the new function is at worst equal to the Willmore energy of u. Indeed, thanks to formula (1.10) it is enough to look at the hyperbolic Willmore energy. The function u is changed only on $[-x_0, x_0]$ where we have substituted its graph with an arc of a geodesic of the hyperbolic half-plane which does not contribute to the hyperbolic Willmore energy. Finally, by construction the new function satisfies (1.13).

The case $\alpha\beta < 1$ and $\beta \geq 0$ is in some sense dual to the one just described. Indeed, again the graph is increasing on $(-1, 0)$ while S_α (the arc of semicircle explicit solution of the boundary value problem for $\alpha\beta = 1$) is now a barrier from above and the satisfied differential inequality is $x + u(x)u'(x) \geq 0$ in $[0, 1]$.

As we have seen, the geodesics of the hyperbolic half plane play an important role when studying the case $\beta \geq 0$. In some sense, spheres are the dominating shapes. When studying the case $\beta < 0$, both catenoids and spheres influence the shape of minimisers. For $|\beta|$ large, numerical calculations clearly display almost catenoidal and almost spherical (hyperbolically geodesic) parts of solutions. A catenoid symmetric with respect to zero is obtained rotating around the x-axis the graph of $x \mapsto \cosh(bx)/b$ for $b \in \mathbb{R}_+$ which is called a *catenary*. In the following the word catenary refers both to the function $x \mapsto \cosh(bx)/b$, for some $b > 0$, as well as to its graph. In the geometric constructions with $\beta < 0$ catenaries come into play in addition to the hyperbolic geodesics. For $\beta < 0$ given and $\alpha = \alpha_\beta$ with

$$\alpha_\beta := \frac{\sqrt{1 + \beta^2}}{\operatorname{arsinh}(-\beta)}\,, \tag{1.14}$$

an explicit solution is given by the catenary $x \mapsto \cosh(bx)/b$ with $b = \operatorname{arsinh}(-\beta)$. This explicit solution plays for $\beta < 0$ the role that the semicircle S_α plays for $\beta \geq 0$. Then, we distinguish the cases $\alpha > \alpha_\beta$ and $\alpha < \alpha_\beta$. These are cases 3. and 4. in Theorem 1.1. For $\alpha > \alpha_\beta$ there exist two catenaries c_1 and c_2 with height α at the boundary. Concerning the slopes at the extrema of the interval, one finds $c_1'(-1) < \beta < c_2'(-1)$ (see [10, Figure 4]). In this case, the boundary conditions force the graph to remain initially between the two catenaries. Notice that one catenary is relatively flat while the other is quite deep, i.e. it gets near to the x-axis. In analogy with the case $\beta \geq 0$ and the behavior of the 'good' graphs with respect to the spheres, one may expect that these catenaries could serve as barriers: one from above and the other from below. However the situation is more complicated than this. One can prove that the flatter of the two catenaries is a barrier from above for the elements of the modified minimising sequence, while the deep catenary is only on a subset of $[-1,1]$ (not containing 0) a barrier from below (see [10, Lemma 4.7]). Similarly as in the case $\beta \geq 0$ this observation follows from the fact that the elements of the modified minimising sequence satisfy an ordinary differential inequality (see [10, Lemma 4.5]). Still, the solutions we obtain resemble these catenaries since they satisfy $u' > 0$ in $(0,1]$. Further the fact that the graph starts between two catenaries suggests that compactness problems may arise. Indeed, we need further to distinguish the case $-\beta \geq \alpha$ and $-\beta < \alpha$. The parameter range $-\beta \geq \alpha$ can be studied with ideas similar to the case $\beta \geq 0$ using catenaries instead of geodesic semicircles. The case $-\beta < \alpha$ is special since we can prevent loss of compactness only by further restricting the class of functions over which we minimise (see the definition of the space $N_{\alpha,\beta}$ in (1.11)). The fact that for parameters in this range something special is happening is suggested also by numerical computations. Indeed, for a value of β in this range there is numerical evidence of the existence of two graphs both minimising the Willmore energy and with comparatively very different qualitative behavior. These numerical experiments suggest also that in general we cannot expect uniqueness of the minimiser in the class of surfaces we consider.

The case $\alpha < \alpha_\beta$ is not simply the dual of the case $\alpha > \alpha_\beta$. We need to further differentiate between the cases $\alpha^* \leq \alpha < \alpha_\beta$ and $\alpha < \alpha^*$. Here α^* defined in (1.12) is the smallest boundary height where for some boundary angle one may have a catenoid as solution. Notice that $\alpha_\beta \geq \alpha^*$ for all $\beta < 0$. In the case $\alpha < \alpha_\beta$ in order to achieve a priori information on suitably modified minimising sequences both hyperbolic geodesics and catenaries are used in the constructions. This interplay between these two prototypes of Willmore surfaces gives rise to some technical difficulties.

The case $\alpha^* \leq \alpha < \alpha_\beta$ is in some sense dual to $\alpha > \alpha_\beta$. Here we still have the two catenaries c_1 and c_2 with height α at the boundary. If $-\beta < \alpha$ the graph starts above both catenaries and these are barriers from below. This follows again from a differential inequality (see [10, Lemma 4.28]). For $-\beta > \alpha$ the graph starts below both catenaries and these are in general not barriers from above. The constructions leading to minimising sequences satisfying strong a priori bounds are similar to those for $\alpha > \alpha_\beta$. The case $\alpha = \alpha^*$ is special since there is only one catenary with height α but the constructions still work. As can be seen from the statement of Theorem 1.1, the first order derivative of the elements of the modified minimising sequence could be chosen to be of a fixed sign on $[-1,0]$ for $\beta \geq 0$ and for $\beta < 0$ but $\alpha \geq \alpha_\beta$. This is not the case for the range of parameters such that $\beta < 0$ and $\alpha < \alpha_\beta$. In this case the elements of the modified sequence satisfy either $u' > 0$ in $(0,1]$ or that u' has a change of sign on $(0,1]$. Numerical experiments indicate that both phenomena occur. We do not have a good understanding on when which occur. For $\beta < 0$ and small values of α, we can prove that the first order derivative changes sign in $[-1,0]$. Due to the boundary conditions the graph is, starting from $x = -1$, at first approaching the x-axis but when this becomes energetically too expensive (as can be seen looking at the second term inside the brackets in (1.5)), the graph tends to move away from the x-axis causing a change of sign of the derivative. From the studies of the case $\beta \geq 0$, we then know that there is no further change of sign of the first order derivative (see [10, Lemma 3.20]).

It remains to discuss the case $\alpha < \alpha^*$. This turns out to be the most complicated range of parameters. The main problem is that here we do not have natural comparison functions since there are no catenaries with height α at the boundary. The quantity we study in this case is the quotient $u(x)/x$ for $x \in (0,1]$. When this quotient is bigger than or equal to α^*, we are in the situation already studied in the case $\alpha^* \leq \alpha < \alpha_\beta$ and we can derive bounds for the function and its derivative. For the other values of x, the quotient is below the corresponding quotient of any catenary centered at 0 (i.e. $u(x)/x < \cosh(bx)/(bx)$ for any $b \in \mathbb{R}_+$). This is energetically expensive since the only way to approach the x-axis with small Willmore energy and bounded derivative is as a catenary. With this observation, we prove that on the set $x \in (0,1]$ where $u(x)/x < \alpha^*$ the quotient $u(x)/x$ is increasing moving from the right to the left starting at $x = 1$ (see [10, Proposition 4.43]). In these constructions we need to further restrict the space over which we minimise (see [10, Definition 4.26]). Also in this case the constructions are different for the cases $\alpha > -\beta$ and $\alpha \leq -\beta$. The quotient $u(x)/x$ is particularly important due to the scale invariance of the Willmore functional.

Via the strong a priori bounds for the elements of the modified minimising sequence, we obtain not only the existence of a minimiser, but also a qualitative description of it. Further, starting from a weak formulation of the Euler-Lagrange equation the regularity of the minimiser is obtained by a clever choice of test functions. The details of the proof of regularity are given in [8, Proof of Theorem 4, Step 2].

In the geometric constructions we have used the conformal invariance of the Willmore functional via reflections, translations, rotations and scaling. We do not employ inversions. However, for certain choices of the boundary conditions inversion could have been employed but it would not have covered all the cases. Considering inversions of the Willmore surfaces of revolution generated by graphs constructed in Theorem 1.1 yield parametric Willmore surfaces of revolution which are not necessarily generated by graphs.

Via the geometric constructions we also have a good understanding of the monotonicity behavior of the energy.

Proposition 1.3 (Cf. Propositions 3.12, 3.19, 4.18, 4.40 and 4.49 in [10])**.** *For $\alpha > 0$ and $\beta \in \mathbb{R}$, let $M_{\alpha,\beta}$ be as defined in Theorem 1.1 and, for $\beta < 0$, let α_β be defined as in* (1.14).

(i) For $\beta > 0$ the energy $M_{\alpha,\beta}$ is strictly monotonically increasing in α for $\alpha\beta \geq 1$ and strictly monotonically decreasing in α for $\alpha\beta \leq 1$.

(ii) For $\beta = 0$ the energy $M_{\alpha,\beta}$ is strictly monotonically decreasing in α.

(iii) For $\beta < 0$ the energy $M_{\alpha,\beta}$ is strictly monotonically increasing in α for $\alpha \geq \alpha_\beta$ and strictly monotonically decreasing in α for $\alpha \leq \alpha_\beta$.

The explicit solutions given by the spheres for $\alpha\beta = 1$ and by the catenary for $\alpha = \alpha_\beta$ mark the values of the parameters where there is a change in the monotonicity behavior of the energy. A natural question is if the minimiser in the class of symmetric graphs is also a minimiser in the bigger class of surfaces of revolution generated by (symmetric) curves. That this is in general not the case can be seen from the asymptotic behavior of the energy. For $\beta \neq 0$ the energy $M_{\alpha,\beta}$ diverges when α grows to infinity while one can construct surfaces of revolution generated by (symmetric) curves with bounded energy.

Solutions of (1.8) for $\kappa_h(0)$ given and $\kappa_h'(0) = 0$ are oscillating for $|\kappa_h(0)| \neq 2$ and with a fixed sign if $|\kappa_h(0)| \leq 2$. Solutions with $|\kappa_h(0)| = 2$ are the catenaries. Concerning the hyperbolic curvature of minimisers for $M_{\alpha,\beta}$, defined in Theorem 1.1, we have the following result.

Theorem 1.4 (Cf. Theorems 6.4, 6.7, 6.9 and 6.11 in [10])**.** *For $\alpha > 0$ and $\beta \in \mathbb{R}$ let $u_{\alpha,\beta}$ be a smooth positive even function minimiser for $M_{\alpha,\beta}$ (defined in Theorem 1.1) with $u(-1) = \alpha$ and $u'(-1) = \beta$. Let $\kappa_h[u_{\alpha,\beta}]$ denote the hyperbolic curvature of the graph of $u_{\alpha,\beta}$ as defined in* (1.6)*. Then we have*

1. *For $\beta > 0$ and $\alpha\beta > 1$: either $\kappa_h[u_{\alpha,\beta}] < 0$ in $[0,1)$ or there exists an $a \in (0,1)$ such that $\kappa_h[u_{\alpha,\beta}] < 0$ in $[0,a)$ and $\kappa_h[u_{\alpha,\beta}] > 0$ in $(a,1)$.*

2. *For $\beta \geq 0$ and $\alpha\beta \leq 1$: $\kappa_h[u_{\alpha,\beta}] > 0$ in $(-1,1)$.*

3. *For $\beta < 0$ and $\alpha \geq \alpha_\beta$: either $\kappa_h[u_{\alpha,\beta}] > 0$ in $[0,1)$ or there exists an $a \in (0,1)$ such that $\kappa_h[u_{\alpha,\beta}] > 0$ in $[0,a)$ and $\kappa_h[u_{\alpha,\beta}] < 0$ in $(a,1)$.*

4. *For $\beta < 0$ and $\alpha < \alpha_\beta$: $\kappa_h[u_{\alpha,\beta}] > 0$ in $(-1,1)$.*

Concerning the asymptotic behavior of the solutions constructed in Theorem 1.1 when $\beta \in \mathbb{R}$ is fixed and α goes to 0, we prove that they converge to the unit sphere centered at the origin.

Theorem 1.5 (Cf. Theorem 5.8 in [10])**.** *Fix $\beta \in \mathbb{R}$. For $\alpha > 0$ let u_α be a minimiser for $M_{\alpha,\beta}$. Then, u_α converges for $\alpha \searrow 0$ to $x \mapsto \sqrt{1-x^2}$ in $C^m_{loc}(-1,1)$ for any $m \in \mathbb{N}$.*

In a recent paper [30], Grunau presents a more refined study of the asymptotic behavior of the minimisers near to $x = 1$ as α goes to zero. In a boundary layer the properly rescaled minimisers are shown to converge to a piece of a catenary. The two results together confirm the numerical computations showing that for α small the solutions have almost a catenoidal part and almost a spherical part. It is here worth remarking how useful the numerical computations have been in understanding the behavior of the solutions.

Scholtes in [63] studies the functional obtained by adding to the Wilmore functional the area functional. Using also the geometric constructions just described above, he proves the existence of minimisers in the class of surfaces of revolution generated by symmetric graphs satisfying prescribed (but not arbitrary) Dirichlet boundary data.

1.1.2 Natural boundary conditions

In this paragraph we discuss the results proved in [3, 4]. In these works surfaces of revolution with only the position of the boundary fixed are considered. That is, only the two circles constituting the boundary are prescribed. The second boundary condition arises then naturally when considering critical points of the Willmore functional in this class of surfaces. This can be seen by looking at the first variation of $\mathcal{W}$. Given a smooth function $u : [-1,1] \to \mathbb{R}_+$ which is a critical point of the Willmore functional one finds for any $\varphi \in H^2(-1,1) \cap H^1_0(-1,1)$

$$\begin{aligned} 0 = \frac{d}{dt}\mathcal{W}(u+t\varphi)\Big|_{t=0} = \langle \mathcal{W}'(u), \varphi \rangle \quad &= \quad -2\pi \left[H(x)\frac{u(x)\varphi'(x)}{1+u'(x)^2} \right]_{-1}^{1} \\ & \quad -2\pi \int_{-1}^{1} u\varphi \left(\Delta_g H + 2H^3 - 2HK \right) dx \,, \end{aligned}$$

(See [3, Appendix A].) where Δ_g denotes the Laplace-Beltrami operator on Γ, the surface of revolution generated by u. Hence, it is necessary that Γ is solution of (1.1) and that its mean curvature is equal to zero at the boundary ($H(\pm 1) = 0$) in order that $\langle \mathcal{W}'(u), \varphi \rangle = 0$ for all admissible test functions φ. These (and more general) boundary conditions are discussed in [56].

With symmetry In [3] we study the existence of Willmore surfaces of revolution satisfying *symmetric* natural boundary conditions and generated by *symmetric* graphs. In this work a more general functional than the Willmore functional is considered. For a smooth, immersed two-dimensional surface $\Gamma \subset \mathbb{R}^3$ and a real parameter $\gamma \in [0,1]$ we study the functional

$$\mathcal{W}_\gamma(\Gamma) := \int_\Gamma H^2 \, dS - \gamma \int_\Gamma K \, dS \,, \tag{1.15}$$

with, as before, $H = (\kappa_1 + \kappa_2)/2$ the mean curvature of the immersion (κ_1, κ_2 the principal curvatures of Γ), $K = \kappa_1\kappa_2$ its Gauss curvature, and dS its area element. This is a special choice of the functional proposed by Nitsche in [56] that to a two-dimensional surface Γ associates the value

$$\mathcal{F}(\Gamma) = \int_\Gamma \Phi(H,K)\, dS \quad \text{with } \Phi(H,K) = \mu + (H - H_0)^2 - \gamma K, \tag{1.16}$$

with real parameters μ, γ and H_0 satisfying $\mu \geq 0$, $0 \leq \gamma \leq 1$ and $\gamma H_0^2 \leq \mu(1-\gamma)$. These conditions on the parameters are needed for the definiteness of the functional. That is, the existence of a constant $C > -\infty$ such that $\mathcal{F}(\Gamma) \geq C$ holds true for all connected and orientable surfaces of regularity class C^2. In 1973, Helfrich [33] studied a functional quite similar to $\mathcal{F}$ in (1.16) as a model for biological bilayer membranes. Since then, $\mathcal{F}$ is often referred to as *Helfrich functional.* The functional $\mathcal{W}_\gamma$ is non-negative for $\gamma \in [0,1]$ since

$$4(H^2 - \gamma K) = (1-\gamma)(\kappa_1 + \kappa_2)^2 + \gamma(\kappa_1 - \kappa_2)^2 \geq 0 \quad \text{for } \gamma \in [0,1]\,. \tag{1.17}$$

Moreover, the strict inequality $\mathcal{W}_\gamma(\Gamma) > 0$ holds for every non-planar surface Γ if $0 < \gamma < 1$.

As in the case of Dirichlet boundary conditions we study surfaces of revolution generated by symmetric graphs. Let Γ be the surface of revolution generated by the graph of an even smooth function $u : [-1,1] \to \mathbb{R}_+$. The Gauss curvature of Γ and the energy are given respectively by

$$K = \frac{u''(x)}{(1+u'^2)^{\frac{3}{2}}} \quad \text{and} \quad \mathcal{W}_\gamma(u) := \mathcal{W}_\gamma(\Gamma) = \mathcal{W}_0(u) + 2\pi\gamma \left[\frac{u'(x)}{\sqrt{1+u'^2}}\right]_{-1}^{1}, \tag{1.18}$$

with $\mathcal{W}_0(u) = \mathcal{W}(u)$ the Willmore energy of u defined in (1.5). Identity (1.18) shows that also the case $\gamma = 1$ is special. Indeed, up to some constant, $\mathcal{W}_1(u)$ equals $\mathcal{W}_h(u)$, the hyperbolic Willmore energy of u defined in (1.7). Thus, varying γ within $[0,1]$, we interpolate between the "Euclidean" Willmore functional with $\gamma = 0$, and the "hyperbolic" Willmore functional for $\gamma = 1$.

Critical points of $\mathcal{W}_\gamma$ satisfy the Willmore equation (1.1). The Euler-Lagrange equation of $\mathcal{W}_\gamma$ is independent of the value of γ since the integral over the Gauss curvature only contributes to the boundary terms on account of the Gauss-Bonnet Theorem. The boundary value problem under consideration is then

$$\begin{cases} \Delta_g H + 2H(H^2 - K) = 0 \quad \text{on } \Gamma, \\ u(\pm 1) = \alpha \ \text{ and } \ H(\pm 1) = \dfrac{\gamma}{\alpha\sqrt{1+u'(\pm 1)^2}}\,, \end{cases} \tag{1.19}$$

with Δ_g the Laplace-Beltrami operator on the surface of revolution generated by the graph of u. Here, as for the case of Dirichlet boundary conditions, the parameter $\alpha > 0$ gives the radius of the circles constituting the boundary. The derivation of the second boundary condition is given in [3, Appendix A] together with a geometric interpretation. The second boundary condition can be rewritten as $H(\pm 1) = \gamma\kappa_n(\pm 1)$ with $\kappa_n(1)$ the normal curvature of the boundary curve $\varphi \mapsto (1, u(1)\cos(\varphi), u(1)\sin(\varphi))$ and similarly for $\kappa_n(-1)$.

The main result is the following.

Theorem 1.6 (Cf. Theorem 1.1 in [3])**.** *For each $\alpha > 0$ and for each $\gamma \in [0,1]$, there exists a positive and symmetric function $u \in C^\infty([-1,1], \mathbb{R}_+)$ satisfying $u(\pm 1) = \alpha$ such that the corresponding surface of revolution $\Gamma \subset \mathbb{R}^3$ solves* (1.19).

For special values of α and γ, explicit solutions of problem (1.19) are known. For example, if $\gamma = 1$ then the piece of sphere described by the circular arc $u(x) = \sqrt{\alpha^2 + 1 - x^2}$, $x \in [-1,1]$, provides an explicit solution of (1.19) for arbitrary $\alpha > 0$. When $\gamma = 0$ the second boundary condition is $H(\pm 1) = 0$. Then for $\alpha > \alpha^*$, with α^* defined as in (1.12), there exist two catenoid solutions of (1.19) generated by catenaries $x \mapsto \cosh(bx)/b$ with $b > 0$ suitably chosen. These explicit examples show that the solutions of problem (1.19) are, in general, not unique. Theorem 1.6 becomes particularly interesting for $\gamma = 0$ and $\alpha < \alpha^*$, as minimal surface solutions do no longer exist. For $\gamma = 0$ and $\alpha = 1$ there still exists an explicit solution given by $u(x) = 2 - \sqrt{2 - x^2}$, a piece of the well-known Clifford torus.

Existence of rotationally symmetric Willmore surfaces solutions of (1.19) for $\gamma = 0$ and for all values of α was observed numerically in [28]. In [38] the presence of a third solution for $\alpha > \alpha^*$ was numerically observed, suggesting that α^* is a bifurcation point on the branch of minimal surface solutions. In [16] Deckelnick and Grunau prove that α^* is indeed a bifurcation point and so, at least locally, the existence also of a non-minimal solution for α near to α^* is settled. In the same paper, using a linearisation around the Clifford torus they prove existence of a solution to (1.19) for $\gamma = 0$ and α close to 1. Theorem 1.6 states existence of solutions for the same boundary value problem for all $\alpha \in (0, \alpha^*)$. Without some uniqueness results on the minimisers, we cannot say that these solutions are on the numerically computed branch. Uniqueness is a delicate issue since for $\alpha > \alpha^*$ it is not valid.

A natural approach to prove existence of solutions to (1.19) is by solving a minimisation problem. The set over which we minimise is given by $\bigcup_{\beta \in \mathbb{R}} N_{\alpha,\beta}$ with $N_{\alpha,\beta}$ defined as in (1.11). That is, we minimise among symmetric smooth graphs satisfying $u(\pm 1) = \alpha$ and with arbitrary slope at the boundary. Then, if a minimiser is a graph, the corresponding surface of revolution is a solution of the Willmore Dirichlet boundary value problem (1.9) for some value β of the derivative at the boundary. For the last problem we have already proven existence, estimates and regularity.

The crucial part in the proof of Theorem 1.6 consists then in showing that a minimiser is a proper graph. This follows from the study of the monotonicity and continuity property of the energy

$$T_{\gamma,(\alpha,\beta)} := \inf \left\{ \mathcal{W}_\gamma(u) \,:\, u \in N_{\alpha,\beta} \right\},$$

for $\gamma \in [0, 1]$, $\alpha > 0$ and $\beta \in \mathbb{R}$. The fact that this energy is attained and a minimiser exists is a direct consequence of Theorem 1.1 and (1.18).

Lemma 1.7 (Cf. Corollary 3.3 in [3])**.** *Let $\gamma \in [0, 1]$ and $\alpha > 0$ be fixed. Then $\beta \mapsto T_{\gamma,(\alpha,\beta)}$ is continuous in $\mathbb{R}$ if $\alpha \leq \alpha^*$ while for $\alpha > \alpha^*$ it is continuous in $\mathbb{R} \backslash \{-\alpha\}$.*

The energy is not necessarily continuous in $-\alpha$ for $\alpha > \alpha^*$ since for $0 > \beta > -\alpha$ and $\alpha \operatorname{arsinh}(-\beta) \geq \sqrt{1 + \beta^2}$ we restrict the set over which we minimise (see the definition of $N_{\alpha,\beta}$ in (1.11)). Numerical experiments indicate that the energy $M_{\alpha,\beta}$ has a discontinuity at this point. That is, for $\beta > -\alpha$ but near to $-\alpha$, numerically we observe two branches of solutions to (1.9): one branch of solutions that are qualitatively as the solutions we construct in Theorem 1.1 and a second branch of solutions not satisfying the extra condition and with lower energy. The energy appears to be continuous along this second branch.

Having informations on the continuity of the energy in β, we now need to show that we may restrict to a compact subset of β containing in its interior the slope that the minimisers have at the boundary. This we reach by studying the monotonicity behavior of the energy in β. Before stating the result we need to introduce some notation. For $\alpha > \alpha^*$ there exist $b_1 < b_2$, $b_i = b_i(\alpha)$ for $i = 1, 2$, real numbers such that

$$\alpha = \frac{\cosh(b_1)}{b_1} = \frac{\cosh(b_2)}{b_2}.$$

These are the two parameters that describe the two catenoids with height α at the boundary. In the following $\beta_1 = \beta_1(\alpha)$ and $\beta_2 = \beta_2(\alpha)$ give the slope at the boundary of the catenoid associated to b_1 and b_2 respectively; that is $\beta_1 := -\sinh(b_1)$ and $\beta_2 := -\sinh(b_2)$.

Lemma 1.8 (Cf. Corollary 3.13 and 3.14 in [3]). *For $\gamma \in [0,1]$ and $\alpha \leq \alpha^*$ the mapping $\beta \mapsto T_{\gamma,(\alpha,\beta)}$ is decreasing for $-\infty < \beta \leq -\alpha$ and increasing for $\alpha^{-1} \leq \beta < +\infty$.*

For $\gamma \in [0,1]$ and $\alpha > \alpha^*$ the mapping $\beta \mapsto T_{\gamma,(\alpha,\beta)}$ is decreasing on $(-\infty, \beta_2(\alpha)]$ and $(-\alpha, \beta_1(\alpha)]$ while it is increasing on $[\alpha^{-1}, \infty)$.

In the particular cases $\gamma = 0$ and $\gamma = 1$ the monotonicity behavior in β of the energy can be described more precisely. The mapping $\beta \mapsto T_{0,(\alpha,\beta)}$ achieves its global minimum at $\beta = -\alpha$ for $\alpha \leq \alpha^*$. For $\alpha > \alpha^*$, the catenoids are the obvious minima that are attained at $\beta = \beta_2(\alpha)$ and $\beta = \beta_1(\alpha)$. For $\alpha > 0$, the mapping $\beta \mapsto T_{1,(\alpha,\beta)}$ achieves its global minimum at $\beta = \alpha^{-1}$. The proof of Lemma 1.8 is based on gluing pieces of semicircles and catenaries (as for the Dirichlet boundary value problem), the monotonicity behavior of the energy in α and the scale invariance of the energy. For $\gamma \in (0,1)$ the monotonicity behavior of the energy in β is not completely characterised. One may conjecture that there exists some $\tilde{\beta} = \tilde{\beta}(\alpha,\gamma) \in [\beta_1(\alpha), \alpha^{-1}]$ such that $\beta \mapsto T_{\gamma,(\alpha,\beta)}$ is decreasing on $(-\alpha, \tilde{\beta}]$ and increasing on $[\tilde{\beta}, +\infty)$. The difficulty lies in the fact that for $\gamma \in (0,1)$ there do no exist graphs (or even curves) such that the energy $\mathcal{W}_\gamma$ is equal to zero (see (1.17)).

It is interesting that for $\alpha \leq \alpha^*$ and $\gamma = 0$ the monotonicity property of the energy in β yields that the constructed solution of (1.19) satisfies $u'(-1) = -\alpha$ for each α. This confirms to a certain extent that the case $\beta = -\alpha$ is special as already observed in the study of the Dirichlet boundary value problem. The asymptotic behavior of the solutions for α going to 0 in the case $\gamma = 0$ has been studied in [37] where convergence to the sphere is proven.

The general case In [4] we construct connected annular type Willmore surfaces of revolution spanned by two concentric circles contained in two parallel planes by minimising the Willmore functional in this class of surfaces. The first boundary condition is that the boundary of the surface is given by these circles, while the second one is that the mean curvature is equal to zero at the boundary. Comparing the problem to the one studied in [3] here the two circles do not need to have the same radius. Moreover, we do not restrict to graphs, neither to symmetric curves. On the other hand, here we study only the Willmore functional and not the more general one studied in [3] (see (1.15)).

Let $S_r := \{re^{i\varphi} : \varphi \in \mathbb{R}\}$ be a circle of radius r centered at the origin. Given two positive parameters α_l and α_r we consider the circles $C_{\alpha_l} := \{-1\} \times S_{\alpha_l}$ and $C_{\alpha_r} := \{1\} \times S_{\alpha_r}$ centered at $(-1,0,0)$ and $(1,0,0)$ and with radii α_l and α_r, respectively. The boundary problem we consider is

$$\begin{cases} \Delta_\Gamma H + 2H(H^2 - K) = 0 & \text{on } \Gamma, \\ \partial\Gamma = C_{\alpha_l} \cup C_{\alpha_r}, & H = 0 \text{ on } \partial\Gamma\,, \end{cases} \tag{1.20}$$

with Δ_Γ the Laplace-Beltrami operator on Γ. We first observe for which values of the parameters there exists a minimal surface solution. Piece of catenoids having C_{α_l} as boundary components are those generated by rotating the graphs

$$x \mapsto \frac{\alpha_l}{\cosh(\gamma)} \cosh\left(\frac{\cosh(\gamma)}{\alpha_l}(x+1) + \gamma\right), \quad x \in [-1,1]\,, \tag{1.21}$$

for arbitrary $\gamma \in \mathbb{R}$. Studying this function one sees that there exists $\gamma \in \mathbb{R}$ such that the catenoid generated by (1.21) is a solution to (1.20) if and only if $\alpha_r \geq \alpha_r^*(\alpha_l)$ with

$$\alpha_r^*(\alpha_l) := \inf_{\gamma\in\mathbb{R}} \frac{\alpha_l}{\cosh(\gamma)} \cosh\left(\frac{2\cosh(\gamma)}{\alpha_l} + \gamma\right). \tag{1.22}$$

Notice that $\alpha_r^*(\alpha_l) > 0$. One can further say that for $\alpha_r > \alpha_r^*(\alpha_l)$ there are two such minimal surfaces, while for $\alpha_r = \alpha_r^*(\alpha_l)$ there is only one.

The main result is the following.

Theorem 1.9. *For each $\alpha_l, \alpha_r > 0$ there exists some smooth, annular type Willmore surface $\Gamma \subset \mathbb{R}^3$ minimising the Willmore energy among all rotationally symmetric, annular type surfaces with boundary $C_{\alpha_l} \cup C_{\alpha_r}$. The surface Γ is embedded into $\mathbb{R}^3$ and admits the representation*

$$\Gamma = \{(x, u(x)\cos\varphi, u(x)\sin\varphi) \,:\, x \in [-1,1]\ ,\ \varphi \in \mathbb{R}\}$$

with some function $u \in C^\infty([-1,1], \mathbb{R}_+)$. The surface Γ is a solution of the boundary value problem (1.20).

Finally, one of the following three alternatives holds:

a) If $\alpha_r > \alpha_r^*(\alpha_l)$, there exist precisely two such solutions Γ, both being catenoids with $H \equiv 0$.

b) If $\alpha_r = \alpha_r^*(\alpha_l)$, there exists precisely one such solution Γ, a catenoid with $H \equiv 0$.

c) If $\alpha_r < \alpha_r^*(\alpha_l)$, there exists at least one such solution Γ. Its mean curvature satisfies $H = 0$ on $C_{\alpha_l} \cup C_{\alpha_r}$ and $H \neq 0$ on $\Gamma \backslash (C_{\alpha_l} \cup C_{\alpha_r})$.

Naturally, alternative *c)* is the interesting part of this result as the constructed Willmore surface is not a minimal surface (as it corresponds to the case where no annular type minimal surface spanning the two concentric circles exists). Also note that the solution from part *c)* minimises under rotationally symmetric, annular type variations but is only stationary under general variations. Presently, we do not know whether there exists some non-rotationally symmetric, annular type surface spanning $C_{\alpha_l} \cup C_{\alpha_r}$ with smaller Willmore energy than that constructed in Theorem 1.9.

Theorem 1.9 is proven by solving a minimisation problem. Let $\widetilde{T}_{\alpha_l,\alpha_r}$ denote the set of all regular curves $c \in W^{2,2}([-1,1], \mathbb{R} \times \mathbb{R}_+)$ connecting the points $(-1, \alpha_l)$ and $(1, \alpha_r)$, i.e. $c(-1) = (-1, \alpha_l)$, $c(1) = (1, \alpha_r)$. Let T_{α_l,α_r} denote the set of all functions $u \in W^{2,2}([-1,1], \mathbb{R}_+)$ with boundary conditions $u(-1) = \alpha_l$, $u(1) = \alpha_r$. The minimisation problems we consider are

$$\widetilde{M}_{\alpha_l,\alpha_r} = \inf_{c \in \widetilde{T}_{\alpha_l,\alpha_r}} \mathcal{W}(c) \quad \text{and} \quad M_{\alpha_l,\alpha_r} = \inf_{u \in T_{\alpha_l,\alpha_r}} \mathcal{W}(u)\,. \tag{1.23}$$

It is of course clear that $\widetilde{M}_{\alpha_l,\alpha_r} \leq M_{\alpha_l,\alpha_r}$. Of greatest interest is that the two infima are actually equal.

Lemma 1.10 (Cf. Corollary 1 in [4])**.** *The equality $\widetilde{M}_{\alpha_l,\alpha_r} = M_{\alpha_l,\alpha_r}$ holds for any $\alpha_l, \alpha_r > 0$, i.e. any minimiser within the small class T_{α_l,α_r} is also a minimiser in the larger class $\widetilde{T}_{\alpha_l,\alpha_r}$.*

By an explicit construction (see [4, Lemma 2.3]), for any given curve in $\widetilde{T}_{\alpha_l,\alpha_r}$ one can construct a curve admitting a non-parametric representation with almost the same Willmore energy and lower boundary values. The lemma above then follows from the fact that the energy M_{α_l,α_r} is decreasing in α_l with α_r fixed and vice-versa. It is here worth noticing that the construction in [4, Lemma 2.3] could also be applied to the Dirichlet boundary value problem studied in [8, 10]. So that, in studying the minimisation problem for general curves with Dirichlet boundary conditions one may restrict to graphs *whenever* the energy is decreasing in the boundary height α. On the other hand, this reduction is not always possible. In the case of Dirichlet boundary conditions the energy of the minimiser in the class of graphs becomes unbounded when the boundary height grows to infinity and the boundary slope is kept fixed and different from zero, while the energy remains bounded if one considers the minimisation problem in the larger class of curves.

In order to prove existence of a minimiser for the minimisation problem for graphs in (1.23) we use a different approach than that used for Dirichlet boundary conditions. Instead of starting from a minimising sequence and modifying it so that strong a priori bounds are satisfied, we begin by first restricting further the set over which we minimise. That is for $L > 0$ we consider the subset of T_{α_l,α_r} defined by

$$T_{\alpha_l,\alpha_r,L} := \left\{u \in T_{\alpha_l,\alpha_r} \ : \ u(x) \geq L^{-1} \text{ and } |u'(x)| \leq L \text{ in } [-1,1]\right\}$$

and the energy

$$M_{\alpha_l,\alpha_r,L} := \inf_{u \in T_{\alpha_l,\alpha_r,L}} \mathcal{W}(u) \ .$$

Choosing L sufficiently large, $T_{\alpha_l,\alpha_r,L}$ is non-empty and hence $M_{\alpha_l,\alpha_r,L}$ well-defined. The reason for working within the smaller class $T_{\alpha_l,\alpha_r,L}$ is that it is relatively simple to construct minimisers $u = u_L$ in this class. By definition the elements in $T_{\alpha_l,\alpha_r,L}$ already satisfy the estimates needed for the compactness argument, thus yielding the existence of a minimiser. The main task consists then in proving a priori estimates on these minimisers u_L that are independent of L. This ensures that the minimiser is a point in the "interior" of $T_{\alpha_l,\alpha_r,L}$ and hence that the corresponding surface of revolution is a solution of the boundary value problem (1.20).

In the proof of the a priori estimates on the minimisers the relation between the Willmore functional and the hyperbolic Willmore functional is again useful. As a first step we prove that the hyperbolic curvature of minimisers satisfies the pointwise bound $0 \leq \kappa_h(x) \leq 2$ for $x \in [-1,1]$. This is obtained using semicircles (geodesics of the hyperbolic half-plane) as barriers from below and catenaries as barriers from above. Notice that semicircles have hyperbolic curvature identically equal to zero, while the hyperbolic curvature of catenaries is equal to two at the center of symmetry of the catenary and decreases to zero on both sides. This pointwise estimate yields a bound from above for the minimiser. Moreover, it shows that the values of the (first order) derivative on the interval $(-1,1)$ are bounded by the values of the derivative in $x = \pm 1$ and by a bound from below of the minimiser. These other bounds are obtained with more refined geometric constructions using catenaries as barriers from above. Another property of which we make use is that the energy $M_{\alpha_l,\alpha_r,L}$ is bounded by 4π for L sufficiently large. This smallness of the energy gives direct and explicit bounds on the length of an interval where the graph could approach the x-axis. In the constructions we have more freedom than in the Dirichlet boundary value problem since we may change the slope of the derivative at the boundary. This method cannot therefore be directly applied to the study of the Dirichlet boundary value problem with non-symmetric boundary data.

In the case of symmetric boundary conditions $\alpha = \alpha_l = \alpha_r$ and minimising only among symmetric graphs ([3]) we could prove that for $\alpha < \alpha^*$ with α^* defined in (1.12) the minimisers satisfy $u'(-1) = -u'(1) = -\alpha$. We cannot expect the same behavior in this more general case, but we can still show the following.

Lemma 1.11. *Given $\alpha_l > 0$ and $\alpha_r > 0$ such that $\alpha_r < \alpha_r^*(\alpha_l)$, let u be a minimiser of the Willmore energy in T_{α_l,α_r}. Then $u'(-1) < 0$ and $u'(1) > 0$.*

A second main result considers the limit case when both α_l and α_r converge to zero, i.e. the bounding circles C_{α_l} and C_{α_r} collapse to the points $(-1,0,0)$ and $(1,0,0)$ respectively.

Theorem 1.12 (Cf. Theorem 5.4 in [4]). *For α_l, $\alpha_r > 0$ let u_{α_l,α_r} be a minimiser of M_{α_l,α_r}. Then u_{α_l,α_r} converges uniformly to the function $x \mapsto \sqrt{1-x^2}$ on $[-1,1]$.*

Comparing to [10, Theorem 5.8] we obtain here uniform convergence up to the boundary. This we prove by showing that $\varphi_{\alpha_l,\alpha_r} := x^2 + u^2_{\alpha_l,\alpha_r}$ converges uniformly to $\varphi \equiv 1$.

1.2 A uniqueness result for graphs

In [7] a two-dimensional surface Γ that admits a parametrisation as a graph over a two-dimensional domain is considered. As boundary condition we study the zero Dirichlet boundary value problem: the boundary of Γ is given by the boundary of the domain over which the surface is given as a graph, and the tangent planes along the boundary are given by the plane containing the domain. The surface $\Gamma \subset \mathbb{R}^3$ can then be parametrised by $f(x,y) = (x, y, u(x,y))$ for $(x,y) \in \Omega$, the two-dimensional domain, and $u : \bar{\Omega} \to \mathbb{R}$ a smooth function. The boundary conditions require that $u|_{\partial\Omega} = 0$ and $\nabla u|_{\partial\Omega} = 0$. The question we address is the following. Is it true that Γ is a Willmore surface if and only if Γ is a subset of the plane $\{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_3 = 0\}$? Or in other words, does Γ being a Willmore surface imply and require u being constant? A uniqueness result of this kind has been studied by Palmer in [58]. He proves that a Willmore surface of disk type which has its boundary on a circle and which intersects the plane of the circle in a constant angle is a spherical cap or a flat disk. We extend the result of Palmer in the case of zero Dirichlet boundary data.

The result is the following.

Theorem 1.13 (Cf. Theorem 1.1 [7]). *Let $\Omega \subset \mathbb{R}^2$ be a smooth bounded strictly star-shaped domain with respect to $z_0 \in \Omega$. Let $u : \Omega \to \mathbb{R}$ be a smooth function with $u|_{\partial\Omega} = 0$ and $\nabla u|_{\partial\Omega} = 0$ and let $\Gamma \subset \mathbb{R}^3$ be the surface given by the graph of u.*

Then Γ is a Willmore surface if and only if $u \equiv 0$ in Ω.

We recall that a domain Ω is strictly star-shaped with respect to z_0 ($z_0 \in \Omega$) when $(z - z_0) \cdot \nu > 0$ for every $z \in \partial\Omega$ with ν the exterior normal to $\partial\Omega$ in z. Of course, due to the conformal invariance of the equation, it is not a restriction that we consider the plane $\{z = 0\} \subset \mathbb{R}^3$. The result of Palmer in [58] is for general parametrised surfaces of disk type, while here we have so far to restrict to graphs.

In general we do not expect uniqueness for the Willmore Dirichlet boundary value problem, not even in the presence of some extra symmetries. Indeed, in the case of surfaces of revolution generated by symmetric graphs with symmetric boundary data one can numerically find two different minimisers. Therefore, there is numerical evidence not only of two solutions to the boundary value problem but also of two different Willmore surfaces satisfying the same boundary value problem and having both minimal Willmore energy in a certain class. On the other hand, it is not yet clear what to expect in the case of graphs.

The proof of Theorem 1.13 consists of two steps. In the first we prove that if Γ is a Willmore surface, the mean curvature and all second order derivatives of u are zero at the boundary. This is done in the spirit of Pohozaev's identity (see [71, Chapter III, Sect.1]). Starting from the fact that Γ is a solution to (1.1) one multiplies the equation by test functions and then integrates. The first test function is the function u itself, while the second is $\varphi(x) := (x - x_0)u_x + (y - y_0)u_y = (z - z_0) \cdot \nabla u$ in the case that the domain Ω is strictly star-shaped with respect to $z_0 = (x_0, y_0)$. The test functions we choose are related to the conformal invariance of the problem (see [60]). Integrating by parts twice and using the boundary conditions yields two integral identities that combined give the crucial identity

$$\int_{\partial\Omega} H^2((x - x_0)\nu_x + (y - y_0)\nu_y)\, d\omega = 0\,,$$

involving only a boundary term. Here $\nu = (\nu_x, \nu_y)$ denotes the exterior normal field to $\partial\Omega$. This is where the assumption that Ω is strictly star-shaped with respect to z_0 is used.

Since the Willmore equation is an elliptic partial differential equation of fourth order the Dirichlet boundary conditions together with the information that also all the second derivatives of u vanish at the boundary is not sufficient to conclude that $u \equiv 0$ in Ω. We would also need that the third derivatives of u are zero at the boundary and this seems to be difficult to prove via suitable choices of test functions. In the second step of the proof we follow the ideas in [58]. By a result of Bryant [5] we may associate to an immersed Willmore surface in $\mathbb{R}^3$ a holomorphic function q (or a quartic holomorphic differential $q(z)dz^4$). This is similar to the case of surfaces of constant mean curvature to which one can associate a holomorphic function (or a quadratic holomorphic differential), the so-called Hopf function (or Hopf differential). From the fact that the mean curvature is equal to zero at the boundary it follows that also the holomorphic function q is equal to zero at the boundary. Hence, q is identically equal to zero. Then, the classification theorem of Bryant ([5]) yields that either Γ is a piece of a sphere or it is, after a conformal transformation, a minimal surface. By the boundary conditions the first alternative is excluded. The fact that Γ after a conformal transformation cannot be a non-planar minimal surface is due to the fact that, by the first step of the proof, the boundary of Γ consists only of umbilic points and this is a conformal invariant. Here we use concepts derived from the correspondence between Willmore surfaces in $\mathbb{R}^3$ and harmonic maps with values in the unit sphere in a suitably defined five-dimensional Minkowski space. These ideas from conformal differential geometry seem to be very useful in the study of Willmore surfaces and are sketched in [7, Appendix].

2 Hartree Fock theory for pseudo-relativistic atoms

A model for an atom with N electrons and a nucleus of charge Z fixed (at the origin) is in Schrödinger theory given by the Hamiltonian (operator)

$$H = \sum_{j=1}^{N} \left(T_j - V_j\right) + \sum_{1 \le i < j \le N} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|} \,. \tag{2.1}$$

The operator $T_j - V_j$ is the one-particle operator acting on the j-th electron. Since the electrons are all identical particles, the one-particles operators are all equal, that is $T_j - V_j = T - V$ for all $j \in \{1, \ldots, N\}$ with T and V some operators. Here T denotes the kinetic energy of an electron, while V describes the nuclear potential, i.e. the attraction that the electron feels to the nucleus. Usually, $V(\mathbf{x}) = Z/|\mathbf{x}|$. For the sake of the presentation, we defer the discussion of the choice of the kinetic energy and of the nuclear potential until after the presentation of the Hartree-Fock approximation. The operators $1/|\mathbf{x}_i - \mathbf{x}_j|$ describe the repulsion between the electrons. For a description of this model and an explanation of the Born-Oppenheimer approximation we refer to [50]. Here and in the following we use units where the reduced Planck constant $\hbar = 1$ and $e = m = 1$ with e and m the charge and the mass of an electron, respectively.

The electrons are described by a "wavefunction" $\Psi : \mathbb{R}^{3N} \to \mathbb{C}$. For the sake of clear presentation we do not consider the spin although all that we are going to say holds also with a number $q \in \mathbb{N}$ of spin-states. (In nature $q = 2$.) Since by the Heisenberg uncertainty principle, we cannot know at the same time the position and the speed of the electrons the function $|\Psi|^2$ has to be interpreted as a probability density. That is for a (measurable) region $S \subset \mathbb{R}^{3N}$ the quantity

$$\int_S |\Psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)|^2 \, d\mathbf{x}_1 \ldots d\mathbf{x}_N \,,$$

gives the probability of finding the N electrons in S. In particular, we have the normalisation $\|\Psi\|_{L^2(\mathbb{R}^{3N})} = 1$. Due to the Pauli exclusion principle the wavefunctions have also to be antisymmetric, that is

$$\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_j, \ldots, \mathbf{x}_i, \ldots, \mathbf{x}_N) = -\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_i, \ldots, \mathbf{x}_j, \ldots, \mathbf{x}_N) \text{ for all } i, j \in \{1, .., N\} \,,$$

so that the N-particle Hilbert space (the space of wavefunctions) is $\mathcal{H}_F = \wedge_{i=1}^N L^2(\mathbb{R}^3)$.

The operator H defined in (2.1) acts on a dense subspace of the N-particle Hilbert space $\mathcal{H}_F$ and, by appropriate choices of the kinetic energy and of the nuclear potential, it is bounded from below on this subspace. The *(quantum) ground state energy* is the infimum of the spectrum of H considered as an operator acting on $\mathcal{H}_F$:

$$E^{\mathrm{QM}}(N,Z) := \inf \sigma_{\mathcal{H}_F}(H) = \inf\{\, \langle \Psi, H\Psi\rangle \mid \Psi \in \mathcal{D}(H) \subset \mathcal{H}_F, \langle \Psi, \Psi\rangle = 1\}\,, \tag{2.2}$$

where $\langle\cdot,\cdot\rangle$ denotes the scalar product in $L^2(\mathbb{R}^{3N})$ and $\mathcal{D}(H)$ is the domain of the Hamiltonian. One of the aims of quantum mechanics is the study of the ground state energy and, if there are any, of the wavefunctions minimising it. Unfortunately this task turns out to be too complicated and so many approximations have been studied since the beginning of the theory.

In a first class of approximations instead of considering wavefunctions the objects over which one minimises are the so-called *densities*. A density is a non-negative function $\rho : \mathbb{R}^3 \to \mathbb{R}$ such that $\|\rho\|_{L^1(\mathbb{R}^3)} = N$. To a wavefunction $\Psi \in \mathcal{H}_F$ there is a natural way to associate a density:

$$\rho(\mathbf{x}) := N \int_{\mathbb{R}^{3(N-1)}} |\Psi(\mathbf{x}, \mathbf{x}_2, \dots, \mathbf{x}_N)|^2 \, d\mathbf{x}_2..d\mathbf{x}_N \,.$$

The art then consists in finding a functional acting on densities such that its infimum of the energy gives a good approximation of the quantum ground state energy. This approach is often used in numerical computations since it reduces considerably the dimension of the problem. It is known under the name *density functional theory*. One of the first models in this class is the well known Thomas-Fermi model. One minimises the functional (called Thomas-Fermi functional)

$$\mathcal{E}_V^{\mathrm{TF}}(\rho) = \tfrac{3}{10}(6\pi^2)^{\frac{2}{3}} \int_{\mathbb{R}^3} \rho(\mathbf{x})^{\frac{5}{3}} d\mathbf{x} - \int_{\mathbb{R}^3} V(\mathbf{x})\rho(\mathbf{x}) d\mathbf{x} + \tfrac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\rho(\mathbf{x})\rho(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{x} d\mathbf{y}\,,$$

over the set $R_N := \{\rho \in L^{5/3}(\mathbb{R}^3) : \rho \geq 0 \text{ and } \int_{\mathbb{R}^3} \rho = N\}$. The Thomas-Fermi energy is then given by

$$E_V^{\mathrm{TF}}(N) := \inf\{\, \mathcal{E}_V^{\mathrm{TF}}(\rho) \mid \rho \in R_N\}\,.$$

This is an approximation for the quantum ground state energy defined in (2.2) when the kinetic energy of the electrons in the Hamiltonian H is given by $T_j = -\frac{1}{2}\Delta_j$. This method was introduced at the same time and separately by Fermi and Thomas in 1927 [24, 73]. The mathematical theory of the model has been developed in 1977 by Lieb and Simon in [52]. In this fundamental work, among other results, it is proven the existence of a minimiser under the relaxed condition $\int_{\mathbb{R}^3} \rho \leq N$ and the assumption that the nuclear potential satisfies $V \in L^{5/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. By this we mean that V may be written as $V = V_1 + V_2$ with $V_1 \in L^{5/2}(\mathbb{R}^3)$ of compact support and $V_2 \in L^\infty(\mathbb{R}^3)$. In the case that the nuclear potential is the standard one given by $V(\mathbf{x}) = Z/|\mathbf{x}|$, they can prove existence and uniqueness of the minimiser under the condition $\int_{\mathbb{R}^3} \rho = N \leq Z$. For $N > Z$ (and $\int_{\mathbb{R}^3} \rho = N$) the minimum is not attained. Although the results are very nice, a limitation of the model is already evident. The Thomas-Fermi theory cannot describe negative ions (atoms negatively charged) that are present in nature. Moreover, it turns out that the model cannot describe molecules. That is, it is energetically more convenient for two atoms to stay at an infinite distance to each other than to link and form a molecule. On the other hand, Lieb and Simon [52] also prove that developing the quantum ground state energy in powers of Z one finds

$$E^{\mathrm{QM}}(Z,Z) = E^{\mathrm{TF}}(Z,Z) + \mathrm{o}(Z^{7/3}) \ \text{ for } Z \to \infty\,,$$

with $E^{\mathrm{TF}}(Z,Z) = E^{\mathrm{TF}}(1,1)Z^{7/3}$ and $E^{\mathrm{TF}}(1,1)$ the energy of a neutral Thomas-Fermi atom of unit nuclear charge. That is, this model gives the leading order term of the real quantum ground state energy. Here, we use the usual convention $E^{\mathrm{TF}}(N,Z) = E_V^{\mathrm{TF}}(N)$ and $\mathcal{E}^{\mathrm{TF}}(\rho) = \mathcal{E}_V^{\mathrm{TF}}(\rho)$ for $V(\mathbf{x}) = Z/|\mathbf{x}|$. For completeness, we recall that so far the known expansion of the energy is

$$E^{\mathrm{QM}}(Z,Z) = E^{\mathrm{TF}}(1,1)Z^{7/3} + \frac{1}{8}Z^2 + c_s Z^{5/3} + \mathrm{o}(Z^{5/3}) \ \text{ for } Z \to \infty\,.$$

The first correction term to the Thomas Fermi energy is known as the Scott correction. In the case of kinetic energy given by $-\frac{1}{2}\Delta$ it was proven by Hughes [36] and Siedentop and Weikard [65, 66] while the last correction is due to Fefferman and Seco (see the announcement [22]). These results are for neutral atoms and have been generalised to ions and molecules as also to other choices of the kinetic energy, see e.g. [25, 70].

In other approximations to (2.2) the minimisation problem is restricted to subsets of the N-particle Hilbert space $\mathcal{H}_F$. One of the most famous and the one we are interested in is the Hartree-Fock approximation. In this approximation, one restricts the minimisation problem given in (2.2) minimising only over the simplest antisymmetric wavefunctions. These are pure wedge products (also called Slater determinants), i.e. wavefunctions Ψ that admit a representation as

$$\Psi(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N) = \frac{1}{\sqrt{N!}}\,\det(u_i(\mathbf{x}_j))_{i,j=1}^N\,, \tag{2.3}$$

with $\{u_i\}_{i=1}^N$ orthonormal in $L^2(\mathbb{R}^3)$. These functions u_i are called *orbitals*. Notice that this way, $\Psi \in \mathcal{H}_F$ and $\|\Psi\|_{L^2(\mathbb{R}^{3N})} = 1$. For Ψ a Slater determinant as in (2.3), $\Psi \in \mathcal{D}(H)$ and H as in (2.1) one finds that

$$\begin{aligned}\langle \Psi, H\Psi\rangle \;=\;& \sum_{i=1}^N \int_{\mathbb{R}^3} \overline{u_i(\mathbf{x})}\big(T - V(\mathbf{x})\big)u_i(\mathbf{x})\,d\mathbf{x} \\ &+ \sum_{i,j=1}^N \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|u_i(\mathbf{x})|^2|u_j(\mathbf{y})|^2 - \overline{u_i(\mathbf{x})u_j(\mathbf{y})}u_i(\mathbf{y})u_j(\mathbf{x})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}d\mathbf{y}\,.\end{aligned}$$

The *Hartree-Fock ground state energy* is defined by

$$E_V^{\mathrm{HF}}(N) := \inf\{\,\langle\Psi, H\Psi\rangle \,|\, \Psi \text{ Slater determinant and } \Psi \in \mathcal{D}(H)\}\,. \tag{2.4}$$

This approximation and its generalisation are frequently used in quantum chemistry. A generalisation of this model is the *multiconfiguration method* of rank K where linear combinations of Slater determinants built with up to K orthonormal orbitals are considered (see e.g. [26, 47]).

Another way of defining the Hartree-Fock approximation is via projections. One makes use of the one-to-one correspondence between Slater determinants and projections onto finite dimensional subspaces of $L^2(\mathbb{R}^3)$. This correspondence is given associating to Ψ given in (2.3), with $\{u_i\}_{i=1}^N$ orthonormal in $L^2(\mathbb{R}^3)$, the projection γ onto the subspace spanned by $u_1,\ldots,u_N$ and vice-versa. Notice that the (integral) kernel of such a projection γ is given by $\gamma(\mathbf{x},\mathbf{y}) = \sum_{j=1}^N u_j(\mathbf{x})\overline{u_j(\mathbf{y})}$. Its one-particle density is given by $\rho_\gamma(\mathbf{x}) = \sum_{j=1}^N |u_j(\mathbf{x})|^2$, $\rho_\gamma \in L^1(\mathbb{R}^3)$. What is crucial is that the energy expectation of a Slater determinant depends only on γ: $\langle\Psi, H\Psi\rangle = \mathcal{E}_V^{\mathrm{HF}}(\gamma)$ where $\mathcal{E}_V^{\mathrm{HF}}$ is the *Hartree-Fock energy functional* defined by

$$\mathcal{E}_V^{\mathrm{HF}}(\gamma) = \mathrm{Tr}[T\gamma] - \mathrm{Tr}[V\gamma] + \mathcal{D}(\gamma) - \mathcal{E}x(\gamma)\,, \tag{2.5}$$

where, with t the quadratic form associated to the kinetic energy,

$$\mathrm{Tr}[T\gamma] := \sum_{i=1}^N\ t(u_i,u_i)\ , \quad \mathrm{Tr}[V\gamma] = \int_{\mathbb{R}^3} \rho_\gamma(\mathbf{x})V(\mathbf{x})\,d\mathbf{x}\,,$$

$\mathcal{D}(\gamma)$ is the *direct* Coulomb energy,

$$\mathcal{D}(\gamma) = \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\rho_\gamma(\mathbf{x})\rho_\gamma(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{x}\, d\mathbf{y}\,, \tag{2.6}$$

and $\mathcal{E}x(\gamma)$ is the *exchange* Coulomb energy,

$$\mathcal{E}x(\gamma) = \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|\gamma(\mathbf{x},\mathbf{y})|^2}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{x}\, d\mathbf{y}\,.$$

This way,

$$E_V^{\mathrm{HF}}(N) = \inf\{\, \mathcal{E}_V^{\mathrm{HF}}(\gamma) \,|\, \gamma : L^2(\mathbb{R}^3;\mathbb{C}) \to L^2(\mathbb{R}^3;\mathbb{C}) \text{ a projection with } \mathrm{Tr}[\gamma] = N \}\,.$$

This reformulation will be useful in the minimisation problem.

In the works [9, 11, 12] we study the Hartree-Fock theory for pseudo-relativistic atoms. The term pseudo-relativistic refers to the fact that we wish to take into account some relativistic effects. The classical choice of the kinetic energy T in (2.1) is $T = -\frac{1}{2}\Delta$ (i.e. the kinetic energy is quadratic in the momentum). In this case, $u_i \in H^1(\mathbb{R}^3)$, for all $i \in \{1,\ldots,N\}$, ensures that $\mathcal{E}^{\mathrm{HF}}(\gamma)$ is bounded from above. Moreover, the inequality $\mathcal{D}(\gamma) \geq \mathcal{E}x(\gamma)$ (see [11, Top of page 5]) and Hardy inequality imply the boundedness from below in the case of a nuclear potential given by $V(\mathbf{x}) = Z/|\mathbf{x}|$. For this model Lieb and Simon in [53] prove the existence of a Hartree-Fock minimiser when $Z < N+1$. Furthermore they prove the regularity of the orbitals away from the origin. The existence of infinitely many other critical points was proven by Lions in [55].

When taking into account some relativistic effects (due to the high speed of the electrons), the kinetic energy should be linear in the momentum, that is a (pseudo-)differential operator of order one. In the literature several choices are made. One, and the one we make, is to consider the kinetic energy given by the operator

$$T = \sqrt{-\alpha^{-2}\Delta + \alpha^{-4}} - \alpha^{-2}\,,$$

with α Sommerfeld's fine structure constant; physically, $\alpha \simeq 1/137.036$. This operator is defined in Fourier spaces as the multiplication operator $\sqrt{2\pi\alpha^{-2}|\mathbf{p}|^2 + \alpha^{-4}} - \alpha^{-2}$, i.e.:

$$(\sqrt{-\alpha^{-2}\Delta + \alpha^{-4}}f)\hat{}\ (\mathbf{p}) := \sqrt{2\pi\alpha^{-2}|\mathbf{p}|^2 + \alpha^{-4}}\,\hat{f}(\mathbf{p})\,,$$

for any $f \in C_0^\infty(\mathbb{R}^3)$ where $\hat{f}$ denotes the Fourier transform of f. The domain of the operator is $H^1(\mathbb{R}^3)$ and its quadratic form domain is $H^{1/2}(\mathbb{R}^3)$. This operator is non-local in the sense that it does not necessarily preserve the support of a function.

Another possible choice is to consider the Dirac operator $D_0 = \boldsymbol{\alpha}\cdot(-i\nabla) + \boldsymbol{\beta}\alpha^{-1}$ with $\boldsymbol{\alpha} = (\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\boldsymbol{\alpha}_3), \boldsymbol{\beta}$ the Dirac matrices and α Sommerfeld's fine structure constant (see [72]). This operator is local but it has a *negative continuous spectrum* which is not bounded from below. The analogue of the Hartree-Fock approximation in this model is called the Dirac-Fock model. Esteban and Séré in [19] proved that the Dirac-Fock functional has infinitely many critical points. In this model the rigorous definition of a ground state is a delicate problem since the energy functional is not bounded from below; see [20, 21]. Nevertheless, there are Hartree-Fock-type models, coming from the Dirac operator, that do have a minimiser. We refer to [2, 31, 32], and the references therein, for the description of these models.

Here we study the Hartree-Fock functional defined in (2.5) with the following choices of kinetic energy T and nuclear potential V

$$T = \sqrt{-\alpha^{-2}\Delta + \alpha^{-4}} - \alpha^{-2} \text{ and } V(\mathbf{x}) = \frac{Z}{|\mathbf{x}|}\,, \tag{2.7}$$

with $Z > 0$. The minimisation problem we study is then

$$E^{\mathrm{HF}}(N, Z, \alpha) = \inf\{\, \mathcal{E}^{\mathrm{HF}}(\gamma) \,|\, \gamma : L^2(\mathbb{R}^3;\mathbb{C}) \to L^2(\mathbb{R}^3;\mathbb{C}) \text{ a projection with } \operatorname{Tr}[\gamma] = N\}\,, \tag{2.8}$$

where $\mathcal{E}^{\mathrm{HF}}(\gamma)$ denotes the Hartree-Fock functional defined in (2.5) with the choice of kinetic energy and nuclear potential given in (2.7). Concerning the one-particle operator $T - Z/|\mathbf{x}|$ Herbst in [34] shows that it is bounded from below *if and only if* $Z\alpha \leq 2/\pi$. This follows from the inequality [39, Formula (5.33) p. 307]

$$\int_{\mathbb{R}^3} \frac{|f(\mathbf{x})|^2}{|\mathbf{x}|}\, d\mathbf{x} \leq \frac{\pi}{2} \int_{\mathbb{R}^3} |\mathbf{p}||\hat{f}(\mathbf{p})|^2\, d\mathbf{p} \quad \text{for} \quad f \in H^{1/2}(\mathbb{R}^3)\,. \tag{2.9}$$

Similarly, the operator H defined in (2.1) is bounded from below if $Z\alpha \leq 2/\pi$ (see [34] for $N = 1$, [13] and [54] for $N \geq 1$), so that there is a bound on the nuclear charges that we can describe. Let us notice here that to define the one-particle operator $T - V$ there is an issue. Indeed while for $Z\alpha < \frac{1}{2}$ the nuclear potential V is a small operator perturbation of the kinetic energy T, for $1/2 \leq Z\alpha < 2/\pi$ the nuclear potential is only a small form perturbation of the kinetic energy and hence one needs to work with forms to define the operator H. For the sake of the presentation we do not give the correct definition of the operators and of their domains here. This has been done in detail in [11].

2.1 Existence of the Hartree-Fock minimiser and regularity of the orbitals

We present here the results in [11]. The aim in this work is to prove the existence of a minimiser for the minimisation problem given in (2.8). Further, regularity is established.

We first extend the definition of the Hartree-Fock energy functional $\mathcal{E}^{\mathrm{HF}}$, in order to turn the minimisation problem (2.8) (that is, (2.4)) into a convex problem. A *density matrix* $\gamma : L^2(\mathbb{R}^3;\mathbb{C}) \to L^2(\mathbb{R}^3;\mathbb{C})$ is a self-adjoint trace class operator that satisfies the operator inequality $0 \leq \gamma \leq \mathrm{Id}$. A density matrix γ has integral kernel

$$\gamma(\mathbf{x}, \mathbf{y}) = \sum_j \lambda_j u_j(\mathbf{x})\overline{u_j(\mathbf{y})}\,, \tag{2.10}$$

where λ_j, u_j are the eigenvalues and corresponding eigenfunctions of γ. We choose the u_j's to be orthonormal in $L^2(\mathbb{R}^3;\mathbb{C})$. As before, $\rho_\gamma \in L^1(\mathbb{R}^3)$ denotes the one-particle density associated to γ given by $\rho_\gamma(\mathbf{x}) = \sum_j \lambda_j\, |u_j(\mathbf{x})|^2$. We consider then the set

$$\mathcal{A} := \big\{\gamma \text{ density matrix : } \operatorname{Tr}\big[T\gamma\big] < +\infty\,\big\}\,, \tag{2.11}$$

where, by definition, for γ written as in (2.10), $\operatorname{Tr}[T\gamma] := \sum_j \lambda_j t(u_j, u_j)$ with t the quadratic form associated to the kinetic energy T. This condition implies that the orbitals u_j are elements of $H^{1/2}(\mathbb{R}^3)$. One may see that all the terms in $\mathcal{E}^{\mathrm{HF}}(\gamma)$ (see (2.5)) are finite if $\gamma \in \mathcal{A}$. For the details we refer to the introduction in [11].

Thanks to this first extension we may consider the study of the minimisation problem for the Hartree-Fock functional over the *convex* set $\{\gamma \in \mathcal{A} :\, \operatorname{Tr}[\gamma] = N\}$. Still, the conservation of the number of particles (i.e. the condition $\operatorname{Tr}[\gamma] = N$) could be violated in the limit procedure due to some possible loss of compactness. It is then convenient to extend further the set over which we minimise considering the set $\{\gamma \in \mathcal{A} :\, \operatorname{Tr}[\gamma] \leq N\}$.

The following theorem states the existence of the Hartree-Fock minimiser.

Theorem 2.1 (Cf. Theorem 1 in [11]). *Let $Z\alpha < 2/\pi$, and let $N \geq 2$ be a positive integer such that $N < Z + 1$.*

Then there exists an N-dimensional projection $\gamma^{\mathrm{HF}} = \gamma^{\mathrm{HF}}(N, Z, \alpha)$ minimising the Hartree-Fock energy functional $\mathcal{E}^{\mathrm{HF}}$ given by (2.5) *with the choice of kinetic energy and nuclear potential given in* (2.7)*. That is, $E^{\mathrm{HF}}(N, Z, \alpha)$ in* (2.8) *(and therefore, in* (2.4)*) is attained. In fact,*

$$\begin{aligned}\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) = E^{\mathrm{HF}}(N, Z, \alpha) &= \inf\left\{\mathcal{E}^{\mathrm{HF}}(\gamma) \,\middle|\, \gamma \in \mathcal{A}, \gamma^2 = \gamma, \mathrm{Tr}[\gamma] = N\right\} \\ &= \inf\left\{\mathcal{E}^{\mathrm{HF}}(\gamma) \,\middle|\, \gamma \in \mathcal{A},\ \ \mathrm{Tr}[\gamma] = N\right\} \\ &= \inf\left\{\mathcal{E}^{\mathrm{HF}}(\gamma) \,\middle|\, \gamma \in \mathcal{A},\ \ \mathrm{Tr}[\gamma] \le N\right\}. \end{aligned} \tag{2.12}$$

The statements of Theorem 2.1 (appropriately modified) also hold for molecules. More explicitely, for a molecule with K nuclei of charges $Z_1, \ldots, Z_K$, fixed at $R_1, \ldots, R_K \in \mathbb{R}^3$, the nuclear potential is given by $V(\mathbf{x}) = \sum_{k=1}^{K} Z_k \alpha / |\mathbf{x} - R_k|$. Then a Hartree-Fock minimiser exists for $N < 1 + \sum_{k=1}^{K} Z_k$ under the condition $Z_k \alpha < 2/\pi$, $k = 1, \ldots, N$.

As discussed above, in the proof of existence it is convenient to start considering the minimisation problem as in the last equation in (2.12). That is, one minimises the Hartree-Fock functional over the class of density matrices with trace satisfying $\mathrm{Tr}[\gamma] \le N$. Given a minimising sequence $\{\gamma_n\}_{n\in\mathbb{N}}$ the idea is to associate to it a (uniformly bounded) sequence of Hilbert-Schmidt operators, in order to use the compactness theorem available for this class of operators. The condition $\mathrm{Tr}[T\gamma_n] \le N$ and moreover the fact that $\mathrm{Tr}[T\gamma_n]$ are uniformly bounded yield naturally candidates for the Hilbert-Schmidt operators to consider. This construction gives a candidate for the minimiser. What is left to prove is the lower semicontinuity of the functional. In the pseudo-relativistic context one faces the problem that the Coulomb potential is not relatively compact with respect to the kinetic energy. This has been already addressed in [2]. A way to overcome the problem is to consider the one-particle operator $h_0 := T - V$ together with the projections onto the pure points spectrum and the absolutely continuous spectrum, respectively. This splitting allows the passage to the limit. The assumption $Z\alpha < 2/\pi$ is needed in the proof when showing that $\mathrm{Tr}[E(\mathbf{p})\gamma_n]$ is uniformly bounded for a minimising sequence $\{\gamma_n\}_{n\in\mathbb{N}}$. The idea of establishing existence of Hartree-Fock minimisers by solving the minimisation problem on the set of density matrices was introduced in [48, 68]. The same method was used in [2] in the Dirac-Fock case.

So far we have proved the existence of a minimiser for the Hartree-Fock functional in the class of density matrices with $\mathrm{Tr}[\gamma] \le N$. To get back to the original problem, we need to show that a minimiser satisfies $\mathrm{Tr}[\gamma] = N$ (possibly under some extra hypothesis) and moreover that a minimiser can be choosen to be a projection (instead of a general density matrix). Let γ^{HF} be a minimiser under the condition $\mathrm{Tr}[\gamma] \le N$. This density matrix may be written as

$$\gamma^{\mathrm{HF}}(\mathbf{x}, \mathbf{y}) = \sum_{k=1}^{K} \lambda_k \varphi_k(\mathbf{x}) \overline{\varphi_k(\mathbf{y})},$$

with $1 \ge \lambda_k > 0$ and φ_k orthonormal in $L^2(\mathbb{R}^3)$. Since γ^{HF} is a minimiser, the orbitals φ_k may be chosen to be eigenfunctions of the *Hartree-Fock operator* $h_{\gamma^{\mathrm{HF}}} \varphi_i = \epsilon_i \varphi_i$ with

$$(h_{\gamma^{\mathrm{HF}}} u)(\mathbf{x}) = (Tu)(\mathbf{x}) - (Vu)(\mathbf{x}) + u(\mathbf{x}) \int_{\mathbb{R}^3} \frac{\gamma^{\mathrm{HF}}(\mathbf{y}, \mathbf{y})}{|\mathbf{x} - \mathbf{y}|}\, d\mathbf{y} - \int_{\mathbb{R}^3} \frac{\gamma^{\mathrm{HF}}(\mathbf{x}, \mathbf{y})}{|\mathbf{x} - \mathbf{y}|} u(\mathbf{y})\, d\mathbf{y}, \tag{2.13}$$

for $u \in C^\infty(\mathbb{R}^3)$ (See the construction in [11, Introduction]. Notice that the definition given here for the operator $h_{\gamma^{\mathrm{HF}}}$ differs by a factor α from the one given in [11].). Here the eigenvalues ϵ_i are ordered in increasing order: $\epsilon_1 \le \epsilon_2 \le \ldots$. A useful observation at this point is that writing

$$\gamma^{\mathrm{HF}}(\mathbf{x}, \mathbf{y}) = \sum_{k=2}^{K} \lambda_k \varphi_k(\mathbf{x}) \overline{\varphi_k(\mathbf{y})} + \lambda_1 \varphi_1(\mathbf{x}) \overline{\varphi_1(\mathbf{y})} = \gamma_{k-1}^{\mathrm{HF}}(\mathbf{x}, \mathbf{y}) + \lambda_1 \varphi_1(\mathbf{x}) \overline{\varphi_1(\mathbf{y})}, \tag{2.14}$$

for the Hartree-Fock energy one finds $\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) = \mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}_{k-1}) + \alpha^{-1}\lambda_1\epsilon_1$. Similar formulas hold isolating the other orbitals. Being γ^{HF} a minimiser this immediately shows that the eigenvalues ϵ_k need to be non-positive and that it is convenient to choose $\lambda_k = 1$. The lower energy values should be filled before going to higher energy values. In order to prove that the minimiser is a projection, it is then important to study how many negative eigenvalues $h_{\gamma^{\mathrm{HF}}}$ has. By [11, Lemma 2] we see that $h_{\gamma^{\mathrm{HF}}}$ has infinitely many negative eigenvalues if $\mathrm{Tr}[\gamma] < Z$. This result together with some more refined reasonings similar to the one in (2.14) yield that if $N < Z+1$ the minimiser γ^{HF} of the problem $\inf\{\mathcal{E}^{\mathrm{HF}}(\gamma) : \gamma \in \mathcal{A},\ \mathrm{Tr}[\gamma] \leq N\}$ satisfies $\mathrm{Tr}[\gamma] = N$ and it can be chosen to be a projection.

The minimisers of the Hartree-Fock functional are in generally not unique. The existence of infinitely many distinct critical points of the functional $\mathcal{E}^{\mathrm{HF}}$ was proved recently (under the same conditions) in [18].

In the next result some regularity properties of the orbitals are given.

Theorem 2.2 (Cf. Theorem 1 in [11])**.** *Let $Z\alpha < 2/\pi$, and let $N \geq 2$ be a positive integer such that $N < Z+1$. Let $\gamma^{\mathrm{HF}} = \gamma^{\mathrm{HF}}(N, Z, \alpha)$ be the projection with $\mathrm{Tr}[\gamma^{\mathrm{HF}}] = N$ minimising the Hartree-Fock energy constructed in Theorem 2.1. One can write*

$$\gamma^{\mathrm{HF}}(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^{N} \varphi_i(\mathbf{x})\overline{\varphi_i(\mathbf{y})}$$

with $\varphi_i \in H^{1/2}(\mathbb{R}^3; \mathbb{C}), i = 1, \ldots, N$, orthonormal in $L^2(\mathbb{R}^3)$, such that the Hartree-Fock orbitals *$\{\varphi_i\}_{i=1}^N$ satisfy:*

(i) With $h_{\gamma^{\mathrm{HF}}}$ as defined in (2.13)*,*

$$h_{\gamma^{\mathrm{HF}}}\varphi_i = \varepsilon_i\varphi_i \ , \ i = 1, \ldots, N \, , \tag{2.15}$$

with $0 > \varepsilon_N \geq \ldots \geq \varepsilon_1 > -\alpha^{-1}$ the N lowest eigenvalues of $h_{\gamma^{\mathrm{HF}}}$.

(ii) For $i = 1, \ldots, N$, $\varphi_i \in C^\infty(\mathbb{R}^3 \setminus \{0\}; \mathbb{C})$.

(iii) For all $R > 0$ and $\beta < \nu_{\varepsilon_N} := \sqrt{-\varepsilon_N(2\alpha^{-1} + \varepsilon_N)}$, there exists a constant $C = C(R, \beta) > 0$ such that for $i = 1, \ldots, N$, $|\varphi_i(\mathbf{x})| \leq C\, e^{-\beta|\mathbf{x}|}$ for $|\mathbf{x}| \geq R$.

Theorem 2.2 can be extended also to molecules. Of course, in this case the orbitals are smooth away from each of the nuclei. The proof of the regularity result (*ii*) works for *any* eigenfunction φ of $h_{\gamma^{\mathrm{HF}}}$. Further, the proof of the exponential decay (*iii*) yields the same claim for those corresponding to *negative* eigenvalues ε. More precisely, if $h_{\gamma^{\mathrm{HF}}}\varphi = \varepsilon\varphi$ for some $\varepsilon \in [\varepsilon_N, 0)$, then $|\varphi(\mathbf{x})| \leq C\, e^{-\beta|\mathbf{x}|}$ for all $\beta < \nu_\varepsilon := \sqrt{-\varepsilon(2\alpha^{-1} + \varepsilon)}$ for some $C = C(R, \beta) > 0$. Note that, in general, eigenfunctions of $h_{\gamma^{\mathrm{HF}}}$ can be unbounded at $\mathbf{x} = 0$ and hence the regularity can only be expected to hold away from the origin. Both the regularity and the exponential decay above are similar to the results in the non-relativistic case (see [53]). However, the proof of Theorem 2.2, part (*ii*) $-$ (*iii*), is considerably more complicated due to the non-locality of the kinetic energy operator, the fact that the kinetic energy is a pseudo-differential operator of order one, and the fact that the Hartree-Fock operator $h_{\gamma^{\mathrm{HF}}}$ is only given as a *form* sum for $Z\alpha \in [1/2, 2/\pi)$.

In the non-relativistic case the regularity of the orbitals follows from the elliptic regularity theory for systems. Indeed the system of equations $h_{\gamma^{\mathrm{HF}}}\varphi_i = \epsilon_i\varphi_i$ may be rewritten as

$$\left\{ \begin{array}{rcl} -\Delta\varphi_i - V\varphi_i + \displaystyle\sum_{j=1}^{N}(\Phi_{j,j}\varphi_i - \Phi_{i,j}\varphi_j) & = & \epsilon_i\varphi_i \, , \text{ for } i \in \{1, \ldots, N\} \, , \\ -\Delta\Phi_{i,j} & = & 4\pi\varphi_i\overline{\varphi_j} \, , \text{ for } i, j \in \{1, \ldots, N\} \, , \end{array} \right. \tag{2.16}$$

introducing new variables $\Phi_{i,j}$ defined by

$$\Phi_{i,j}(\mathbf{x}) := \int_{\mathbb{R}^3} \frac{\varphi_i(\mathbf{y})\overline{\varphi_j(\mathbf{y})}}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y} \text{ for all } \mathbf{x} \in \mathbb{R}^3 \text{ and } i,j \in \{1,\dots,N\}\,.$$

In the case of pseudo-relativistic atoms, this transformation does not yield immediately regularity. In this case the system is a mixed system: some of the equations have leading term $-\Delta$ (a differential operator of order two) while the others have as leading term the kinetic energy and hence a pseudo-differential operator of order one. We prove regularity working directly with the eigenvalue equations and showing that $\varphi_i \in H^k(\Omega)$ for all $k \in \mathbb{N}$ and $\Omega \subset \mathbb{R}^3 \setminus \{0\}$. This we do by induction. The main difficulty is due to the non-locality of the kinetic energy. For this several localisations are needed in order to use the smoothing properties of the pseudo-differential operators of the kind $\chi T \eta$ with χ, η localisation functions with disjoint supports. In [11, Appendix] the needed properties of pseudo-differential operators are presented shortly.

The exponential decay of the orbitals in L^2-sense is proven via perturbation theory (see [11, Proposition 1]). Already at this point the upper bound on the rate of the exponential decay appears. Starting from the eigenvalue equation $h_{\gamma^{\mathrm{HF}}}\varphi_i = \epsilon_i \varphi_i$ we get to a pointwise exponential decay for the φ_i inverting the operator $T - \epsilon_N$. The information on the decay of the kernel of $(T-\epsilon_N)^{-1}$ and the exponential decay in L^2 of the orbitals, yield then the pointwise estimate.

2.2 Real-Analyticity of the orbitals

In [9] we continue the study of the regularity of the Hartree-Fock orbitals (see Theorem 2.2) by showing that all of these orbitals are, in fact, real analytic away from the origin. Apart from inherent mathematical interest, analyticity of solutions has important consequences. For example, in the non-relativistic case, the analyticity of the orbitals and the regularity properties of the true quantum mechanical eigenfunction was used in [27] to prove that the quantum mechanical ground state is never a Hartree-Fock state. We expect the same kind of result in this situation.

The main theorem is the following, which completely settles the question of regularity away from the origin of solutions to the equations (2.15).

Theorem 2.3 (Cf. Theorem 1.1 in [9])**.** *Let $Z\alpha < 2/\pi$, and let $N \geq 2$ be a positive integer such that $N < Z+1$. Let $\varphi_1, \dots, \varphi_N$, $\varphi_i \in H^{1/2}(\mathbb{R}^3)$ for $i = 1, \dots, N$, be solutions to the pseudo-relativistic Hartree-Fock equations in* (2.15) *with γ^{HF} the projection onto span$\{\varphi_1, \dots, \varphi_N\}$, a minimiser for the Hartree-Fock functional. Then, for $i = 1, \dots, N$, $\varphi_i \in C^\omega(\mathbb{R}^3 \setminus \{0\})$, that is, the Hartree-Fock orbitals are real analytic away from the origin in $\mathbb{R}^3$.*

Although in this theorem regularity is only stated for the orbitals giving a Hartree-Fock minimiser, the proof works also for the infinitely many critical points of the Hartree-Fock functional constructed in [18] and for all the eigenfunctions of the corresponding Hartree-Fock operators. Also, the proof yields real-analyticity of any $H^{1/2}(\mathbb{R}^3)$-solution $\varphi : \mathbb{R}^3 \to \mathbb{C}$ to equations of the kind

$$\sqrt{-\Delta+1}\,\varphi - \frac{Z}{|\mathbf{x}|}\varphi \pm |\varphi^2| * |\cdot|^{-1}\varphi = \lambda\varphi\,.$$

(see [9, Remark 1.2] for more general equations.). In Theorem 2.3 the restrictions $Z\alpha < 2/\pi$ and $N \geq 2$ are only made to ensure existence of a Hartree-Fock minimiser and hence of solutions to (2.15). Of course, this does not play a role in the proof of regularity and in fact, our proof proves analyticity away from $\mathbf{x} = 0$ for $H^{1/2}$-solutions to (2.15) for any $Z\alpha$. In particular, in the case $N = 1$, the Hartree-Fock equations reduce to $T\varphi - V\varphi = \epsilon\varphi$ and our result also holds for $H^{1/2}$-solutions to this equation. As for Theorems 2.1 and 2.2, the statement of Theorem 2.3 (appropriately modified) also holds for molecules. In fact, the only assumption needed on the nuclear potential is its analyticity away from finitely many points in $\mathbb{R}^3$, and certain (possibly different) integrability properties in the vicinity of each of these points, and at infinity; for more details, see [9, Remark 4.19]. The results hold also for other choices of the kinetic energy, see [9, Remark 1.2(vi)].

The proof of Theorem 2.3 is inspired by the classical Morrey-Nirenberg proof of analyticity of solutions to elliptic partial differential equations with real analytic coefficients by 'nested balls'. We first present the ideas of Morrey and Nirenberg's proof. We then discuss the difficulties in our situation, and the way we solve those.

The aim is to prove L^2-bounds on derivatives of order k of the solution in a ball of some radius r around a given point. These bounds should behave suitably in k in order to make the Taylor series of the solution converge locally, thereby proving analyticity. The proof of these bounds is inductive. In fact, for some ball B_R with $R > r$, one proves the bounds on all balls B_ρ with $r \leq \rho \leq R$, with the appropriate (with respect to k) behaviour in the distance to the boundary $R - \rho$. The induction basis is provided by standard elliptic estimates. In the induction step, one has to bound $k+1$ derivatives of the solution in the ball B_ρ. To do so, one divides the difference $B_R \setminus B_\rho$ into $k+1$ nested balls using $k+1$ localization functions with successively larger supports. Commuting m of the k derivatives (in the case of an operator of order m) with these localization functions produces (local) differential operators of order $m-1$, with support in a larger ball. These local commutator terms are controlled by the induction hypothesis, since they contain one derivative less. For the last term (the term where no commutators occur) one then uses the equation.

This method of Morrey and Nirenberg poses new technical difficulties in our case, due to the non-locality of the kinetic energy and the presence of the terms

$$(R_{\gamma^{\mathrm{HF}}}\varphi_i)(\mathbf{x}) := \int_{\mathbb{R}^3} \frac{\gamma^{\mathrm{HF}}(\mathbf{y},\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y}\varphi_i(x) \ \text{ and } \ (K_{\gamma^{\mathrm{HF}}}\varphi_i)(\mathbf{x}) := \int_{\mathbb{R}^3} \frac{\gamma^{\mathrm{HF}}(\mathbf{x},\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\varphi_i(\mathbf{y})\, d\mathbf{y}\,.$$

The non-locality of the operator $\sqrt{-\Delta+\alpha^{-2}}$ implies that, as opposed to the case of a differential operator, the commutator of the kinetic energy with a localization function is not localized in the support of the localization function. That is, when resorting to prove analyticity by differentiating the equation, the localization argument described above introduces commutators which are (non-local) pseudo-differential operators. Now the induction hypothesis does not provide control of these terms. Furthermore, it is far from obvious that the singularity of the potential V outside B_R does not influence the regularity in B_R of the solution through these operators. Loosely speaking, the singularity of the nuclear potential can be felt everywhere. We overcome this problem by a new localization argument which enables us to capture in more detail the action of high order derivatives on nested balls, [9, Lemma B.1]. We present the ideas considering, for the sake of presentation, the equation $E(\mathbf{p})\varphi - V\varphi = 0$ with $E(\mathbf{p}) = \sqrt{-\Delta+\alpha^{-2}}$ and V a potential that is real-analytic in $\overline{B_R}$. Notice that $T = \alpha^{-1}(E(\mathbf{p}) - \alpha^{-1})$ ((2.7)). We choose to invert $E(\mathbf{p})$ (turning the equation into an integral operator equation). One starts from the equation $\varphi = E(\mathbf{p})^{-1}V\varphi$ and in order to get, in the induction step, estimates for the $(k+1)$-derivative of φ in B_r we differentiate the equation and localise it. The term on the right hand side of the equation is then given by $\Phi E(\mathbf{p})^{-1}D^\beta V\varphi_i$ with $|\beta| = k+1$ and Φ a smooth function with support in B_R and satisfying $\Phi \equiv 1$ in B_r. Due to the non-locality of $E(\mathbf{p})^{-1}$, the behavior of $D^\beta Vu$ over all of $\mathbb{R}^3$ influences this term. We can control the derivatives of φ_i only where we have the induction hypothesis (i.e. inside B_R) and the estimate becomes singular when approaching ∂B_R. Let ρ be such that Φ has support on B_ρ, $r < \rho < R$. We divide B_R in $k+1$ nested balls

$$B_R = \bigcup_{j=0}^{k} B_{R-j\epsilon} \quad \text{with } \ \epsilon \ \text{ such that } \ \rho < R - k\epsilon\,.$$

To this covering of B_R we associate a partition of unity with $k+1$-localisation functions χ_j, $j \in \{0, \ldots, k\}$. The function χ_{k-j} has support on $B_{R-j\epsilon}$ (see [9, Figure 1 and 2]) and, by the induction hypothesis, in this ball we can control up to i-derivatives of the solution, with the right order in ϵ and i. Lemma B.1 in [9] gives that $\Phi E(\mathbf{p})^{-1} D^\beta V \varphi_i$ can be written as a sum of terms (also) of the following kind

$$\sum_{j=0}^{k} \Phi E(\mathbf{p})^{-1} D^{j+1} \chi_j D^{\beta-j-1} V \varphi_i \,.$$

By this special localisation, on the j-th term of the sum we take only as many derivatives on φ_i as we can bound on the support of χ_j. When j is big we are (relatively) far away from the boundary and we can control more derivatives. Then, the terms $\chi_j D^{\beta-j-1} V \varphi_i$ can be estimated directly via the induction hypothesis. Here one uses that the potential V is real-analytic in B_R. The term $\Phi E(\mathbf{p})^{-1} D^{j+1} \chi_j$ is taken care of with very explicit bounds (see [9, Lemma C.2]). Indeed, by construction Φ and χ_j have disjoint supports for $j \in \{1, \ldots, k\}$ and hence the operator $\Phi E(\mathbf{p})^{-1} D^{j+1} \chi_j$ can be bounded by a constant depending on j (the number of derivatives) and the distance between the supports of the localisation functions to the power j. Notice that, for proving analyticity it is not sufficient to know that the operator $\Phi E(\mathbf{p})^{-1} D^{j+1} \chi_j$ is smoothing, but one needs a quantified estimate on the smoothing effect.

The second major obstacle is due to the presence of the terms $R_{\gamma^{\mathrm{HF}}} \varphi_i$ and $K_{\gamma^{\mathrm{HF}}} \varphi_i$ that are morally cubic in the φ_i's. To illustrate the problem, we discuss proving analyticity by the above method (local L^2-estimates) for solutions u to the equation $-\Delta u = u^3$. When differentiating this equation, the application of Leibniz rule introduces a sum of terms on the right hand side. After using Hölders inequality on each term (the product of three factors, each a number of derivatives on u), one needs to use a Sobolev inequality to 'get back to L^2' in order to use the induction hypothesis. Summing the many terms, the needed estimate does not come out. For the equation $-\Delta u = u^2$ this problem does not occur, but in the cubic case, one looses too many derivatives when using Sobolev inequality. This problem of loss of derivatives may be overcome by characterizing analyticity by growth of derivatives in some L^p with $p > 2$. By choosing p sufficiently large the loss of derivatives in the Sobolev inequality mentioned above is less and allows us to prove the needed estimate. Additional technical difficulties occur due to the fact that the cubic terms, $R_{\gamma^{\mathrm{HF}}} \varphi_i$ and $K_{\gamma^{\mathrm{HF}}} \varphi_i$ are actually non-local. Note that in the proof that non-relativistic Hartree-Fock orbitals are analytic away from the positions of the nuclei (see [26, 47]), these terms are dealt with by cleverly re-writing the Hartree-Fock equations as a system as done in (2.16). This eliminates the terms $R_{\gamma^{\mathrm{HF}}} \varphi_i$ and $K_{\gamma^{\mathrm{HF}}} \varphi_i$ turning these into quadratic products in the functions φ_i, $\Phi_{i,j}$. One then obtains a non-linear system of elliptic second order equations with coefficients analytic away from the positions of the nuclei. This idea cannot readily be extended to our case as already observed at the end of the previous section.

2.3 The ionization conjecture

In Theorem 2.1 the existence of a pseudo-relativistic Hartree-Fock minimiser under the condition $N < Z + 1$ is proved. The same condition is needed in the case of non-relativistic atoms. In the Hartree-Fock theory one can then describe atoms with total charge almost equal to minus one. These are negatively charged ions. As we have already observed, the Thomas-Fermi theory (see page 18) does not describe negatively charged atoms. A long standing open problem in the mathematical physics literature is the characterisation of the *maximal* number of electrons N that a nucleus of charge Z can bind. This is known as the *Ionization conjecture* and the number $N - Z$ is called the *maximal negative ionization*. The conjecture can be formulated as follows. Consider atoms with arbitrarily large nuclear charge Z, is it true that the maximal negative ionization remain bounded? That is, is it true that there exists a universal constant Q such that the number N of electrons that a nucleus of charge Z can bind is bounded by $Z+Q$? In nature negative ions with charge minus one are present. In the theory of atomic structures, the answer to the question depends of course on the model one considers. For the Thomas-Fermi model, the answer is trivially yes. For the full Schrödinger model the answer is still open. Lieb in [49] with a very elegant and short proof shows that $N \leq 2Z+1$ is necessary for the existence of a ground state both for the problem (2.2) as for the Hartree-Fock approximation. In [51] the authors prove that, denoting by $N(Z)$ the number of electrons that a nucleus of charge Z binds in non-relativistic quantum theory, the quotient $N(Z)/Z$ approaches one at the limit Z to infinity. This result was then improved in [23, 64], where it is shown that $N(Z) \leq Z + CZ^{1-a}$ with $a = 9/56$.

Finally in 2003 Jan Philip Solovej [69] proved the ionization conjecture in the non-relativistic Hartree-Fock model. In [12] the result is extended to the pseudo-relativistic Hartree-Fock theory. One of the main results is the following.

Theorem 2.4 (Cf. Theorem 1.1 in [12]). *Let $Z \geq 1$ and $\alpha > 0$. Let $Z\alpha = \kappa$ and assume that $0 \leq \kappa < 2/\pi$. There is a constant $Q > 0$ depending only on κ such that if N, the number of electrons, is such that a Hartree-Fock minimiser for* (2.8) *exists, then $N \leq Z + Q$.*

As in Theorem 2.1, the condition $\kappa = Z\alpha < 2/\pi$ is needed to control with the kinetic energy the nucleus potential and to have still a bit of the kinetic energy left (see (2.9)). The case $\kappa = 0$ corresponds to the non-relativistic limit.

We present the basic idea for the proof of Theorem 2.4. Let N, the numbers of electrons, satisfy $N \geq Z$ and be such that a Hartree-Fock minimiser exists. That is, there exists a density matrix $\gamma^{\mathrm{HF}} \in \mathcal{A}$ (defined in (2.11)) such that $\mathrm{Tr}[\gamma^{\mathrm{HF}}] = N$ and

$$\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) = \inf\left\{\mathcal{E}^{\mathrm{HF}}(\gamma) : \gamma \in \mathcal{A} \text{ and } \mathrm{Tr}[\gamma] = N\right\}.$$

At this point, we consider ρ^{TF} the Thomas-Fermi minimiser with potential $V(\mathbf{x}) = Z/|\mathbf{x}|$ and under the condition $\int \rho^{\mathrm{TF}} = Z$. (See the description of the Thomas-Fermi model at page 18.) Existence and uniqueness of the minimiser are proved in [52]. Denoting by ρ^{HF} the density of the minimiser γ^{HF}, we find for all $r > 0$

$$\begin{aligned} N &= \int_{\mathbb{R}^3} \rho^{\mathrm{HF}}(\mathbf{x})\, d\mathbf{x} \\ &= \int_{|\mathbf{x}|<r} \left[\rho^{\mathrm{HF}}(\mathbf{x}) - \rho^{\mathrm{TF}}(\mathbf{x})\right] d\mathbf{x} + \int_{|\mathbf{x}|<r} \rho^{\mathrm{TF}}(\mathbf{x})\, d\mathbf{x} + \int_{|\mathbf{x}|>r} \rho^{\mathrm{HF}}(\mathbf{x})\, d\mathbf{x}. \end{aligned} \tag{2.17}$$

By the equalities above and since $\int_{|\mathbf{x}|<r} \rho^{\mathrm{TF}}(\mathbf{x}) d\mathbf{x} \leq Z$, Theorem 2.4 follows from the following result.

Theorem 2.5 (Cf. Theorem 1.16 in [12]). *There exist $r > 0$ and positive constants c_1 and c_2 independent of N and Z but possibly depending on κ such that*

$$\int_{|\mathbf{x}|<r} \left[\rho^{\mathrm{HF}}(\mathbf{x}) - \rho^{\mathrm{TF}}(\mathbf{x})\right]\, d\mathbf{x} \leq c_1 \ \textit{and} \ \int_{|\mathbf{x}|>r} \rho^{\mathrm{HF}}(\mathbf{x})\, d\mathbf{x} \leq c_2.$$

As can be seen from the statement of Theorem 2.5 and the formula in (2.17), the main idea is to compare the Hartree-Fock minimiser to the Thomas-Fermi minimiser for the neutral atom. It turns out that for this comparison the following functions are important. For γ^{HF} a Hartree-Fock minimiser, the function

$$\varphi^{\mathrm{HF}}(\mathbf{x}) := \frac{Z}{|\mathbf{x}|} - \int_{\mathbb{R}^3} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y} \ \text{ for } \ \mathbf{x} \in \mathbb{R}^3,$$

is called the *Hartree-Fock-mean field potential* and

$$\Phi_R^{\mathrm{HF}}(\mathbf{x}) := \frac{Z}{|\mathbf{x}|} - \int_{|\mathbf{y}|<R} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y} \quad \text{for} \quad \mathbf{x} \in \mathbb{R}^3,$$

is the *Hartree-Fock-screened nuclear potential*. Similarly, one defines the Thomas-Fermi mean field potential φ^{TF} and the Thomas-Fermi-screened nuclear potential Φ_R^{TF}. Notice that the screened nuclear potential describes the charge that an electron feels at a distance larger than R from the nucleus. The following theorem is the principal ingredient in the proof of Theorem 2.5 and is the main technical estimate in [12].

Theorem 2.6 (Cf. Theorem 1.17 in [12])**.** *Let $Z\alpha = \kappa$, $0 \le \kappa < 2/\pi$. Assume $N \ge Z \ge 1$.*

Then there exist universal constants $\alpha_0 > 0$, $0 < \varepsilon < 4$ and C_M and C_Φ depending on κ such that for all $\alpha \le \alpha_0$

$$\left| \Phi_{|\mathbf{x}|}^{\mathrm{HF}}(\mathbf{x}) - \Phi_{|\mathbf{x}|}^{\mathrm{TF}}(\mathbf{x}) \right| \le C_\Phi |\mathbf{x}|^{-4+\varepsilon} + C_M \textit{ for all } \mathbf{x} \in \mathbb{R}^3.$$

The meaning of the estimate above can be understoood when comparing it to the Sommerfeld's estimate for the Thomas-Fermi screened nuclear potential

$$\Phi_{|\mathbf{x}|}^{\mathrm{TF}}(\mathbf{x}) \le 3^4 2\pi^2 |\mathbf{x}|^{-4} \quad \text{for all } \mathbf{x} \in \mathbb{R}^3$$

(see [12, Corollary 1.14]). Theorem 2.6 gives that the Thomas-Fermi screened nuclear potential is a good approximation to the Hartree-Fock screened nuclear potential near to the nucleus.

The main estimate in Theorem 2.6 is proven by an iterative procedure. Near the nucleus we expect the Thomas-Fermi minimiser to be a good approximation to the Hartree-Fock minimiser. By a direct comparison and via some semiclassical estimates, the claim of Theorem 2.6 follows for small $\mathbf{x}$, or, more precisely, up to a distance of order $Z^{-1/3}$. At a bigger distance, a direct comparison between the two minimisers does not give the needed behavior. Then for bigger distances, but still not too far away, one compares the Hartree-Fock minimiser with the minimiser of an 'ad hoc' chosen Thomas-Fermi model. This model differs from the previous one on the choice of the nuclear potential. It takes into account that, being at a certain distance from the nucleus, the nuclear charge is screened by the electrons nearer to the nucleus. This construction yields the estimate in an intermediate zone (i.e. up to a fixed distance independent of Z). At a unitary distance estimates of the exterior integral of the density yield that the number of electrons can be bounded independently of Z. In all the steps, the estimates are proved by semiclassical methods.

The main steps of the proof of the results above are as in [69]. What is interesting here is the proof that, up to a unitary distance (in Z) to the nucleus, the Thomas-Fermi model is a good approximation of the Hartree-Fock model also in the case of pseudo-relativistic atoms. This was known for the leading order (in Z) of the energy but not for the mean field and screened nuclear potential. In this case the proof is technically considerably more complicated due to the non-locality of the kinetic energy. Several difficulties poses the fact that, while in the non-relativistic case the density ρ^{HF} is in $L^{5/3}(\mathbb{R}^3)$, in our case $\rho^{\mathrm{HF}} \in L^{4/3}(\mathbb{R}^3) + L^{5/3}(\mathbb{R}^3)$. This is in fact the point where some relativistic effects appear. This is taken care of with Theorem 2.10 in [12]. This result is an improved Daubechies-Lieb-Yau inequality which allows us to bound the term

$$\int_{|\mathbf{x}-\mathbf{y}|<R} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y}$$

via the kinetic energy and a sum of terms depending on κ, Z and R. Choosing, at each step, R appropriately the right order is obtained.

By proving Theorem 2.6 we also get the following interesting results.

Theorem 2.7 (Cf. Theorem 1.19 in [12]). *Let $Z\alpha = \kappa$, $0 \le \kappa < 2/\pi$ and $Z \ge 1$. The ionization energy of a neutral atom $E^{\mathrm{HF}}(Z-1, Z, \alpha) - E^{\mathrm{HF}}(Z, Z, \alpha)$ is bounded by a universal constant.*

Here as in (2.8) $E^{\mathrm{HF}}(N, Z, \alpha)$ denotes the Hartree-Fock energy for a system of N electrons and a nucleus of charge Z.

Theorem 2.8 (Cf. Theorem 1.20 in [12]). *Let $Z\alpha = \kappa$, $0 \le \kappa < 2/\pi$. For all $Z \ge 1$ and N with $N \ge Z$ for which a HF minimiser exists with $\int \rho^{\mathrm{HF}} = N$, we have*

$$|\varphi^{\mathrm{TF}}(\mathbf{x}) - \varphi^{\mathrm{HF}}(\mathbf{x})| \le A_\varphi |\mathbf{x}|^{-4+\varepsilon_0} + A_1,$$

with A_0, A_1 and ε_0 universal constants.

The method of proof gives also an asymptotic formula for the atomic radius. The Hartree-Fock-radius $R^{\mathrm{HF}}_{Z,N}(\nu)$ to the ν last electrons is defined by

$$\int_{|\mathbf{x}| \ge R^{\mathrm{HF}}_{Z,N}(\nu)} \rho^{\mathrm{HF}}(\mathbf{x})\, d\mathbf{x} = \nu.$$

It describes the radius of the ball in $\mathbb{R}^3$ outside of which ν electrons are present.

Theorem 2.9 (Cf. Theorem 1.18 in [12]). *Let $Z\alpha = \kappa$, $0 \le \kappa < 2/\pi$. Both $\liminf_{Z\to\infty} R^{\mathrm{HF}}_{Z,Z}(\nu)$ and $\limsup_{Z\to\infty} R^{\mathrm{HF}}_{Z,Z}(\nu)$ are bounded and behave asymptotically as*

$$3^{\frac{4}{3}} 2^{\frac{1}{2}} \pi^{\frac{2}{3}} \nu^{-\frac{1}{3}} + o(\nu^{-\frac{1}{3}}) \text{ as } \nu \to \infty.$$

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Part 1

Boundary value problems for Willmore surfaces

This part consists of the following five papers.

- A. Dall'Acqua, K. Deckelnick, H.-Ch. Grunau, Classical solutions to the Dirichlet problem for Willmore surfaces of revolution, *Adv. Calc. Var.* **1** (2008) 379–397.
- A. Dall'Acqua, S. Fröhlich, H.-Ch. Grunau, F. Schieweck, Symmetric Willmore surfaces of revolution satisfying arbitrary Dirichlet boundary data, *Adv. Calc. Var.* **4** (2011) 1–81.
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Classical solutions to the Dirichlet problem for Willmore surfaces of revolution[1]

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Abstract

We consider the Willmore equation with Dirichlet boundary conditions for a surface of revolution obtained by rotating the graph of a positive smooth even function. We show existence of a regular solution by minimisation. Instead of minimising the Willmore functional we reformulate the problem in the hyperbolic half plane and we minimise the corresponding "hyperbolic Willmore functional".

Keywords. Dirichlet boundary conditions, Willmore surfaces of revolution.
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1 Introduction

Recently, the Willmore functional and the associate L^2–gradient flow, the so–called Willmore flow, have attracted a lot of attention. Given a smooth immersed surface $f : M \to \mathbb{R}^3$, the Willmore functional is defined by

$$\mathcal{W}(f) := \int_{f(M)} H^2 dA,$$

where $H = (\kappa_1 + \kappa_2)/2$ denotes the mean curvature of $f(M)$. Apart from being of geometric interest, the functional $\mathcal{W}$ is a model for the elastic energy of thin shells or biological membranes. Furthermore, it is used in image processing for problems of surface restoration and image inpainting. In these applications one is usually concerned with minima, or more generally with critical points of the Willmore functional. It is well–known that the corresponding surface Γ has to satisfy the Willmore equation

$$\Delta_g H + 2H(H^2 - K) = 0 \qquad \text{on } \Gamma, \tag{1}$$

where Δ_g denotes the Laplace–Beltrami operator on Γ and K its Gauss curvature with respect to the induced metric g. A particular difficulty arises from the fact that Δ_g depends on the unknown surface so that the equation is highly nonlinear. Moreover, it is of fourth order where many of the established techniques do not apply. A solution of (1) is called a Willmore surface. Existence of closed Willmore surfaces of prescribed genus has been proved by Simon [19] and Bauer-Kuwert [1]. Recently, Rivière [17] proved a far reaching regularity result. Also, local and global existence results for the Willmore flow of closed surfaces are available, see e.g. [9, 10, 11, 20]. On the other hand, Mayer and Simonett [15] gave a numerical example providing evidence that the Willmore

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flow may develop singularities in finite time. An analytic proof for occurence of a singularity in finite or infinite time for particular initial data was given by Blatt [3]. The Willmore flow for one dimensional closed curves was studied by [7, 16].

If one is interested in surfaces with boundaries, then appropriate boundary conditions have to be added to (1). Since this equation is of fourth order one requires two sets of conditions and a discussion of possible choices can be found in [14] along with corresponding existence results. These results, however, are based on perturbation arguments and hence require severe smallness conditions on the data, which are by no means explicit. Thus the question arises whether it is possible to specify more general conditions on the boundary data that will guarantee the existence of a solution to (1). Such a task seems to be quite difficult since the problem is highly nonlinear and in addition lacks a maximum principle. Quite recently, Schätzle [18] proved an important general result concerning existence of branched Willmore immersions in $\mathbb{S}^n$ with boundary which satisfy Dirichlet boundary conditions. Assuming the boundary data to obey some explicit geometrically motivated smallness condition these immersions can even be shown to be embedded. By working in $\mathbb{S}^n$, some compactness problems could be overcome; on the other hand, when pulling pack these immersions to $\mathbb{R}^n$ it cannot be excluded that they contain the point ∞. Moreover, in general, the existence of branch points cannot be ruled out, and due to the generality of the approach, it seems to us that no topological information about the solutions can be extracted from the existence proof. We think that it is quite interesting to identify situations where it is possible to work with a-priori-bounded minimising sequences or where solutions with additional properties like e.g. being a graph or enjoying certain symmetry properties can be found. In order to outline possible directions of further research and to see, which kind of phenomena and results concerning compact embedded solutions in $\mathbb{R}^3$ of boundary value problems for the Willmore equation might be expected, we investigate boundary value problems for (1) in a specific symmetric situation. More precisely, we look at surfaces of revolution, which are obtained by rotating a graph over the $x = x_1$-axis in $\mathbb{R}^3$ around the x_1-axis. These are described by a sufficiently smooth function

$$u : [-1, 1] \to (0, \infty)$$

and are parametrised as follows:

$$(x, \varphi) \mapsto f(x, \varphi) = (x, u(x) \cos \varphi, u(x) \sin \varphi), \quad x \in [-1, 1], \quad \varphi \in [0, 2\pi].$$

Numerical experiments concerning such kind of Willmore surfaces were performed by Fröhlich [8]. In the present article we consider the Willmore problem under Dirichlet boundary conditions, where the height $u(\pm 1) = \alpha > 0$ and a horizontal angle $u'(\pm 1) = 0$ are prescribed at the boundary:

Theorem 1. *For every $\alpha > 0$, there exists a smooth function $u \in C^\infty([-1, 1], (0, \infty))$ such that the corresponding surface of revolution solves the Dirichlet problem for the Willmore equation*

$$\begin{cases} \Delta_g H + 2H(H^2 - K) = 0 & \text{in } (-1, 1), \\ u(\pm 1) = \alpha, \qquad u'(\pm 1) = 0. \end{cases} \tag{2}$$

This solution u is even and has the following additional properties:

$$\forall x \in [0, 1]: \quad 0 \le x + u(x)u'(x), \qquad u'(x) \le 0.$$

$$\forall x \in [-1, 1]: \qquad \alpha \le u(x) \le \alpha + 1, \qquad |u'(x)| \le \frac{1}{\alpha}.$$

When comparing this result with the situation for minimal surfaces of revolution one may be surprised that existence holds true even for $\alpha \searrow 0$.

We solve (2) by minimising the Willmore functional in the class of surfaces of revolution, which are given by even functions $u : [-1,1] \to (0,\infty)$. In the following section we reformulate this problem in the hyperbolic half plane. In Section 3, taking advantage of using geodesic arcs in the hyperbolic half plane and refined energy reducing constructions, we show that one may pass to suitable minimising sequences satisfying quite strong a-priori-estimates. The latter ensure the required compactness. Further interesting properties of minimising sequences and the minimal Willmore energy as e.g. monotonicity in α are also proved in Section 3. In developing these techniques we benefit from previous works on related one-dimensional problems [5], [6].

Langer and Singer [12] gave explicit expressions for the curvature of elastic curves in the hyperbolic half plane in terms of the arclength of the unknown curve. However, there does not seem to be a direct way to use these results for the question being studied in the present article. Moreover, we think that the constructions made below in order to improve the properties of minimising sequences are of independent interest and *explain* to a good extent the shape of solutions.

2 Geometric background

2.1 Geometric quantities for surfaces of revolution

The calculations below are based on the formulas given in [2]. Let

$$u : [-1,1] \to (0,\infty)$$

be a sufficiently smooth function. We consider the surface generated by the graph of u, the parametrisation of which is given by

$$(x,\varphi) \mapsto f(x,\varphi) = (x, u(x)\cos\varphi, u(x)\sin\varphi).$$

Here, we consider $x = x_1$ as first and $\varphi = x_2$ as second parameter. First and second fundamental form and the interior normal on the surface of revolution are given as follows:

$$\begin{aligned}
(g_{ij}) &= \begin{pmatrix} 1+u'(x)^2 & 0 \\ 0 & u(x)^2 \end{pmatrix}, \qquad g = u(x)^2\left(1+u'(x)^2\right) \\
(L_{ij}) &= \frac{1}{\sqrt{1+u'(x)^2}} \begin{pmatrix} -u''(x) & 0 \\ 0 & u(x) \end{pmatrix} \\
\nu(x,\varphi) &= \frac{1}{\sqrt{1+u'(x)^2}} \left(u'(x), -\cos\varphi, -\sin\varphi\right).
\end{aligned}$$

We use the sign convention that the mean curvature H is positive if the surface is mean convex and negative if it is mean concave with respect to the interior normal ν. The mean curvature and Gauss curvature are then given respectively by

$$\begin{aligned}
H &= -\frac{u''(x)}{2\left(1+u'(x)^2\right)^{3/2}} + \frac{1}{2u(x)\sqrt{1+u'(x)^2}} = \frac{1}{2u(x)u'(x)}\left(\frac{u(x)}{\sqrt{1+u'(x)^2}}\right)', \\
K &= -\frac{u''(x)}{u(x)\left(1+u'(x)^2\right)^2}.
\end{aligned} \tag{3}$$

The Laplace-Beltrami operator on the surface of revolution acts on smooth functions h as follows

$$\begin{aligned}
\Delta_g h &= \frac{1}{\sqrt{g}} \sum_{i,j=1}^{2} \partial_i\left(\sqrt{g}\, g^{ij}\partial_j h\right) \\
&= \frac{1}{u(x)\sqrt{1+u'(x)^2}}\left(\partial_x\left(\frac{u(x)}{\sqrt{1+u'(x)^2}}\,\partial_x h\right) + \partial_\varphi\left(\frac{\sqrt{1+u'(x)^2}}{u(x)}\,\partial_\varphi h\right)\right),
\end{aligned}$$

where g^{ij} are the entries of the inverse of $(g_{ij})_{i,j}$. The terms in the Willmore equation (1) for a surface of revolution are then

$$\begin{aligned}\Delta_g H &= \frac{1}{u(x)\sqrt{1+u'(x)^2}}\\ &\quad \partial_x\left(\frac{u(x)}{\sqrt{1+u'(x)^2}}\,\partial_x\left(\frac{1}{2u(x)\sqrt{1+u'(x)^2}}-\frac{u''(x)}{2\,(1+u'(x)^2)^{3/2}}\right)\right),\\ 2H(H^2-K) &= \frac{1}{4\,(1+u'(x)^2)^{3/2}}\left(\frac{1}{u(x)}-\frac{u''(x)}{1+u'(x)^2}\right)\left(\frac{1}{u(x)}+\frac{u''(x)}{1+u'(x)^2}\right)^2.\end{aligned}$$

So, for surfaces Γ of revolution as described above, the Willmore functional reads as follows

$$\mathcal{W}(\Gamma)=\int_\Gamma H^2\,dS=\frac{\pi}{2}\int_{-1}^{1}\left(\frac{1}{u(x)\sqrt{1+u'(x)^2}}-\frac{u''(x)}{(1+u'(x)^2)^{3/2}}\right)^2 u(x)\sqrt{1+u'(x)^2}\,dx. \tag{4}$$

2.2 Surfaces of revolution as elastic curves in the hyperbolic half plane

The following formulae and calculations are mainly based on [13]. We will recall a different and for our purposes more suitable interpretation and reformulation of the Willmore functional.

The hyperbolic half plane $\mathbb{R}^2_+ := \{(x,y) : y>0\}$ is equipped with the metric

$$ds_h^2=\frac{1}{y^2}(dx^2+dy^2).$$

Geodesics are circular arcs centered on the x-axis and lines parallel to the y-axis; the first will play a crucial role in choosing suitable minimising sequences for the modified Willmore functional.

Let $s\mapsto\gamma(s)=(\gamma_1(s),\gamma_2(s))$, where we do not raise the indices, be a curve in $\mathbb{R}^2_+$ parametrised with respect to its arclength, i.e.

$$1\equiv\frac{\gamma_1'(s)^2+\gamma_2'(s)^2}{\gamma_2(s)^2}.$$

Then, its curvature is given by

$$\kappa_h(s)=-\frac{\gamma_2(s)^2}{\gamma_2'(s)}\frac{d}{ds}\left(\frac{\gamma_1'(s)}{\gamma_2(s)^2}\right)=\frac{\gamma_2(s)^2}{\gamma_1'(s)}\left(\frac{1}{\gamma_2(s)}+\frac{d}{ds}\left(\frac{\gamma_2'(s)}{\gamma_2(s)^2}\right)\right). \tag{5}$$

We think that this is the most frequently used sign convention. However, our arguments would not be affected by choosing the opposite sign. For graphs $[-1,1]\ni x\mapsto(x,u(x))\in\mathbb{R}^2_+$, formula (5) yields

$$\kappa_h(x)=-\frac{u(x)^2}{u'(x)}\frac{d}{dx}\left(\frac{1}{u(x)\sqrt{1+u'(x)^2}}\right)=\frac{u(x)u''(x)}{(1+u'(x)^2)^{3/2}}+\frac{1}{\sqrt{1+u'(x)^2}}. \tag{6}$$

Concerning the Willmore energy (in this metric) we find:

$$\begin{aligned}\mathcal{W}_h(u) &:= \int_{-1}^{1}\kappa_h(x)^2\,ds_h(x)=\int_{-1}^{1}\kappa_h(x)^2\frac{\sqrt{1+u'(x)^2}}{u(x)}\,dx\\ &= \int_{-1}^{1}\left(\frac{u''(x)}{(1+u'(x)^2)^{3/2}}-\frac{1}{u(x)\sqrt{1+u'(x)^2}}\right)^2 u(x)\sqrt{1+u'(x)^2}\,dx\\ &\quad +4\int_{-1}^{1}\frac{u''(x)}{(1+u'(x)^2)^{3/2}}\,dx\\ &= \frac{2}{\pi}\int_\Gamma H^2\,dS-\frac{2}{\pi}\int_\Gamma K\,dS=\frac{2}{\pi}\int_\Gamma H^2\,dS+4\left[\frac{u'(x)}{\sqrt{1+u'(x)^2}}\right]_{-1}^{1},\end{aligned}$$

with H and K as given in (3). This means that

$$\mathcal{W}(\Gamma) = \frac{\pi}{2}\mathcal{W}_h(u) - 2\pi \left[\frac{u'(x)}{\sqrt{1+u'(x)^2}} \right]_{-1}^{1},$$

where $\mathcal{W}(\Gamma)$ is defined in (4) and Γ is the surface of revolution generated by u. In our situation where we assume Dirichlet data

$$u(\pm 1) = \alpha, \qquad u'(\pm 1) = 0,$$

we even have

$$\mathcal{W}(\Gamma) = \frac{\pi}{2}\mathcal{W}_h(u). \tag{7}$$

In proving Theorem 1, we benefit a lot from considering $\mathcal{W}_h$ instead of $\mathcal{W}$. We do not only take technical advantage from this point of view, but we think that it is geometrically more suitable as the constructions in Section 3 will make clear.

Concerning the Euler-Lagrange equation for critical points of the "hyperbolic Willmore functional" $\mathcal{W}_h$ one has:

Lemma 1. *Assume that $u \in C^4([-1,1])$ is such that that $\frac{d}{dt}\mathcal{W}_h(u+t\varphi)|_{t=0} = 0$ for all $\varphi \in C_0^\infty(-1,1)$. Then u satisfies the following Euler-Lagrange equation:*

$$\frac{u(x)}{\sqrt{1+u'(x)^2}}\frac{d}{dx}\left(\frac{u(x)}{\sqrt{1+u'(x)^2}}\kappa_h'(x)\right) - \kappa_h(x) + \frac{1}{2}\kappa_h(x)^3 = 0, \qquad x \in (-1,1), \tag{8}$$

with κ_h as defined in (6).

This observation was formulated in [12, 13] and goes back to U. Pinkall and R. Bryant, P. Griffiths [4]. For the reader's convenience and because it will be used in the proof of regularity, we present the proof of Lemma 1 in Appendix A.

3 Minimisation of the Willmore functional

For $\alpha \in (0,\infty)$ we denote

$$N_\alpha = \{u \in C^{1,1}([-1,1]), u \text{ is even and positive}, u(1) = \alpha, u'(1) = 0\}, \tag{9}$$

and

$$M_\alpha := \inf\{\mathcal{W}_h(u) : u \in N_\alpha\}. \tag{10}$$

In this section, we will show that M_α is attained: i.e there exists $u_\alpha \in N_\alpha$, which is even in $C^\infty([-1,1])$, such that $\mathcal{W}_h(u_\alpha) = M_\alpha$.

According to (7) we have for all $u \in N_\alpha$

$$\mathcal{W}(\Gamma) = \frac{\pi}{2}\int_{-1}^{1} \kappa_h(x)^2\, ds_h(x) = \frac{\pi}{2}\mathcal{W}_h(u),$$

with Γ the surface of revolution generated by the graph u. Hence, the surface of revolution generated by the graph of u_α is a minimizer of the Willmore functional in the class of surfaces of revolution generated by the graph of functions in N_α. The corresponding Willmore equation is the following Dirichlet problem

$$\begin{cases} \Delta_g H + 2H^3 - 2HK = 0 & \text{in } (-1,1), \\ u(\pm 1) = \alpha, \qquad u'(\pm 1) = 0. \end{cases} \tag{11}$$

By minimising the functional $\mathcal{W}_h$ on N_α we construct a symmetric solution to (11).

Remark 1. *We will use the following rescaling property. If u is a positive function in $C^{1,1}([-r,r])$, for some $r>0$, then the function $v \in C^{1,1}([-1,1])$ defined by $v(x) = \frac{1}{r}u(rx)$ is such that*

$$\mathcal{W}_h(v) = \int_{-r}^{r} \kappa_h^2[u]ds_h[u].$$

Here and in the following $\kappa_h[u]$ denotes the curvature of the graph of u in the hyperbolic half plane (defined in (6)) and $ds_h[u]$ denotes the corresponding line element.

3.1 Upper bound for M_α

Lemma 2. *Let M_α be defined as in (10). Then*

$$M_\alpha \leq 8 \int_0^{\arctan(1/(2\alpha))} \frac{d\varphi}{2-\cos\varphi} \leq \frac{16}{9}\sqrt{3}\pi.$$

In particular,

$$\lim_{\alpha\to\infty} M_\alpha = 0.$$

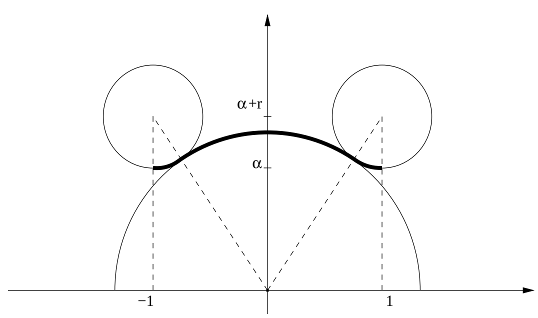

Figure 1: Comparison functions

Proof. Let $r>0$ to be suitably chosen. On the circle centered at $(1,\alpha+r)$ with radius r we consider the shortest arc starting at P, point of intersection between the circle and the segment from $(0,0)$ to $(1,\alpha+r)$, and ending in $(1,\alpha)$. This arc has opening angle $\arctan(1/(\alpha+r))$. Then we extend the curve in a $C^{1,1}$-way by considering on the geodesic circle centered at the origin and going through the point P the arc that starts at the intersection point between the circle and the y-axis and ends in P. Notice that the geodesic arc touches the original arc tangentially. Then we extend the curve on $[-1,0]$ by symmetry. This yields a curve $u_{\alpha,r}$ in N_α with equation

$$u_{\alpha,r}(x) := \begin{cases} \left((\sqrt{1+(\alpha+r)^2}-r)^2-|x|^2\right)^{\frac{1}{2}}, & \text{if } 0\leq |x| < 1-\frac{r}{\sqrt{1+(\alpha+r)^2}},\\ \alpha+r-\sqrt{r^2-(|x|-1)^2}, & \text{if } 1-\frac{r}{\sqrt{1+(\alpha+r)^2}} \leq |x| \leq 1. \end{cases}$$

The part of the curve given by the geodesic circular arc does not contribute to the Willmore energy. The graph of the other circular arcs has hyperbolic curvature

$$\kappa_h = \frac{\alpha+r}{r},$$

and line element

$$ds_h = \frac{r}{\alpha+r(1-\cos\varphi)}\,d\varphi.$$

Then $u_{\alpha,r}$ has Willmore energy:

$$\mathcal{W}_h(u_{\alpha,r}) = 2\frac{(\alpha+r)^2}{r}\int_0^{\arctan(1/(\alpha+r))}\frac{1}{\alpha+r(1-\cos\varphi)}\,d\varphi,$$

and the claim follows choosing $r=\alpha$. □

3.2 Monotonicity of the optimal Willmore energy

We show that $M_{\alpha'} \le M_\alpha$ for $\alpha' > \alpha$.

Lemma 3. *Fix $a>0$. Assume that $u \in C^{1,1}([-a,a])$ has only finitely many critical points and it is positive and symmetric with $u'(a)=0$ and such that $u'(x)\le 0$ for all $x\in[0,a]$. Then, for each $\rho\in(0,a]$, there exists a positive symmetric function $u_\rho \in C^{1,1}([-\rho,\rho])$ such that $u_\rho(\rho)=u(a)$, $u_\rho'(\rho)=0$, u_ρ has at most as many critical points as u and*

$$\forall x\in[0,\rho]:\ u_\rho'(x)\le 0 \ \text{ as well as } \int_{-\rho}^{\rho}\kappa_h[u_\rho]^2\,ds_h[u_\rho] \le \int_{-a}^{a}\kappa_h[u]^2\,ds_h[u].$$

In particular if $a=1$

$$\int_{-\rho}^{\rho}\kappa_h[u_\rho]^2\,ds_h[u_\rho]\le \mathcal{W}_h(u).$$

Proof. Let $r\in(0,a)$ be a parameter. The normal to the graph of u in $(r,u(r))$ has direction $(-u'(r),1)$. The straight line generated by the normal intersects the x-axis left of r, since u is decreasing. We take this intersection point $(c(r),0)$ as center for a geodesic circular arc, where the radius is chosen such that the arc is tangential to the graph of u in $(r,u(r))$ (i.e. the radius is given by the distance between $(c(r),0)$ and $(r,u(r))$). We build a new symmetric function with smaller curvature integral as follows. On $[c(r),r]$ we take this geodesic arc, which has horizontal tangent in $c(r)$, while on $[r,a]$ we take u. By construction, this function is $C^{1,1}([c(r),a])$ and decreasing. We shift it such that $c(r)$ is moved to 0, and extend this to an even function, which is again $C^{1,1}$, now on a suitable interval $[-\ell(r),\ell(r)]$. This function has the same boundary values as u, at most as many critical points as u and, by construction, a smaller curvature integral. This construction yields the claim since $r\mapsto \ell(r)$ is continuous and $\lim_{r\searrow 0}\ell(r)=a$, $\lim_{r\nearrow a}\ell(r)=0$. □

Lemma 4. *Fix $a>0$. Assume that $u\in C^{1,1}([-a,a])$ has only finitely many critical points and it is symmetric, positive with $u'(a)=0$ and such that $u'(x)\ge 0$ for all $x\in[0,a]$. Then there exists a positive symmetric function $v\in C^{1,1}([-a,a])$ with $v(a)=u(a)$, $v'(a)=0$, v has at most as many critical points as u and*

$$\forall x\in[0,a]:\ v'(x)\le 0 \ \text{ as well as } \int_{-a}^{a}\kappa_h[v]^2\,ds_h[v]\le\int_{-a}^{a}\kappa_h[u]^2\,ds_h[u].$$

In particular if $a=1$, $\mathcal{W}_h(v)\le\mathcal{W}_h(u)$.

Proof. We may assume that $u(0)<u(a)$. We consider

$$\tilde u(x) := \begin{cases} u(x+a), & \text{if } x\in[-a,0]\\ u(x-a), & \text{if } x\in[0,a].\end{cases}$$

We apply the procedure of Lemma 3 to $\tilde u$ and find for all $\rho\in(0,a]$ a symmetric positive function $\tilde u_\rho\in C^{1,1}([-\rho,\rho])$ with lower Willmore energy, at most as many critical point as $\tilde u$ and such that $\tilde u_\rho(\rho)=\tilde u(a)=u(0)$, $\tilde u_\rho'(\rho)=0$ and $\tilde u_\rho'(x)\le 0$ for all $x\in[0,\rho]$. Let $\rho_0\in(0,a]$ be such that $\tilde u(a)=u(0)=\frac{\rho_0}{a}u(a)$. Then, by rescaling (Remark 1), the function $v(x)=\frac{a}{\rho_0}\tilde u_{\rho_0}(\frac{\rho_0}{a}x)$ defined on $[-a,a]$ is the desired decreasing function with smaller Willmore energy. □

Lemma 5. *Fix $a > 0$. Assume that $u \in C^{1,1}([-a,a])$ is a symmetric, positive function having only finitely many critical points and satisfying $u'(a) = 0$. Then, for each $\rho \in (0,a]$, there exists a symmetric positive function $u_\rho \in C^{1,1}([-\rho,\rho])$ with $u'_\rho(\rho) = 0$ and $u_\rho(\rho) = u(a)$ with at most as many critical points as u such that*

$$\int_{-\rho}^{\rho} \kappa_h[u_\rho]^2\, ds_h[u_\rho] \le \int_{-a}^{a} \kappa_h[u]^2\, ds_h[u].$$

If $u'(x) < 0$ for x close to a, the same may be achieved for $u'_\rho(x)$ for x close to ρ. In particular if $a = 1$

$$\int_{-\rho}^{\rho} \kappa_h[u_\rho]^2\, ds_h[u_\rho] \le \mathcal{W}_h(u).$$

Proof. We may assume that u is not a constant. Let $x_0 > 0$ be such that $[-x_0, x_0]$ is the smallest possible symmetric interval with $u'(x_0) = 0$. In $[0, x_0]$ the derivative of u has a fixed sign. If $u'(x) \ge 0$ in $[0, x_0]$ then by Lemma 4 there is a positive symmetric function $v \in C^{1,1}([-x_0, x_0])$ with lower Willmore energy such that $v(x_0) = u(x_0)$, $v'(x_0) = 0$ and $v'(x) \le 0$ in $[0, x_0]$. Hence we may assume that $u'(x) \le 0$ in $[0, x_0]$. By Lemma 3 for all $r \in (0, x_0]$ there exists a positive symmetric function $v_r \in C^{1,1}([-r,r])$ such that $v_r(r) = u(x_0)$ and $v'_r(r) = 0$ and $v'_r(x) \le 0$ in $[0,r]$. Hence the function

$$u_r(x) := \begin{cases} u(x + x_0 - r), & \text{if } \ r < x \le a + r - x_0, \\ v_r(x), & \text{if } \ -r \le x \le r, \\ u(x - x_0 + r), & \text{if } \ -a - r + x_0 < x \le -r, \end{cases}$$

is in $C^{1,1}([-a - r + x_0, a + r - x_0])$, is symmetric , $u'_r(a + r - x_0) = 0$, $u_r(a + r - x_0) = u(a)$ and

$$\int_{-(a+r-x_0)}^{a+r-x_0} \kappa_h[u_r]^2\, ds_h[u_r] \le \int_{-a}^{a} \kappa_h[u]^2\, ds_h[u].$$

With this construction the claim is proved for $\rho \ge a - x_0$.

For $\rho < a - x_0$ we start from the function just constructed obtained at the limit for r going to zero. That is $v(x) = u(x + x_0)$ for $x \in [0, a - x_0]$ and extended by symmetry on $[-a + x_0, 0]$. This function is in $C^{1,1}([-a+x_0, a-x_0])$, positive and symmetric. We can repeat the same construction just done. We continuously decrease the interval of definition and, at the same time, the curvature integral. Since we have only finitely many critical points and at each iteration step we do not increase the number of critical points, this procedure is well defined and terminates after finitely many iterations.

If $u' < 0$ close to a the same may be achieved for u'_ρ since in the construction we do not change the function near the end-points of the interval of definition. ∎

Corollary 1. *Fix $a > 0$ and $\alpha > 0$. For each positive symmetric $u \in C^{1,1}([-a,a])$ having only finitely many critical points and satisfying*

$$u(\pm a) = \alpha, \qquad u'(\pm a) = 0$$

and for each $\beta \ge \alpha$, we find a symmetric $v \in C^{1,1}([-a,a])$ having at most as many critical points as u, satisfying

$$v(\pm a) = \beta, \qquad v'(\pm a) = 0$$

and

$$\int_{-a}^{a} \kappa_h[v]^2\, ds_h[v] \le \int_{-a}^{a} \kappa_h[u]^2\, ds_h[u].$$

If $u'(x) < 0$ for x close to a, the same may be achieved for v'. In particular if $a = 1$, $\mathcal{W}_h(v) \le \mathcal{W}_h(u)$.

Proof. By Lemma 5 for each $\rho \in (0, a]$, there exists a symmetric positive function $u_\rho \in C^{1,1}([-\rho, \rho])$ having at most as many critical points as u with $u_\rho'(\rho) = 0$ and $u_\rho(\rho) = u(a) = \alpha$ such that

$$\int_{-\rho}^{\rho} \kappa_h[u_\rho]^2 \, ds_h[u_\rho] \leq \int_{-a}^{a} \kappa_h[u]^2 \, ds_h[u].$$

Choosing ρ_0 such that $\frac{a}{\rho_0}\alpha = \beta$ the function $v(x) = \frac{a}{\rho_0} u_{\rho_0}(\frac{\rho_0}{a}x)$ for $x \in [-a, a]$ yields the claim. □

Theorem 2. *Let M_α for $\alpha \in \mathbb{R}^+$ be as defined in* (10)*. Then for $0 < \alpha < \hat{\alpha}$ we have that*

$$M_{\hat{\alpha}} \leq M_\alpha.$$

Proof. Since the polynomials are dense in H^2, a minimising sequence for M_α may be chosen (in N_α), which consists of symmetric positive polynomials. Corollary 1 yields the claim. □

3.3 Properties of minimising sequences

The first main step consists in finding a procedure which does not increase the Willmore energy but allows to restrict to functions v in N_α (defined in (9)) such that $v'(x) \leq 0$ for all $x \in [0, 1]$. Here, the techniques developed in subsection 3.2 are used essentially.

Theorem 3. *Let N_α be as defined in* (9)*. For each $u \in N_\alpha$ having only finitely many critical points, we find $v \in N_\alpha$ having at most as many critical points as u, satisfying*

$$v'(x) \leq 0 \text{ for all } x \in [0, 1] \quad \text{and} \quad \mathcal{W}_h(v) \leq \mathcal{W}_h(u).$$

Proof. If u does not have the claimed property then there exist $x_0, x_1 \in [0, 1]$, $x_0 < x_1$, with $u'(x) > 0$ in (x_0, x_1), $u'(x_0) = u'(x_1) = 0$ and $u'(x) \leq 0$ in $[x_1, 1]$. Using that $u(x_0) < u(x_1)$, we construct a positive symmetric function $v_1 \in C^{1,1}([-x_1, x_1])$ such that v_1 has at most as many critical points as $u|_{[-x_1,x_1]}$, $v_1'(x) \leq 0$ in $[x_0, x_1]$ and

$$v_1'(x_1) = 0, \quad v_1(x_1) = u(x_1), \quad \int_{-x_1}^{x_1} \kappa_h[v_1]^2 ds_h[v_1] \leq \int_{-x_1}^{x_1} \kappa_h[u]^2 ds_h[u]. \tag{12}$$

The claim will then follow by finitely many iterations proceeding from the boundary points towards the central point 0.

We consider $u|_{[-x_0,x_0]}$ and apply Corollary 1 with $\beta = u(x_1)$. If $x_0 = 0$ one simply skips this first step. There exists a symmetric positive function $w_1 \in C^{1,1}([-x_0, x_0])$ with $w_1(x_0) = u(x_1)$, $w_1'(x_0) = 0$, having no more critical points than $u|_{[-x_0,x_0]}$ and satisfying

$$\int_{-x_0}^{x_0} \kappa_h[w_1]^2 ds_h[w_1] \leq \int_{-x_0}^{x_0} \kappa_h[u]^2 ds_h[u].$$

We define on $[-x_1, x_1]$

$$\tilde{v}_1(x) := \begin{cases} u(x + x_1 + x_0), & \text{if } x \in [-x_1, -x_0], \\ w_1(x), & \text{if } x \in [-x_0, x_0], \\ u(x - x_1 - x_0), & \text{if } x \in [x_0, x_1]. \end{cases}$$

Certainly, $\tilde{v}_1 \in C^{1,1}([-x_1, x_1])$ is positive, symmetric and it does not have more critical points than $u|_{[-x_1,x_1]}$. Moreover, $\tilde{v}_1'(x) \leq 0$ for $x \in [x_0, x_1]$ and

$$\int_{-x_1}^{x_1} \kappa_h[\tilde{v}_1]^2 ds_h[\tilde{v}_1] \leq \int_{-x_1}^{x_1} \kappa_h[u]^2 ds_h[u], \quad \tilde{v}_1(x_1) = u(x_0), \quad \tilde{v}_1'(x_1) = 0.$$

Corollary 1 now yields a positive symmetric function $v_1 \in C^{1,1}([-x_1, x_1])$, having no more critical points than $u|_{[-x_1,x_1]}$ and satisfying (12), with $v_1'(x) \leq 0$ in $[x_0, x_1]$. The last property is verified first close to x_1; it holds on the whole interval since no further critical points arise. □

Moreover, in choosing a minimising sequence for M_α we may restrict to functions in N_α satisfying

$$\forall x \in [0,1]: \qquad 0 \le x + v(x)v'(x). \tag{13}$$

For $x = 0$ and $x = 1$, this inequality is trivially satisfied. If for some $x_0 \in (0,1)$ we have that $0 = x_0 + v(x_0)v'(x_0)$, then the normal in $(x_0, v(x_0))$ to the graph of v goes through the origin. Hence, with the same construction as in Lemma 2 we could substitute over $[-x_0, x_0]$ the original graph by a geodesic circular arc lowering the Willmore energy. Observe that this procedure, applied to a positive symmetric $C^{1,1}$-function with $v'(x) \le 0$ for all $x \in [0,1]$ preserves all these properties.

Combining (13) with Theorem 3 we may restrict ourselves to minimising sequences $(v_k)_k$ for M_α (defined in (10)) having the following properties:

$$v_k \in C^{1,1}([-1,1]) \text{ are positive, symmetric and s.t. } \forall x \in [0,1]: \ 0 \le x + v_k(x)v_k'(x), \ v_k'(x) \le 0. \tag{14}$$

This implies immediately the following a-priori-estimates for this suitably chosen minimising sequence:

$$\forall x \in [-1,1]: \qquad \alpha \le v_k(x) \le \sqrt{\alpha^2 + 1 - x^2} \le \alpha + 1 \qquad |v_k'(x)| \le \frac{|x|}{\alpha}. \tag{15}$$

3.4 Attainment of the minimal Willmore energy

We are now able to state and to prove a more precise result than the main existence result Theorem 1 from the introduction:

Theorem 4. *For each $\alpha > 0$, there exists a positive symmetric function $u \in H^2(-1,1) \cap C^1([-1,1])$ satisfying*

$$u(\pm 1) = \alpha, \qquad u'(\pm 1) = 0,$$

such that

$$\mathcal{W}_h(u) = M_\alpha \overset{\text{def}}{=} \inf\{\mathcal{W}_h(v) : v \in C^{1,1}([-1,1]), v \text{ is even}, \ v(\pm 1) = \alpha, v'(\pm 1) = 0\}.$$

This minimum is a weak solution to the Dirichlet problem (11) satisfying

$$\forall x \in [0,1]: \quad 0 \le x + u(x)u'(x), \qquad u'(x) \le 0. \tag{16}$$

$$\forall x \in [-1,1]: \qquad \alpha \le u(x) \le \sqrt{\alpha^2 + 1 - x^2} \le \alpha + 1 \qquad |u'(x)| \le \frac{|x|}{\alpha}. \tag{17}$$

Moreover, u is a classical solution, i.e. $u \in C^\infty([-1,1])$.

Proof. **Step1. Existence and quantitative properties of a minimiser.**
Let $(v_k)_k \subset N_\alpha$ be a minimizing sequence for M_α satisfying (14 – 15). By the uniform bounds in (15) we find

$$\begin{aligned}
\mathcal{W}_h(v_k) &= \int_{-1}^{1} \frac{v_k''(x)^2 v_k(x)}{(1 + v_k'(x)^2)^{5/2}}\, dx + \int_{-1}^{1} \frac{1}{v_k(x)\sqrt{1 + v_k'(x)^2}}\, dx \\
&\ge \frac{\alpha}{\left(1 + \frac{1}{\alpha^2}\right)^{5/2}} \int_{-1}^{1} v_k''(x)^2\, dx + 2\frac{1}{(\alpha+1)\sqrt{1 + \frac{1}{\alpha^2}}}.
\end{aligned}$$

This shows uniform boundedness of $(v_k)_k$ in $H^2(-1,1)$. After passing to a subsequence, we find a positive symmetric function $u \in H^2(-1,1)$ such that

$$v_k \rightharpoonup u \text{ in } H^2(-1,1), \quad v_k \to u \in C^1([-1,1]),$$

and satisfying (16 – 17). Since

$$\begin{aligned} M_\alpha + o(1) &= \mathcal{W}_h(v_k) = \int_{-1}^{1} \frac{v_k''(x)^2 u(x)}{(1+u'(x)^2)^{5/2}}\,dx + \int_{-1}^{1} \frac{1}{u(x)\sqrt{1+u'(x)^2}}\,dx + o(1) \\ &\geq \int_{-1}^{1} \frac{u''(x)^2 u(x)}{(1+u'(x)^2)^{5/2}}\,dx + \int_{-1}^{1} \frac{1}{u(x)\sqrt{1+u'(x)^2}}\,dx + o(1), \end{aligned}$$

it follows that u minimises the hyperbolic Willmore functional $\mathcal{W}_h$ in the class of all positive symmetric $H^2(-1,1)$-functions v, satisfying $v(\pm 1) = \alpha$, $v'(\pm 1) = 0$. So, u weakly solves (11) and hence, also (8) in the sense of (18) below (see also (19)).

Step 2. Regularity of the minimiser.
From the calculations in the Appendix A, concerning the derivation of the Euler-Lagrange equation, we see that for any *even* $\varphi \in C^2([-1,1])$ with $\varphi(1) = 0$, $\varphi'(1) = 0$ one has that

$$\begin{aligned} -2\int_{-1}^{1} \kappa_h \frac{1}{1+u'^2}\varphi''\,dx &= \int_{-1}^{1} \kappa_h^2 \frac{\sqrt{1+u'^2}}{u^2}\varphi\,dx - 5\int_{-1}^{1} \kappa_h^2 \frac{u'}{u\sqrt{1+u'^2}}\varphi'\,dx \\ &\quad -2\int_{-1}^{1} \kappa_h \frac{1}{u^2}\varphi\,dx + 4\int_{-1}^{1} \kappa_h \frac{u'}{u(1+u'^2)}\varphi'\,dx. \end{aligned} \tag{18}$$

First, we observe that (18) is still true for any $\varphi \in C^2([-1,1])$ with $\varphi(\pm 1) = 0$ and $\varphi'(\pm 1) = 0$. This follows by decomposition of φ in its even and odd part and using that they satisfy the same boundary conditions and that integrals over odd functions vanish. We take for arbitrary $\eta \in C_0^\infty(-1,1)$

$$\varphi(x) := \int_{-1}^{x}\int_{-1}^{y} \eta(s)\,ds dy - \beta(x+1)^2 - \gamma(x+1)^3,$$

where

$$\begin{aligned} \beta &= -\frac{1}{2}\int_{-1}^{1} \eta(s)\,ds + \frac{3}{4}\int_{-1}^{1}\int_{-1}^{y} \eta(s)\,ds dy \\ \gamma &= \frac{1}{4}\int_{-1}^{1} \eta(s)\,ds - \frac{1}{4}\int_{-1}^{1}\int_{-1}^{y} \eta(s)\,ds dy \end{aligned}$$

are chosen such that $\varphi(\pm 1) = 0$ and $\varphi'(\pm 1) = 0$. Since $\mathcal{W}_h(u)$ is finite, u obeys (17) and since

$$|\beta|, |\gamma|, \|\varphi\|_{C^1} \leq C\|\eta\|_{L^1},$$

we can conclude from (18) that for each $\eta \in C_0^\infty(-1,1)$,

$$\left| \int_{-1}^{1} \kappa_h \frac{1}{1+u'^2}\eta\,dx \right| \leq C(u)\|\eta\|_{L^1}.$$

By the bounds on u in (17), the inequality above shows that κ_h is bounded and so,

$$u \in W^{2,\infty}(-1,1).$$

Next, for arbitrary $\eta \in C_0^\infty(-1,1)$ we choose

$$\varphi(x) = \int_{-1}^{x} \eta(s)\,ds - \frac{3}{4}\left(\int_{-1}^{1} \eta(s)\,ds\right)(x+1)^2 + \frac{1}{4}\left(\int_{-1}^{1} \eta(s)\,ds\right)(x+1)^3$$

so that

$$\varphi(\pm 1) = 0, \qquad \varphi'(\pm 1) = 0, \qquad \|\varphi\|_{C^0} \leq C\|\eta\|_{L^1}, \qquad \|\varphi'\|_{L^1} \leq C\|\eta\|_{L^1}.$$

Since we already know that κ_h is bounded, we conclude from (18) that for each $\eta \in C_0^\infty(-1,1)$,

$$\left| \int_{-1}^{1} \kappa_h \frac{1}{1+u'^2} \eta'(x)\, dx \right| \leq C(u) \|\eta\|_{L^1}.$$

This proves that

$$\kappa_h \frac{1}{1+u'^2} \in W^{1,\infty}(-1,1), \quad \kappa_h \in W^{1,\infty}([-1,1]) = C^{0,1}([-1,1]),$$
$$\text{and hence } \ u \in W^{3,\infty}([-1,1]) = C^{2,1}([-1,1]).$$

Finally, rewriting (8) as follows

$$\frac{d}{dx}\left(\frac{u(x)}{\sqrt{1+u'(x)^2}} \kappa_h'(x) \right) = \frac{\sqrt{1+u'(x)^2}}{u(x)} \left(\kappa_h(x) - \frac{1}{2}\kappa_h(x)^3 \right) \text{ in } (-1,1),$$

we get an equation for κ_h with $W^{1,\infty}$-coefficients and right hand side. Hence, $\kappa_h \in W^{3,\infty}([-1,1]) = C^{2,1}([-1,1])$, $u \in C^{4,1}([-1,1])$ and finally, by straightforward bootstrapping, $u \in C^\infty([-1,1])$. $\square$

A Proof of Lemma 1

In order to calculate the Euler-Lagrange equation for the functional $\mathcal{W}_h$, we observe first that for arbitrary $\varphi \in C_0^\infty(-1,1)$:

$$\begin{aligned}
\frac{d}{dt}\kappa_h[u+t\varphi]|_{t=0} &= -\frac{d}{dt}\left\{ \frac{(u+t\varphi)^2}{u'+t\varphi'} \frac{d}{dx}\left(\frac{1}{(u+t\varphi)\sqrt{1+(u'+t\varphi')^2}} \right) \right\}\Bigg|_{t=0} \\
&= -2\frac{u\varphi}{u'}\frac{d}{dx}\left(\frac{1}{u\sqrt{1+u'^2}} \right) + \frac{u^2\varphi'}{u'^2}\frac{d}{dx}\left(\frac{1}{u\sqrt{1+u'^2}} \right) \\
&\quad + \frac{u^2}{u'}\frac{d}{dx}\left(\frac{\varphi}{u^2\sqrt{1+u'^2}} \right) + \frac{u^2}{u'}\frac{d}{dx}\left(\frac{u'\varphi'}{u(1+u'^2)^{3/2}} \right)
\end{aligned}$$

and writing it in terms of κ_h

$$\begin{aligned}
\frac{d}{dt}\kappa_h[u+t\varphi]|_{t=0} &= 2\frac{\varphi}{u}\kappa_h - \frac{\varphi'}{u'}\kappa_h - \frac{\varphi}{u}\kappa_h + \frac{u}{u'\sqrt{1+u'^2}}\left(\frac{\varphi}{u} \right)' \\
&\quad - \frac{u'\varphi'}{1+u'^2}\kappa_h + \frac{u}{u'\sqrt{1+u'^2}}\left(\frac{u'\varphi'}{1+u'^2} \right)' \\
&= \frac{\varphi}{u}\kappa_h - \frac{\varphi'}{u'}\kappa_h - \frac{u'\varphi'}{1+u'^2}\kappa_h + \frac{\varphi'}{u'\sqrt{1+u'^2}} - \frac{\varphi}{u\sqrt{1+u'^2}} \\
&\quad + \frac{u}{u'\sqrt{1+u'^2}}\left(\frac{\varphi''u'}{1+u'^2} + \frac{\varphi'u''}{1+u'^2} - 2\frac{\varphi'u'^2u''}{(1+u'^2)^2} \right)
\end{aligned}$$

As for the last large bracket we have

$$\begin{aligned}
&\left(\frac{\varphi''u'}{1+u'^2} + \frac{\varphi'u''}{1+u'^2} - 2\frac{\varphi'u'^2u''}{(1+u'^2)^2} \right) = \frac{\varphi''u'}{1+u'^2} - \frac{\varphi'u''}{1+u'^2} + 2\frac{\varphi'u''}{(1+u'^2)^2} = \\
&= \frac{\varphi''u'}{1+u'^2} + \varphi'\sqrt{1+u'^2}\left(-\frac{\kappa_h}{u} + \frac{1}{u\sqrt{1+u'^2}} \right) - \frac{2\varphi'}{\sqrt{1+u'^2}}\left(-\frac{\kappa_h}{u} + \frac{1}{u\sqrt{1+u'^2}} \right) \\
&= \frac{\varphi''u'}{1+u'^2} - \frac{\kappa_h\varphi'}{u}\sqrt{1+u'^2} + \frac{\varphi'}{u} + \frac{2\kappa_h\varphi'}{u\sqrt{1+u'^2}} - \frac{2\varphi'}{u(1+u'^2)}
\end{aligned}$$

so that

$$\frac{d}{dt}\kappa_h[u+t\varphi]|_{t=0} = \frac{\varphi\kappa_h}{u} - 3\frac{u'\varphi'\kappa_h}{1+u'^2} - \frac{\varphi}{u\sqrt{1+u'^2}} + \frac{2u'\varphi' + u\varphi''}{(1+u'^2)^{3/2}}.$$

So, in view of the assumptions on u we have for all $\varphi \in C_0^\infty(-1,1)$ that

$$\begin{aligned}
0 &= \frac{d}{dt}\mathcal{W}_h(u+t\varphi)|_{t=0} = \frac{d}{dt}\int_{-1}^{1} \kappa_h[u+t\varphi]^2 \frac{\sqrt{1+(u'+t\varphi')^2}}{u+t\varphi}\,dx\Big|_{t=0} \\
&= \int_{-1}^{1} 2\kappa_h \frac{\sqrt{1+u'^2}}{u}\left(\frac{\varphi\kappa_h}{u} - 3\frac{u'\varphi'\kappa_h}{1+u'^2} - \frac{\varphi}{u\sqrt{1+u'^2}} + \frac{2u'\varphi'+u\varphi''}{(1+u'^2)^{3/2}}\right) dx \\
&\quad + \int_{-1}^{1} \kappa_h^2 \left(\frac{u'\varphi'}{u\sqrt{1+u'^2}} - \frac{\varphi\sqrt{1+u'^2}}{u^2}\right) dx \\
&= \int_{-1}^{1} \kappa_h^2 \frac{\sqrt{1+u'^2}}{u^2}\varphi\,dx - 5\int_{-1}^{1} \kappa_h^2 \frac{u'}{u\sqrt{1+u'^2}}\varphi'\,dx - 2\int_{-1}^{1} \kappa_h \frac{1}{u^2}\varphi\,dx \\
&\quad +4\int_{-1}^{1} \kappa_h \frac{u'}{u(1+u'^2)}\varphi'\,dx + 2\int_{-1}^{1} \kappa_h \frac{1}{1+u'^2}\varphi''\,dx = \ldots
\end{aligned} \tag{19}$$

integrating by parts first in the last integral and then in the second one

$$\begin{aligned}
\ldots &= \int_{-1}^{1} \kappa_h^2 \frac{\sqrt{1+u'^2}}{u^2}\varphi\,dx - \int_{-1}^{1} \kappa_h^2 \frac{u'}{u\sqrt{1+u'^2}}\varphi'\,dx - 2\int_{-1}^{1}\kappa_h\frac{1}{u^2}\varphi\,dx - 2\int_{-1}^{1}\kappa_h' \frac{1}{1+u'^2}\varphi'\,dx \\
&= \int_{-1}^{1} \kappa_h^2 \frac{\sqrt{1+u'^2}}{u^2}\varphi\,dx + \int_{-1}^{1}\kappa_h^2 u' \left(\frac{1}{u\sqrt{1+u'^2}}\right)'\varphi\,dx + 2\int_{-1}^{1}\kappa_h\kappa_h'\frac{u'}{u\sqrt{1+u'^2}}\varphi\,dx \\
&\quad + \int_{-1}^{1}\kappa_h^2\frac{u''}{u\sqrt{1+u'^2}}\varphi\,dx - 2\int_{-1}^{1}\kappa_h\frac{1}{u^2}\varphi\,dx - 2\int_{-1}^{1}\kappa_h'\frac{1}{1+u'^2}\varphi'\,dx \\
&= \int_{-1}^{1}\kappa_h^2\varphi\left(\frac{\sqrt{1+u'^2}}{u^2} - \frac{u'^2}{u^2\sqrt{1+u'^2}} - \frac{u'^2u''}{u(1+u'^2)^{3/2}} + \frac{u''}{u\sqrt{1+u'^2}}\right)dx \\
&\quad -2\int_{-1}^{1}\kappa_h\frac{1}{u^2}\varphi\,dx + 2\int_{-1}^{1}\kappa_h\kappa_h'\frac{u'}{u\sqrt{1+u'^2}}\varphi\,dx - 2\int_{-1}^{1}\frac{u}{\sqrt{1+u'^2}}\kappa_h'\frac{1}{u\sqrt{1+u'^2}}\varphi'\,dx = \ldots
\end{aligned}$$

and, finally, integrating by parts in the last integral

$$\ldots = \int_{-1}^{1}\kappa_h^3\frac{1}{u^2}\varphi\,dx - 2\int_{-1}^{1}\kappa_h\frac{1}{u^2}\varphi\,dx + 2\int_{-1}^{1}\frac{u}{\sqrt{1+u'^2}}\frac{d}{dx}\left(\frac{u}{\sqrt{1+u'^2}}\kappa_h'\right)\frac{1}{u^2}\varphi\,dx.$$

□

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Symmetric Willmore surfaces of revolution satisfying arbitrary Dirichlet boundary data[1]

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Dedicated to Prof. E. Heinz on the occasion of his 85th birthday.

Abstract

We consider the Willmore boundary value problem for surfaces of revolution where, as Dirichlet boundary conditions, any symmetric set of position and angle may be prescribed. Using direct methods of the calculus of variations, we prove existence and regularity of minimising solutions. Moreover, we estimate the optimal Willmore energy and prove a number of qualitative properties of these solutions. Besides convexity-related properties we study in particular the limit when the radii of the boundary circles converge to 0, while the "length" of the surfaces of revolution is kept fixed. This singular limit is shown to be the sphere, irrespective of the prescribed boundary angles.

These analytical investigations are complemented by presenting a numerical algorithm based on C^1-elements and numerical studies. They intensively interact with geometric constructions in finding suitable minimising sequences for the Willmore functional.

Keywords. Dirichlet boundary conditions, Willmore surfaces of revolution.
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1 Introduction

1.1 The Willmore problem

Given a smooth and immersed surface $\Gamma \subset \mathbb{R}^3$, the *Willmore functional* is defined by

$$\mathcal{W}(\Gamma) := \int_\Gamma H^2 \, dA \tag{1.1}$$

with H the mean curvature of the immersion and dA its area element.

The functional $\mathcal{W}$ is of geometric interest, and it models the elastic energy of thin shells or biological membranes. It applies further in image processing and even in string theory (see e.g. [13, 15, 22, 16, 23]). In these applications one is usually concerned with *minima* or, more generally, with *critical points* of the Willmore functional. Such a critical point $\Gamma \subset \mathbb{R}^3$ has to satisfy the *Willmore equation*

$$\Delta_\Gamma H + 2H(H^2 - K) = 0 \quad \text{on } \Gamma, \tag{1.2}$$

where Δ_Γ denotes the Laplace-Beltrami operator on Γ, and K is the Gauss curvature of the surface. A solution of this non-linear fourth-order differential equation is called *Willmore surface.*

Although introduced already in the 19th century (see e.g. [24]), it was Willmore's work [29] which popularised again the investigation of the Willmore functional. Various existence and regularity results for *closed* Willmore surfaces of prescribed genus were extensively discussed in the literature. We want to mention in particular Bauer-Kuwert and Simon [1, 27] for existence of closed Willmore surfaces of prescribed genus, Kuwert-Schätzle and Leschke-Pedit-Pinkall [17, 18, 21] for constrained closed Willmore surfaces of fixed conformal class and Rivière [25] for a far reaching regularity result. We refer to [4] for a more extensive survey.

In the present paper we are interested in surfaces *with boundaries.* Therefore, we need to add to (1.2) appropriate boundary conditions. A discussion of possible choices can be found in Nitsche's survey article [22]. In the present article we prescribe Dirichlet boundary conditions, i.e. $\partial\Gamma$ and the tangential spaces of Γ at $\partial\Gamma$. Nitsche's work [22] contains also some existence results for several kinds of boundary conditions. These are based on perturbation arguments and require severe smallness conditions on the boundary data, which are by no means explicit. Furthermore, using methods from geometric measure theory, Schätzle proved in [26] existence and regularity of branched Willmore immersions in $\mathbb{S}^n$ with prescribed Dirichlet boundary conditions. By working in $\mathbb{S}^n$, some compactness problems could be overcome. On the other hand, when pulling back these immersions to $\mathbb{R}^n$ it cannot be excluded that they contain the point ∞. Due to the generality of his approach it seems to us that, in general, only little topological information of the solution can be extracted from the existence proof. However, under some explicit smallness condition on the Willmore energy of suitable extensions of the Dirichlet boundary data, Schätzle's solutions are shown to be even connected and embedded. For numerical algorithms and numerical analysis for boundary value problems for the Willmore equation and the corresponding parabolic flow we mention Deckelnick, Droske, Rumpf and Dziuk (see [5, 10, 11] and references therein).

To prove existence of a priori bounded solutions to boundary value problems for the Willmore equation (1.2) with some specified further properties like e.g. the topological type or being a graph without imposing smallness conditions on the data seems to be a quite difficult task. Equation (1.2) is highly nonlinear and of fourth order and so, lacking any form of a general maximum or comparison principle. Most of the well established techniques from second order problems like e.g. the De Giorgi-Nash-Moser theory seem to break down completely in higher order problems. In order to start working on a theory of classical bounded smooth solutions for the Willmore boundary value problem we think that it is a good and appropriate strategy to investigate situations enjoying symmetry. Although then, one has an underlying ordinary differential equation, understanding solvability of the corresponding boundary value problems is by no means straightforward. In this spirit the one-dimensional Willmore problem or so called elastica were studied in [6, 7]. Klaus Deckelnick and two of the authors investigated in [4] symmetric Willmore surfaces of revolution where the position and zero slope were prescribed on the boundary. By a number of refined geometric constructions it was possible to work with a priori bounded minimising sequences. Although the differential equation is one-dimensional, the geometry is to a large extent two-dimensional: Great difficulties arising from the interaction between the principal curvatures of the unknown surface are already present.

The previous work [4] was devoted to special Dirichlet boundary data. While the position at the boundary could be prescribed arbitrarily, one had to restrict to a zero boundary angle. Arbitrary boundary angles are subject of the present paper.

1.2 Main results

In the present paper we will investigate a particular Dirichlet boundary value problem for (1.2). Namely, we consider surfaces of revolution $\Gamma \subset \mathbb{R}^3$ which are generated by rotating a smooth function $u\colon [-1,1] \to (0,\infty)$ about the $x = x_1$-axis. Then, Γ can be parametrised as follows:

$$(x,\varphi) \mapsto f(x,\varphi) = (x, u(x)\cos\varphi, u(x)\sin\varphi), \quad x \in [-1,1], \quad \varphi \in [0,2\pi]. \tag{1.3}$$

We consider the Willmore problem under symmetric Dirichlet boundary conditions where the height $u(\pm 1) = \alpha > 0$ and an arbitrary angle $u'(-1) = \beta = -u'(1)$, $\beta \in \mathbb{R}$, are prescribed at the boundary. The case $\beta = 0$ has been studied in [4]. Our main result is the following.

Theorem 1.1 (Existence and regularity). *For each $\alpha > 0$ and each $\beta \in \mathbb{R}$, there exists a positive symmetric function $u \in C^\infty([-1,1],(0,\infty))$, i.e. $u(x) > 0$ and $u(x) = u(-x)$, such that the corresponding surface of revolution $\Gamma \subset \mathbb{R}^3$ solves the Dirichlet problem for the Willmore equation*

$$\begin{cases} \triangle_\Gamma H + 2H(H^2 - K) = 0 \quad \text{in } (-1,1), \\ u(-1) = u(+1) = \alpha, \qquad u'(-1) = -u'(+1) = \beta. \end{cases} \tag{1.4}$$

The solution we find has the following additional properties:

1. *If $\alpha\beta > 1$, then $u' < 0$ in $(0,1]$ and $|u'(x)| \le \beta$ for all $x \in [-1,1]$.*
2. *If $\alpha\beta \le 1$ and $\beta \ge 0$, then $u' < 0$ in $(0,1)$ and $|u'(x)| \le \frac{1}{\alpha}$ for all $x \in [-1,1]$.*
3. *If $\beta < 0$ and $\alpha \operatorname{arsinh}(-\beta) \ge \sqrt{1+\beta^2}$, then $u' > 0$ in $(0,1]$.*
4. *If $\beta < 0$ and $\alpha \operatorname{arsinh}(-\beta) < \sqrt{1+\beta^2}$, then u has at most one critical point in $(0,1)$.*

The proof is obtained by combining Theorems 3.11, 3.18, 4.17, 4.24, 4.39, 4.48 and Lemmas 3.1, 3.20 and 4.1.

It may appear surprising that we find axially symmetric solutions of the Willmore boundary value problem for all values of $\alpha > 0$ and $\beta \in \mathbb{R}$. For example, axially symmetric critical points of the area functional (i.e. minimal surfaces)

$$\mathcal{A}(\Gamma) = 2\pi \int_{-1}^{1} u(x)\sqrt{1+u'(x)^2}\,dx$$

exist only for $u(1) = \alpha \ge \alpha^*$ where

$$\alpha^* := \frac{1}{b^*}\cosh(b^*) = 1.5088795\ldots \tag{1.5}$$

and $b^* > 0$ is the solution of the equation $\cosh(b^*) = b^* \sinh(b^*)$, $b^* = 1.1996786\ldots$. Minimal surfaces of revolution, so called catenoids, are obtained for any $b \in (0,\infty)$ by rotating the curve $x \mapsto \frac{1}{b}\cosh(bx)$ around the x-axis. Not only for boundary data $\alpha \in (0,\alpha^*)$ these catenoids cease to exist, but according to [9, Chapter 6.1, Theorem 3], there is no connected minimal surface solution at all – whether symmetric or not – for $\alpha < 1$.

According to our result, for any set of symmetric Dirichlet boundary data, we always find at least one solution to the Willmore boundary value problem. For non-symmetric Dirichlet data – e.g. $u(1) \neq u(-1)$ – we expect a different picture. Analytical and numerical experiments suggest that one may be forced to impose conditions on the data $u(-1), u(1), u'(-1), u'(1)$ which deviate not too much from the symmetric setting. We feel that it might be even possible to prove nonexistence within the class of surfaces of revolutions generated by graphs for quite unsymmetric sets of data. For these data, however, existence may possibly still hold true in the class of parametric surfaces of revolution.

In order to prove our existence result Theorem 1.1, as in [4], we consider symmetric $C^{1,1}$-functions satisfying the boundary conditions and we study the minimisation problem **in this class**. In this setting, we prove that we may pass from arbitrary to suitable minimising sequences satisfying strong a priori bounds. We obtain these bounds by explicit geometric constructions which lower the Willmore energy. A key observation in doing so is the correspondence between the Willmore functional on surfaces of revolution and a curvature functional (which we call *hyperbolic Willmore functional*) on curves in the hyperbolic half plane. The geometric constructions use geodesics of the hyperbolic half plane as well as catenoids, i.e. minimal surfaces of revolution. The obtained a priori bounds on the elements of the suitably modified minimising sequence ensure the required compactness and yield the desired existence result. In the setting of the hyperbolic half plane a classification of possible curvature functions in terms of elliptic functions of the arc length of the unknown curves is available, see [19, 20]. However, we did not see a possibility to develop these results towards explicit formulae for boundary value problems (1.4). Moreover, we think that the geometric constructions performed in the present paper help to a good extent to understand the geometric shape of minimisers.

It remains as an interesting question whether these solutions minimise the Willmore energy also in the class of all immersed surfaces satisfying the same Dirichlet boundary conditions. For $\beta \neq 0$ and $\alpha \to \infty$ the energy bounds of Chapter 6 indicate that presumably this will not be the case. We expect that there might be parametric Willmore surfaces of revolution with much smaller Willmore energy.

Uniqueness is a further issue we have to leave open.

As can be seen from the statement of Theorem 1.1, the behaviour of those solutions of the Willmore equation constructed there depends not only on whether $\beta \geq 0$ or $\beta < 0$. In both cases we have to make further distinctions. It seems that we have to treat all these cases separately. The switch between the different cases occurs when having explicit solutions. These solutions mark the values of the parameters where the qualitative behaviour of solutions changes. If $\alpha\beta = 1$ then a solution is given by an arc of the circle with centre in the origin and going through the point $(1,\alpha)$. This is a geodesic in the hyperbolic half plane. The corresponding surface of revolution is part of a sphere which is the simplest possible closed Willmore surface. These geodesics of the hyperbolic half plane play an important role when studying the case $\beta \geq 0$. For $\beta < 0$ and $\alpha \operatorname{arsinh}(-\beta) = \sqrt{1+\beta^2}$, the catenoid $u(x) = \cosh(bx)/b$ with $b = \operatorname{arsinh}(-\beta)$ is a minimal surface solution. Catenoids come into play in our constructions in addition to the hyperbolic geodesics when studying the case $\beta < 0$. This interplay between two prototype Willmore surfaces gives rise to some technical difficulties. For $\beta < 0$ and $|\beta|$ large, numerical calculations clearly display almost catenoidal and almost spherical (hyperbolically geodesic) parts of solutions.

Conformal invariance is a key feature of the (hyperbolic) Willmore functional and of Willmore surfaces. Rotation and translation are frequently employed, and scaling invariance is most important throughout the whole paper. On the other hand, inversions are not addressed here since in most cases they do not preserve the particular shape (1.3) of surfaces of revolution generated by graphs. Within this framework, only the relatively simple case $\alpha\beta > 1$ could have been reduced to results in parts of the complementing cases, which are much more involved especially when $\beta < 0$. In particular, boundary data with $\beta \le \frac{1-\alpha^2}{2\alpha}$ cannot be reduced to different cases because here, inversion does not yield graphs. But inversions are nevertheless quite interesting also here. Depending on α, they may yield parametric Willmore surfaces of revolution which are not generated by graphs because they approach the left boundary from the left and the right boundary from the right. This is remarkable in so far as the general discussion of parametric surfaces of revolution is expected to be more difficult than that in the present paper.

Besides existence we also study further qualitative and asymptotic properties of solutions. A natural question is what happens to the solutions constructed in Theorem 1.1 when $\beta \in \mathbb{R}$ is fixed and α goes to 0. We prove that they converge to the sphere centered at the origin with radius 1.

Theorem 1.2. *Fix $\beta \in \mathbb{R}$. For $\alpha > 0$ let u_α be a solution to problem* (1.4) *as constructed in Theorem 1.1. Then, u_α converges for $\alpha \searrow 0$ to $x \mapsto \sqrt{1-x^2}$ in $C^m_{loc}(-1,1)$ for any $m \in \mathbb{N}$.*

For a proof see Theorem 5.8.

With our method of proving existence of solutions we get also information on the qualitative behaviour of the solutions. In particular, we can characterise the sign of the first derivative as stated in Theorem 1.1. Looking at the graph of a solution $u : [-1,1] \to (0,\infty)$ as a curve in the hyperbolic half plane, we study also the sign of its hyperbolic curvature. In Section 2.2 we recall some basic facts from hyperbolic geometry. However, the meaning of the sign of the hyperbolic curvature $\kappa_h[u](x)$ in $(x, u(x))$ is easily explained. One compares the graph of u in $(x, u(x))$ with the tangential geodesic circle centered on the x-axis. Negative $\kappa_h[u](x)$ means that the graph is locally inside this circle while $\kappa_h[u](x) > 0$ means that the graph of u is locally outside this circle. Concerning the sign of the hyperbolic curvature of our solutions we have the following result. We skip the case $\alpha\beta = 1$, where the solution is a geodesic circle.

Theorem 1.3. *For $\alpha > 0$ and $\beta \in \mathbb{R}$ let $u \in C^\infty([-1,1],(0,\infty))$ be a solution to problem* (1.4) *as constructed in Theorem 1.1. Let $\kappa_h[u]$ denote the hyperbolic curvature of the curve $\{(x,u(x)) : x \in [-1,1]\}$. Then, $\kappa_h[u]$ has the following sign properties:*

1. *If $\alpha\beta > 1$, then $\kappa_h[u](0) < 0$ and $\kappa_h[u]$ has at most one change of sign in $(0,1)$.*
2. *If $\alpha\beta < 1$ and $\beta \ge 0$, then $\kappa_h[u] > 0$ in $(-1,1)$.*
3. *If $\beta < 0$ and $\alpha \operatorname{arsinh}(-\beta) > \sqrt{1+\beta^2}$, then $\kappa_h[u](0) > 0$ and $\kappa_h[u]$ has at most one change of sign in $(0,1)$.*
4. *If $\beta < 0$ and $\alpha \operatorname{arsinh}(-\beta) \le \sqrt{1+\beta^2}$, then $\kappa_h[u] > 0$ in $(-1,1)$.*

The proof is obtained by combining Theorems 6.4, 6.7, 6.9 and 6.11.

Numerical calculations give evidence to our feeling that in the case $\alpha\beta > 1$ the hyperbolic curvature may indeed have a change of sign.

It is not only in this respect that the analytical investigations of the present paper benefit a lot from numerical simulations. Numerically calculated solutions help in finding qualitative properties of suitable minimising sequences while, at the same time, analytical insights help to identify suitable initial data such that the numerical gradient flow method indeed converges. In Chapter 7, we explain a C^1-finite element method, which we think is natural in order to deal with Dirichlet boundary conditions. It seems that so far, no C^1-finite element algorithms are available for Willmore surfaces. Like in the analytic part we consider the present paper as a first step also in numerical investigations of Dirichlet problems. We are confident that, basing upon these experiences, we may develop C^1-finite element algorithms also for graphs e.g. over general two-dimensional domains. This will be subject of future research.

We remark that in particular the *Navier boundary value problem* is numerically well investigated, where the position of the surface and its mean curvature are prescribed at the boundary. See e.g. [5, 11] and references therein. In this case the Willmore boundary value problem may be written as a second order system for the position and the mean curvature and continuous finite elements may be used.

Droske and Rumpf [10] proposed a level set formulation for the *Dirichlet problem* and for closed Willmore surfaces and developed a corresponding piecewise linear continuous finite element algorithm.

1.3 Organisation of the paper

In Chapter 2 we recall some basic geometric notions which are relevant for our analysis, and formulate the minimisation problem for the Willmore functional as we shall study it. We explain that the Willmore functional for surfaces of revolution Γ as in (1.3) corresponds to a functional defined on curves in the hyperbolic half plane. We call this second functional the "hyperbolic Willmore functional". This observation was already made by Pinkall and Bryant-Griffiths and used in [2, 3, 20, 4].

In Chapter 3 we prove Theorem 1.1 in the case $\beta \geq 0$ taking advantage of the reformulation of the minimisation problem in the hyperbolic half plane. For $\alpha\beta = 1$ we have a part of a sphere as an explicit solution. We distinguish then the cases $\alpha\beta > 1$ and $\alpha\beta < 1$. In both cases we first prove monotonicity of the energy. The energy is increasing in α for $\alpha\beta > 1$, while it is decreasing in α for $\alpha\beta < 1$. By geometric constructions we prove that we can restrict ourselves to minimising sequences satisfying strong a priori bounds, which are as in Theorem 1.1, Properties 1 and 2 respectively. The key ingredient is to insert suitable parts of hyperbolic geodesic circles. The case $\alpha\beta < 1$ may be viewed as a direct generalisation of the result for $\beta = 0$ from [4]. As for estimates and existence we proceed exactly like there and are quite brief here for this reason. However, we improve it by showing that our solution even satisfies $u' < 0$ in $(0, 1)$. Obtaining a priori estimates in the case $\alpha\beta > 1$ is more involved since the geodesic circle through the boundary points does no longer serve as a comparison function.

In Chapter 4 we prove Theorem 1.1 in the case $\beta < 0$. For $\alpha = \alpha_\beta := \sqrt{1+\beta^2}/\operatorname{arsinh}(-\beta)$ a solution is the catenoid $x \mapsto \cosh(bx)/b$ with $b = \operatorname{arsinh}(-\beta)$. Then, we distinguish the cases $\alpha > \alpha_\beta$ and $\alpha < \alpha_\beta$. Here, the requisite geometric constructions in order to achieve strong enough a priori information on suitably modified minimising sequences do not only involve the hyperbolic geodesics but also the catenoids as minimal surfaces of revolution. These constructions are different not only according to the cases $\alpha > \alpha_\beta$ and $\alpha < \alpha_\beta$, but depend also on whether $-\beta \geq \alpha$ or $-\beta < \alpha$ and whether $\alpha \geq \alpha^*$ or $\alpha < \alpha^*$. The parameter $\alpha^* = \min\{\cosh(b)/b : b \in (0, \infty)\}$ refers to the smallest boundary height where for some boundary angle one may have a catenoid as solution. If $|\beta|$ becomes large and α small it turns out to be somehow delicate to prevent minimising sequences from getting too close to 0 and to obtain bounds from below. Surprisingly, the case where $\alpha > \alpha_\beta$ and $-\beta < \alpha$ is special, because here we can prevent a possible loss of compactness only by further restricting the class of admissible functions.

In Chapter 5 we study the behaviour of minimisers for $\alpha \searrow 0$. We prove that our minimisers converge locally uniformly in $(-1, 1)$ to the sphere. In Chapter 6 we prove bounds on the Willmore energy and we study the sign of the hyperbolic curvature of the constructed solutions.

Chapter 7 gives a description of a C^1-finite element algorithm for the underlying Willmore gradient flow. Moreover, numerical studies are performed, and we provide a series of pictures illustrating typical shapes of solutions within different parameter regimes.

2 Geometric background

2.1 Surfaces of revolution

We consider any function $u \in C^4([-1,1],(0,\infty))$. Rotating the curve $(x,u(x)) \subset \mathbb{R}^2$ about the x-axis generates a *surface of revolution* $\Gamma \subset \mathbb{R}^3$ which can be parametrised by

$$\Gamma\,:\,f(x,\varphi)=\big(x,u(x)\cos\varphi,u(x)\sin\varphi\big)\in\mathbb{R}^3\,,\quad x\in[-1,1],\ \varphi\in[0,2\pi).$$

The term "surface" always refers to the mapping f as well as to the set Γ. The condition $u>0$ implies that f is embedded in $\mathbb{R}^3$ and in particular immersed.

Let κ_1 and κ_2 denote the principal curvatures of the surface $\Gamma \subset \mathbb{R}^3$, that is $\kappa_1 = -u''(x)(1+u'(x)^2)^{-\frac{3}{2}}$ and $\kappa_2 = (u(x)\sqrt{1+u'(x)^2})^{-1}$. Its *mean curvature* H and *Gaussian curvature* K are

$$\begin{aligned} H &:= \frac{\kappa_1+\kappa_2}{2} = -\frac{u''(x)}{2(1+u'(x)^2)^{3/2}}+\frac{1}{2u(x)\sqrt{1+u'(x)^2}} = \frac{1}{2u(x)u'(x)}\left(\frac{u(x)}{\sqrt{1+u'(x)^2}}\right)',\\ K &:= \kappa_1\kappa_2 = -\frac{u''(x)}{u(1+u'(x)^2)^2}\,. \end{aligned}$$

The *Willmore energy* of Γ defined in (1.1) is the integral over the surface of the mean curvature squared. In particular, written in terms of the function u it has the form

$$\mathcal{W}(\Gamma)=\frac{\pi}{2}\int_{-1}^{1}\left(\frac{u''(x)}{(1+u'(x)^2)^{3/2}}-\frac{1}{u(x)\sqrt{1+u'(x)^2}}\right)^2 u(x)\sqrt{1+u'(x)^2}\,dx. \tag{2.1}$$

2.2 Surfaces of revolution as elastic curves in the hyperbolic half plane

Following [2, 3], the construction of axially symmetric critical points Γ of the Willmore functional can be transformed to finding *elastic curves* in the upper half-plane $\mathbb{R}^2_+ := \{(x,y)\in\mathbb{R}^2\,:\,y>0\}$ equipped with the hyperbolic metric $ds_h^2 := \frac{1}{y^2}\,(dx^2+dy^2)$. Geodesics are circular arcs centered on the x-axis and lines parallel to the y-axis; the first will play a crucial role in this work.

Let $s\mapsto\gamma(s)=(\gamma_1(s),\gamma_2(s))$, where we do not raise the indices, be a curve in $\mathbb{R}^2_+$ parametrised with respect to its arc length, i.e.

$$1\equiv\frac{\gamma_1'(s)^2+\gamma_2'(s)^2}{\gamma_2(s)^2}.$$

Then, its curvature is given by

$$\kappa_h(s)=-\frac{\gamma_2(s)^2}{\gamma_2'(s)}\frac{d}{ds}\left(\frac{\gamma_1'(s)}{\gamma_2(s)^2}\right)=\frac{\gamma_2(s)^2}{\gamma_1'(s)}\left(\frac{1}{\gamma_2(s)}+\frac{d}{ds}\left(\frac{\gamma_2'(s)}{\gamma_2(s)^2}\right)\right). \tag{2.2}$$

For graphs $[-1,1]\ni x\mapsto(x,u(x))\in\mathbb{R}^2_+$, formula (2.2) yields

$$\kappa_h[u](x)=-\frac{u(x)^2}{u'(x)}\frac{d}{dx}\left(\frac{1}{u(x)\sqrt{1+u'(x)^2}}\right)=\frac{u(x)u''(x)}{(1+u'(x)^2)^{3/2}}+\frac{1}{\sqrt{1+u'(x)^2}}. \tag{2.3}$$

Using identity (2.3), we compute for the squared hyperbolic curvature times the hyperbolic line element:

$$\begin{aligned}
\kappa_h[u]^2 \frac{\sqrt{1+u'^2}}{u} &= \left\{ \frac{u''}{(1+u'^2)^{3/2}} + \frac{1}{u\sqrt{1+u'^2}} \right\}^2 u\sqrt{1+u'^2} \\
&= \left\{ \frac{u''}{(1+u'^2)^{3/2}} - \frac{1}{u\sqrt{1+u'^2}} \right\}^2 u\sqrt{1+u'^2} + 4\,\frac{u''}{(1+u'^2)^{\frac{3}{2}}} \\
&= 4H^2 u\sqrt{1+u'^2} + 4\,\frac{u''}{(1+u'^2)^{\frac{3}{2}}}.
\end{aligned}$$

We define the *hyperbolic Willmore energy* as the elastic energy of the graph of u in the hyperbolic half plane and compare it with the original Willmore functional $\mathcal{W}(\Gamma)$ defined in (2.1).

$$\mathcal{W}_h(u) := \int_\gamma \kappa_h[u]^2\, ds_h[u] := \int_{-1}^{1} \kappa_h[u]^2 \frac{\sqrt{1+u'^2}}{u}\, dx = \frac{2}{\pi}\,\mathcal{W}(\Gamma) + 4\int_{-1}^{1} \frac{u''}{(1+u'^2)^{3/2}}\, dx, \tag{2.4}$$

where Γ is the surface of revolution obtained by rotating the graph of u.

Lemma 2.1 (Duality of $\mathcal{W}_h(u)$ and $\mathcal{W}(\Gamma)$)**.** *The hyperbolic energy $\mathcal{W}_h(u)$ of a curve $u \in \mathbb{R}^2_+$ and the Willmore energy of the corresponding surface of revolution $\Gamma \subset \mathbb{R}^3$ satisfy*

$$\mathcal{W}_h(u) = \frac{2}{\pi}\,\mathcal{W}(\Gamma) + 4\left[\frac{u'(x)}{\sqrt{1+u'(x)^2}}\right]_{-1}^{1}.$$

This observation goes back to Pinkall (mentioned e.g. in [14]) and Bryant-Griffiths [2, 3], see also [19, 20]. The present derivation is adapted from [4, Section 2.2].

In proving Theorem 1.1, we benefit a lot from this duality between the Willmore functional and the hyperbolic Willmore energy. We do not only take technical advantage from this result, but we think that switching between both functionals helps to a good extent in understanding underlying geometric features.

Concerning the Euler-Lagrange equation for critical points of the hyperbolic Willmore functional $\mathcal{W}_h$ one has:

Lemma 2.2. *Assume that $u \in C^4([-1,1],(0,\infty))$ is such that for all $\varphi \in C_0^\infty([-1,1],(0,\infty))$ one has that $0 = \frac{d}{dt}\mathcal{W}_h(u+t\varphi)|_{t=0}$. Then, u satisfies the following Euler-Lagrange equation*

$$\frac{u(x)}{\sqrt{1+u'(x)^2}}\frac{d}{dx}\left(\frac{u(x)}{\sqrt{1+u'(x)^2}}\kappa_h'(x)\right) - \kappa_h(x) + \frac{1}{2}\kappa_h(x)^3 = 0, \qquad x \in (-1,1), \tag{2.5}$$

with $\kappa_h = \kappa_h[u]$ as defined in (2.3).

When parametrised by the hyperbolic arc length s, equation (2.5) takes the simple form $\frac{d^2}{ds^2}\kappa_h(s) - \kappa_h(s) + \frac{1}{2}\kappa_h(s)^3 = 0$. This equation was discussed in detail in [19] and curvatures of solutions were classified in terms of elliptic functions of the hyperbolic arc length s. However, we do not see any possibility to solve directly and explicitly our Willmore boundary value problem (1.4) basing upon this classification.

2.3 Statement of the Willmore problem

The Willmore boundary value problem (1.4) will be solved by minimising the hyperbolic Willmore functional within the following class of functions:

Definition 2.3. *For $\alpha > 0$ and $\beta \in \mathbb{R}$ we introduce the function space*

$$N_{\alpha,\beta} := \left\{u \in C^{1,1}([-1,1],(0,\infty)) \,:\, u \text{ positive, symmetric, } u(1) = \alpha \text{ and } u'(-1) = \beta\right\} \tag{2.6}$$

as well as

$$M_{\alpha,\beta} := \inf\left\{\mathcal{W}_h(u) \,:\, u \in N_{\alpha,\beta}\right\}. \tag{2.7}$$

Lemma 2.1 gives that

$$\mathcal{W}(\Gamma) = \frac{\pi}{2}\,\mathcal{W}_h(u) + 4\pi\frac{\beta}{\sqrt{1+\beta^2}}$$

for the surface Γ of revolution generated by $u \in N_{\alpha,\beta}$. Since we are working with Dirichlet boundary conditions we may switch between the two functionals depending on which one is more convenient.

In the following sections we will prove existence of solutions $u_{\alpha,\beta} \in N_{\alpha,\beta} \cap C^\infty([-1,1],\mathbb{R})$ such that $\mathcal{W}_h(u_{\alpha,\beta}) = M_{\alpha,\beta}$. Only in the case of parameters treated in Subsection 4.2.3, $N_{\alpha,\beta}$ has for technical reasons to be replaced by a smaller set of admissible functions. The axially symmetric surface $\Gamma_{\alpha,\beta}$ which is generated by $u_{\alpha,\beta}$ is solution of the Willmore boundary value problem (1.4). See [8, Lemma A.1] for an elementary calculation of the Euler-Lagrange equation in this particular setting. For a general survey on the Willmore functional, corresponding Euler-Lagrange equations and natural boundary conditions we refer to the survey article by Nitsche [22], cf. also [28, p. 56]. The Euler-Lagrange equation for the Willmore functional in nonparametric form was already discussed by Poisson [24, p. 224].

Remark 2.4. *The Willmore energy is invariant under rescaling. I.e. if u is a positive function in $C^{1,1}([-r,r],(0,\infty))$ for some $r > 0$, then the function $v \in C^{1,1}([-1,1],(0,\infty))$ defined by $v(x) = u(rx)/r$ has the same hyperbolic Willmore energy as u, that is,*

$$\mathcal{W}_h(v) = \int_{-1}^{1} \kappa_h^2[v]\,ds_h[v] = \int_{-r}^{r} \kappa_h^2[u]\,ds_h[u].$$

Here, $\kappa_h[u]$ is the hyperbolic curvature of u as defined in (2.3) and $\mathcal{W}_h(v)$ is the hyperbolic Willmore energy of v as defined in (2.4).

3 Existence result: The case $\beta \geq 0$

In this section we consider $\beta \geq 0$ and keep it fixed, while α varies in the positive real numbers.

For the value of α such that $\alpha\beta = 1$ we have an explicit solution of (1.4). This is the arc of the circle with centre at the origin and going through the point $(1,\alpha)$. This solution is in particular a geodesic curve in the hyperbolic half plane. It marks the point where there is a change in the behaviour of the energy. For $\alpha\beta > 1$ the energy $M_{\alpha,\beta}$, defined in (2.7), is monotonically increasing in α, while for $\alpha\beta < 1$ it is monotonically decreasing in α.

Minimising sequences are suitably modified by means of parts of geodesic circles in order to achieve strong enough a priori estimates ensuring compactness. In this respect the case $\alpha\beta > 1$ is more involved than the case $\alpha\beta < 1$, because here there is no canonical comparison function from above. However, one can pass to minimising sequences where the derivative is maximal in $x = -1$. The case $\alpha\beta < 1$ is quite similar to and contains the main result Theorem 1.1 from the previous work [4] as a special case. However, this simplicity is due to referring to its main geometric construction. Here, a geodesic circle provides an obvious upper bound. Moreover, we prove an extra property of the solution u constructed there, namely that $u'(x) < 0$ on $(0,1)$.

3.1 The case $\alpha\beta = 1$: The circle

Here, we have an explicit solution.

Lemma 3.1. *For each $\alpha > 0$ and β such that $\alpha\beta = 1$, the part of the sphere $\Gamma \subset \mathbb{R}^3$ generated as a surface of revolution by the function $u(x) = \sqrt{1+\alpha^2 - x^2}$, $x \in [-1,1]$ solves the Dirichlet problem* (1.4)*.*

Moreover, the corresponding surface of revolution is the unique minimiser of the Willmore functional (1.1) *among all axially symmetric surfaces generated by graphs of symmetric functions in $C^{1,1}([-1,1],(0,\infty))$ such that $v(\pm 1) = \alpha$ and $v'(1) = -\beta$.*

Proof. Since $\kappa_h[u] \equiv 0$ in $[-1,1]$, the claim follows from Lemma 2.1 and the definition of the hyperbolic Willmore functional in (2.4). □

3.2 The case $\alpha\beta > 1$

3.2.1 Monotonicity of the optimal energy

In this paragraph we prove that the Willmore energy is increasing in α. The proof is divided into the next four lemmas. First, we prove that it is enough to consider functions in $N_{\alpha,\beta}$ which are decreasing in $[0,1]$. The proof will refer to a main result of the previous work [4, Theorem 3.8], which involves a number of refined geometric constructions. We emphasise that obvious constructions like reflections do *not* yield the following result.

Lemma 3.2. *For each $u \in N_{\alpha,\beta}$ with only finitely many critical points, we find a function $v \in N_{\alpha,\beta}$ having at most as many critical points as u, with lower Willmore energy than u and satisfying $v'(x) \leq 0$ for all $x \in [0,1]$.*

Proof. Assume that u does not have the claimed property. Then, there exists $x_0 \in (0,1)$ such that $[-x_0, x_0]$ is the largest possible symmetric interval with the property $u'(x_0) = 0$ and $u'(x) < 0$ in $(x_0, 1]$. Using a rescaled version of [4, Theorem 3.8] we substitute $u|_{[-x_0,x_0]}$ by a symmetric positive $C^{1,1}$-function defined on the same interval, having the same boundary values as u in x_0, having lower Willmore energy than $u|_{[-x_0,x_0]}$, having at most as many critical points as $u|_{[-x_0,x_0]}$ and decreasing in $[0,x_0]$. The so obtained function v is element of $N_{\alpha,\beta}$, it has at most as many critical points as u, $\mathcal{W}_h(v) \leq \mathcal{W}_h(u)$ and $v'(x) \leq 0$ in $[0,1]$. □

In the proof we need only that $\beta > 0$. Notice further that one could substitute $u|_{[-x_0,x_0]}$ with an appropriately rescaled solution of the Willmore problem with $\beta = 0$ and height $u(x_0)/x_0$ as constructed in [4, Theorem 1.1]. This statement, however, does not give control of the number of critical points. With arguments introduced below we shall see – a posteriori – that we could indeed achieve $u' < 0$ on $(0, x_0)$.

In the next lemma, we construct for any $u \in N_{\alpha,\beta}$ which is decreasing in $[0,1]$ a function with the same boundary values having lower Willmore energy than u and being defined in a larger interval.

Lemma 3.3. *Assume that $u \in N_{\alpha,\beta}$ has only finitely many critical points and satisfies $u'(x) \leq 0$ for all $x \in [0,1]$. Then, for each $\varrho \in [1, \alpha\beta)$, there exists a positive and symmetric function $u_\varrho \in C^{1,1}([-\varrho,\varrho],(0,\infty))$ such that $u_\varrho(\varrho) = \alpha$, $u_\varrho'(\varrho) = -\beta$, $u_\varrho'(x) \leq 0$ for all $x \in [0,\varrho]$, u_ϱ has at most as many critical points as u, and, furthermore, one has*

$$\int_{-\varrho}^{\varrho} \kappa_h[u_\varrho]^2 \, ds_h[u_\varrho] \leq \mathcal{W}_h(u).$$

Proof. The construction is similar to the one of [4, Lemma 3.3]. The situation there differs from the present one in the *non-vanishing* boundary conditions for u'. There we decrease the energy by shortening the interval, while here it is elongated.

Let $r \in (0,1)$ be a parameter. The (euclidian) normal to the graph of u in $(r, u(r))$ has direction $(-u'(r), 1)$. The straight line generated by this normal intersects the x-axis left of r, since u is decreasing. We take this intersection point $(c(r), 0)$ as centre for a geodesic circular arc, where the radius is chosen such that this arc is tangential to the graph of u in $(r, u(r))$. In particular, the radius is given by the distance between $(c(r), 0)$ and $(r, u(r))$. We build a new symmetric function with smaller hyperbolic curvature integral as follows: On $[c(r), r]$ we take this geodesic arc, which has horizontal tangent in $c(r)$, while on $[r, 1]$ we take u. By construction, this function is $C^{1,1}([c(r), 1], (0,\infty))$ and decreasing. We shift it such that $c(r)$ is moved to 0, and extend this to an even function, which is again $C^{1,1}$, now on a suitable interval $[-\ell(r), \ell(r)]$, with $\ell(r) = 1 - c(r)$ and $c(r) = r + u(r)u'(r)$. This new function has the same boundary values as u, at most as many critical points as u, and, by construction, a smaller curvature integral. Our construction yields the claim since $r \mapsto \ell(r)$ is continuous and such that $\lim_{r\searrow 0} \ell(r) = 1$ and $\lim_{r\nearrow 1} \ell(r) = \alpha\beta$. $\square$

Remark 3.4. *Notice that, by concavity of the geodesic circles, $u_\varrho'(x) \geq -\gamma$ in $[0, \varrho]$ if $u'(x) \geq -\gamma$ in $[0,1]$.*

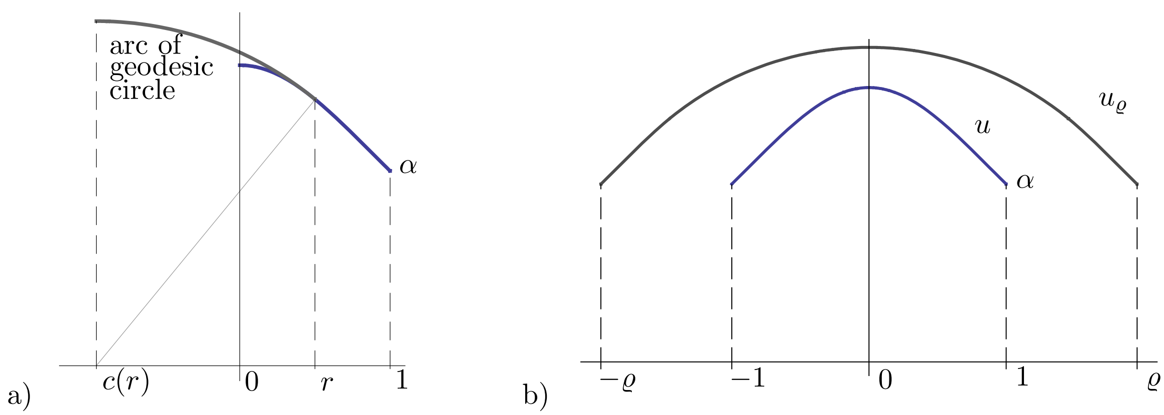


Figure 2: Proof of Lemma 3.3.

By Lemma 3.2, we can remove the assumption that $u'(x) \leq 0$ in $[0,1]$ from Lemma 3.3.

Lemma 3.5. *Assume that $u \in N_{\alpha,\beta}$ has only finitely many critical points. Then, for each $\varrho \in [1, \alpha\beta)$, there exist a positive and symmetric function $u_\varrho \in C^{1,1}([-\varrho, \varrho], (0,\infty))$ such that $u_\varrho(\varrho) = \alpha$, $u_\varrho'(\varrho) = -\beta$, $u_\varrho'(x) \leq 0$ for all $x \in [0, \varrho]$, u_ϱ has at most as many critical points as u, and, furthermore, it holds that*

$$\int_{-\varrho}^{\varrho} \kappa_h[u_\varrho]^2 \, ds_h[u_\varrho] \leq \mathcal{W}_h(u).$$

Proof. By Lemma 3.2 there exists v in $N_{\alpha,\beta}$ having at most as many critical points as u, with lower Willmore energy than u and satisfying $v'(x) \leq 0$ in $[0,1]$. The claim follows from Lemma 3.3 applied to v. $\square$

By rescaling we obtain:

Lemma 3.6. *For each $u \in N_{\alpha,\beta}$ having only finitely many critical points and for each $\gamma \in [\beta^{-1}, \alpha]$ there exists a symmetric function $v \in C^{1,1}([-1,1], (0,\infty))$ having at most as many critical points as u and satisfying: $v(\pm 1) = \gamma$, $v'(1) = -\beta$, $v'(x) \leq 0$ in $[0,1]$ and $\mathcal{W}_h(v) \leq \mathcal{W}_h(u)$.*

Proof. If $\gamma \in (\beta^{-1}, \alpha]$ the claim follows from Lemma 3.5 by rescaling. If $\gamma = \beta^{-1}$ we choose $v(x) := \sqrt{1+\gamma^2 - x^2}$. □

The previous lemma gives that the optimal Willmore energy $M_{\alpha,\beta}$, defined in (2.7), is increasing in α.

Proposition 3.7. *We have $M_{\widetilde{\alpha},\beta} \geq M_{\alpha,\beta}$ for all α, $\widetilde{\alpha}$ such that $\widetilde{\alpha} \geq \alpha \geq \frac{1}{\beta}$.*

Proof. Since polynomials are dense in $H^2(-1,1)$, a minimising sequence for $M_{\tilde{\alpha},\beta}$ may be chosen in $N_{\tilde{\alpha},\beta}$, which consists of symmetric and positive polynomials. Lemma 3.6 proves the statement. □

In Proposition 6.2 we prove that even $\lim_{\alpha\to\infty} M_{\alpha,\beta} = +\infty$.

3.2.2 Properties of minimising sequences

In the next two lemmas we introduce geometric constructions and show that on minimising sequences, by possibly inserting parts of geodesic circles and rescaling, we may assume that $0 \geq u'(x) \geq -\beta$ and $x + u(x)u'(x) \leq 0$ for $x \in [0,1]$.

We first employ the elongation procedure of Lemma 3.3 and rescaling to achieve the derivative bounds.

Lemma 3.8. *For each $u \in N_{\alpha,\beta}$ with only finitely many critical points there exists $v \in N_{\alpha,\beta}$ having at most as many critical points as u, with lower Willmore energy than u and such that*

$$-\beta \leq v'(x) \leq 0 \text{ for all } x \in [0,1].$$

Proof. By Lemma 3.2 there exists $w \in N_{\alpha,\beta}$ having at most as many critical points as u with lower Willmore energy than u and such that $w'(x) \leq 0$ in $[0,1]$. If moreover, $w'(x) \geq -\beta$ the claim follows with $v = w$. Otherwise there exists a first $x_1 \in (0,1)$ with $w'(x_1) = -\beta$ such that in particular $w'(x) \geq -\beta$ on $[0,x_1]$. By using a scaled version of Lemma 3.3 we dilate the function $w|_{[-x_1,x_1]}$ by inserting an arc of a geodesic circle. For each $\varrho \in (x_1, w(x_1)\beta)$ there exists $w_\varrho \in C^{1,1}([-\varrho,\varrho],(0,\infty))$ with lower Willmore energy than $w|_{[-x_1,x_1]}$, with at most as many critical points as $w|_{[-x_1,x_1]}$ and such that $w_\varrho(\pm\varrho) = w(x_1)$ and $w_\varrho'(\varrho) = -\beta$. Notice that by concavity of the geodesic circles $w_\varrho'(x) \geq -\beta$ in $[0,\varrho]$. We choose $\varrho = w(x_1)/\alpha$ and v to be equal to w_ϱ being rescaled to the interval $[-1,1]$. The choice of ϱ is such that we dilate the graph of $w|_{[0,x_1]}$ until we reach the line $y \mapsto \alpha y$. This construction is illustrated in Figure 3. □

We now add the property $x + u(x)u'(x) \leq 0$ for $x \in [0,1]$ to those of the previous lemma by possibly inserting a suitable part of a geodesic circle.

Lemma 3.9. *For each $u \in N_{\alpha,\beta}$ having only finitely many critical points, there exists $v \in N_{\alpha,\beta}$ having at most as many critical points as u, with lower Willmore energy than u and satisfying*

$$0 \geq v'(x) \geq -\beta \text{ and } 0 \geq x + v(x)v'(x) \text{ for all } x \in [0,1].$$

Proof. By Lemma 3.8 there exists $w \in N_{\alpha,\beta}$ with lower Willmore energy than u, having at most as many critical points as u and such that $-\beta \leq w'(x) \leq 0$ in $[0,1]$. We consider the function φ defined in $[0,1]$ by

$$\varphi(x) := x + w(x)w'(x).$$

Note that $\varphi(0) = 0$ and $\varphi(1) < 0$. If $\varphi \leq 0$ in $[0,1]$ then the claim follows with $w = v$. Otherwise, there exists $x_0 \in (0,1)$ such that $\varphi(x_0) = 0$ and $\varphi \not\leq 0$ in a left neighbourhood of x_0. Then, the normal line at $(x_0, w(x_0))$ to the graph of w passes through the origin and we can substitute w over

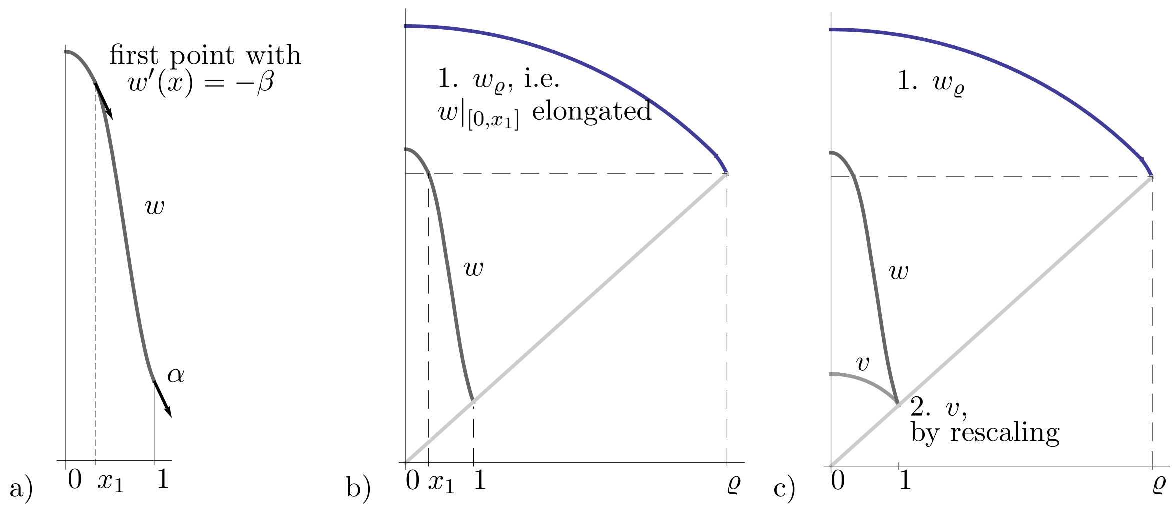


Figure 3: Proof of Lemma 3.8.

$[-x_0, x_0]$ by a geodesic circular arc lowering the hyperbolic Willmore energy. This new function yields the claim. Notice that with this construction, due to the concavity of circles, the property $-\beta \le w' \le 0$ is preserved and that we do not add critical points. $\square$

The following proposition summarises how by making use of Lemmas 3.8 and 3.9 we may pass to minimising sequences satisfying suitable a priori bounds.

Proposition 3.10. *Let $(u_k)_{k\in\mathbb{N}}$ be a minimising sequence for $M_{\alpha,\beta}$ in $N_{\alpha,\beta}$ such that each u_k has only finitely many critical points. Then, there exists a minimising sequence $(v_k)_{k\in\mathbb{N}} \subset N_{\alpha,\beta}$ such that for all $k \in \mathbb{N}$ it holds: v_k has at most as many critical points as u_k, $\mathcal{W}_h(v_k) \le \mathcal{W}_h(u_k)$,*

$$\begin{aligned} & 0 \ge x + v_k(x)v_k'(x) \text{ and } -\beta \le v_k'(x) \le 0 \text{ for all } x \in [0,1] \\ \text{and} \quad & \sqrt{1+\alpha^2-x^2} \le v_k(x) \le \sqrt{(\alpha+\beta)^2 - x^2} \text{ for all } x \in [-1,1]. \end{aligned} \tag{3.1}$$

3.2.3 Proof of the existence theorem

The proof of the following theorem follows the lines of the proof of [4, Theorem 3.9].

Theorem 3.11 (Existence and regularity)**.** *For each $\alpha > 0$ and β such that $\alpha\beta > 1$ there exists a function $u \in C^\infty([-1,1],(0,\infty))$ such that the corresponding surface of revolution $\Gamma \subset \mathbb{R}^3$ solves the Dirichlet problem* (1.4)*. This solution is positive and symmetric, and it has the following properties:*

$$\begin{aligned} & -\beta \le u'(x) < 0 \text{ and } x + u(x)u'(x) < 0 \text{ in } (0,1] \\ \text{as well as} \quad & \sqrt{1+\alpha^2-x^2} \le u(x) \le \sqrt{(\alpha+\beta)^2-x^2} \quad \text{in } [-1,1]. \end{aligned} \tag{3.2}$$

Proof. Let $(u_k)_{k\in\mathbb{N}} \in N_{\alpha,\beta}$ be a minimising sequence for $M_{\alpha,\beta}$ such that $\mathcal{W}_h(u_k) \le M_{\alpha,\beta} + 1$ for all $k \in \mathbb{N}$. By the density of polynomials in $H^2(-1,1)$ and Proposition 3.10 we may assume that each element u_k of the minimising sequence satisfies (3.1). We can estimate the Willmore energy from below as follows:

$$\begin{aligned}\mathcal{W}_h(u_k) &= \int_{-1}^{1} \frac{u_k''(x)^2 u_k(x)}{(1+u_k'(x)^2)^{\frac{5}{2}}}\,dx + 2\int_{-1}^{1} \frac{u_k''(x)}{(1+u_k'(x)^2)^{\frac{3}{2}}}\,dx + \int_{-1}^{1} \frac{1}{u_k(x)\sqrt{1+u_k'(x)^2}}\,dx \\ &\geq \frac{\alpha}{(1+\beta^2)^{\frac{5}{2}}} \int_{-1}^{1} u_k''(x)^2\,dx - \frac{4\beta}{\sqrt{1+\beta^2}}\,.\end{aligned}$$

Thus, $(u_k)_{k\in\mathbb{N}}$ is uniformly bounded in $H^2(-1,1)$, and, eventually, after passing to a subsequence, Rellich's embedding theorem ensures the existence of $u \in H^2(-1,1)$ such that

$$u_k \rightharpoonup u \quad \text{in } H^2(-1,1) \qquad \text{and} \qquad u_k \to u \in C^1([-1,1],(0,\infty)).$$

Making use of the strong convergence in $C^1([-1,1])$ and the weak convergence in $H^2(-1,1)$ of the sequence $(u_k)_{k\in\mathbb{N}}$, we have

$$\begin{aligned}M_{\alpha,\beta} + o(1) &= \mathcal{W}_h(u_k) = \int_{-1}^{1} \frac{u_k''^2 u}{(1+u'^2)^{\frac{5}{2}}}\,dx + \int_{-1}^{1} \frac{1}{u\sqrt{1+u'^2}}\,dx - \frac{4\beta}{\sqrt{1+\beta^2}} + o(1) \\ &\geq \int_{-1}^{1} \frac{u''^2 u}{(1+u'^2)^{\frac{5}{2}}}\,dx + \int_{-1}^{1} \frac{1}{u\sqrt{1+u'^2}}\,dx - \frac{4\beta}{\sqrt{1+\beta^2}} + o(1) = \mathcal{W}_h(u) + o(1).\end{aligned}$$

Thus, u minimises $\mathcal{W}_h$ in the class of all positive and symmetric $H^2(-1,1)$-functions v satisfying $v(\pm 1) = \alpha$, $v'(+1) = -\beta$, and, therefore, u weakly solves (2.5). Moreover, since the elements of the minimising sequence satisfy (3.1) then u satisfies $x + u(x)u'(x) \leq 0$ and $-\beta \leq u'(x) \leq 0$ in $(0,1]$. From the first inequality it follows that $u' < 0$ in $(0,1]$.

The proof of smoothness of the solution is exactly as in [4, Theorem 3.9, Step 2].

Finally we show that u satisfies $x + u(x)u'(x) < 0$ in $(0,1]$. Indeed, if $x_0 + u(x_0)u'(x_0) = 0$ for some $x_0 \in (0,1]$ then reasoning as in Lemma 3.9 and using that $M_{\alpha,\beta} = \mathcal{W}_h(u)$, we see that u equals an arc of a geodesic circle in $[-x_0, x_0]$. But u being a solution of (2.5) implies by uniqueness of the initial value problem that u is a geodesic circular arc on $[-1,1]$. But such an arc cannot satisfy the boundary conditions when $\alpha\beta > 1$. □

In Lemma 6.3 we prove further that u' is a decreasing function in $[0,1]$.

Proposition 3.12. *Let $\alpha\beta > 1$. Then, $M_{\widetilde{\alpha},\beta} > M_{\alpha,\beta}$ for all $\widetilde{\alpha}$ such that $\widetilde{\alpha} > \alpha$.*

Proof. Let $u_{\widetilde{\alpha}}$ be a solution of (1.4) for boundary values $\widetilde{\alpha}$ and β as constructed in Theorem 3.11. By proceeding as in Lemma 3.5, i.e. inserting an appropriately chosen circular arc, we get a function $v \in N_{\alpha,\beta}$ such that $\mathcal{W}_h(v) \leq \mathcal{W}_h(u_{\widetilde{\alpha}})$. We prove that this inequality is in fact strict. As we have seen in the proof of Theorem 3.11, $u_{\widetilde{\alpha}}$ cannot be equal to an arc of a geodesic circle in an interval. Hence, by introducing a piece of a geodesic circle the energy strictly decreases. The claim follows since $\mathcal{W}_h(v) \geq M_{\alpha,\beta}$. Notice that, for the same reason, also this last inequality is strict. □

3.3 The case $\alpha\beta < 1$

The method of proof is related to that for the case $\alpha\beta > 1$ but much simpler. The results are, in some sense, dual. For the monotonicity of the energy in the case $\alpha\beta > 1$, we have constructed a function with lower Willmore energy and defined in a bigger interval. Now, with the same construction, the function is defined in a shorter interval. Moreover, we show that in this case we can confine ourselves to functions satisfying $x + u(x)u'(x) \geq 0$ in $(0, 1]$. A lower bound for the derivative follows directly from this inequality. We proceed quite similarly as in the case $\beta = 0$, which was discussed in the previous paper [4] and which is included here.

3.3.1 Monotonicity of the optimal energy

In this case the Willmore energy is decreasing in α. The proof is as in paragraph 3.2.1. For the sake of conciseness we formulate only the results.

Lemma 3.13. *Assume that $u \in N_{\alpha,\beta}$ has only finitely many critical points. Then, for each $\varrho \in [\alpha\beta, 1]$, there exist a positive and symmetric function $u_\varrho \in C^{1,1}([-\varrho, \varrho], (0, \infty))$ such that $u_\varrho(\varrho) = \alpha$, $u'_\varrho(\varrho) = -\beta$, $u'_\varrho(x) \leq 0$ for all $x \in [0, \varrho]$, u_ϱ has at most as many critical points as u, and, furthermore, one has*

$$\int_{-\varrho}^{\varrho} \kappa_h[u_\varrho]^2 \, ds_h[u_\varrho] \leq \mathcal{W}_h(u).$$

In the next two results, for $\beta = 0$ we interpret $1/\beta$ as ∞.

Lemma 3.14. *For each $u \in N_{\alpha,\beta}$ having only finitely many critical points and for each $\gamma \in [\alpha, \beta^{-1}]$ there exists a symmetric function $v \in C^{1,1}([-1, 1], (0, \infty))$ having at most as many critical points as u and satisfying: $v(\pm 1) = \gamma$, $v'(1) = -\beta$, $v'(x) \leq 0$ in $[0, 1]$ and $\mathcal{W}_h(v) \leq \mathcal{W}_h(u)$.*

Proposition 3.15. *It holds that $M_{\widetilde{\alpha},\beta} \geq M_{\alpha,\beta}$ for all $\alpha, \widetilde{\alpha}$ such that $0 < \widetilde{\alpha} \leq \alpha \leq \frac{1}{\beta}$.*

3.3.2 Properties of minimising sequences

In the next lemma we show that we can restrict ourselves to functions which are decreasing in $(0, 1]$ and satisfy $x + u(x)u'(x) \geq 0$ in $(0, 1]$. A priori bounds follow directly from these observations.

Lemma 3.16. *For each $u \in N_{\alpha,\beta}$ with only finitely many critical points there exists $v \in N_{\alpha,\beta}$ with lower Willmore energy than u, having at most as many critical points as u and such that*

$$0 \leq x + v(x)v'(x) \text{ and } v'(x) \leq 0 \text{ for all } x \in [0, 1].$$

Proof. By Lemma 3.2 and the following remark there exists $w \in N_{\alpha,\beta}$ with lower Willmore energy than u, having at most as many critical points as u and such that $w'(x) \leq 0$ in $[0, 1]$. Let us consider the function φ defined in $[0, 1]$ by $\varphi(x) := x + w(x)w'(x)$. Note that $\varphi(0) = 0$ and $\varphi(1) > 0$. If $\varphi \geq 0$ in $[0, 1]$ then the claim follows with $w = v$. Otherwise, there exists $x_0 \in (0, 1)$ such that $\varphi(x_0) = 0$ and $\varphi \geq 0$ in $(x_0, 1]$. Then, the normal line at $(x_0, w(x_0))$ to the graph of w passes through the origin and we can substitute w over $[-x_0, x_0]$ by a geodesic circular arc lowering the hyperbolic Willmore energy. The new function so obtained yields the claim. With this construction we do not add critical points. $\square$

The following proposition characterises suitably modified minimising sequences.

Proposition 3.17. *Let $(u_k)_{k\in\mathbb{N}}$ be a minimising sequence for $M_{\alpha,\beta}$ in $N_{\alpha,\beta}$ such that each u_k has only finitely many critical points. Then, there exists a minimising sequence $(v_k)_{k\in\mathbb{N}} \subset N_{\alpha,\beta}$ such that for all $k \in \mathbb{N}$: v_k has at most as many critical points as u_k, $\mathcal{W}_h(v_k) \leq \mathcal{W}_h(u_k)$ and satisfying:*

$$\begin{gathered} 0 \leq x + v_k(x)v'_k(x), \; v'_k(x) \leq 0 \text{ and } v'_k(x) \geq -\tfrac{x}{v_k(x)} \geq -\tfrac{x}{\alpha} \text{ for all } x \in [0, 1], \\ \text{and } \; \alpha \leq v_k(x) \leq \sqrt{1 + \alpha^2 - x^2} \text{ for all } x \in [-1, 1]. \end{gathered} \tag{3.3}$$

3.3.3 Proof of the existence theorem

Thanks to Proposition 3.17 we prove now existence of a solution. The following result is a direct generalisation of [4, Theorem 1.1]. Its proof appears to be relatively simple but one should observe that via Lemma 3.2 the main constructions of [4, Theorem 3.8] are essentially used.

Theorem 3.18 (Existence and regularity)**.** *For each $\alpha > 0$ and each $\beta \geq 0$ such that $\alpha\beta < 1$ there exists a function $u \in C^\infty([-1,1],(0,\infty))$ such that the corresponding surface of revolution $\Gamma \subset \mathbb{R}^3$ solves the Dirichlet problem* (1.4)*. This solution is positive and symmetric, and it has the following properties:*

$$-\frac{x}{\alpha} \leq u'(x) \leq 0 \text{ and } x + u(x)u'(x) > 0 \text{ in } (0,1], \text{ and } \alpha \leq u(x) \leq \sqrt{1+\alpha^2-x^2} \text{ in } [-1,1]. \quad (3.4)$$

Proof. Let $(u_k)_{k\in\mathbb{N}} \in N_{\alpha,\beta}$ be a minimising sequence for $M_{\alpha,\beta}$ such that $\mathcal{W}_h(u_k) \leq M_{\alpha,\beta} + 1$ for all $k \in \mathbb{N}$. By Proposition 3.17 and the density of polynomials in $H^2(-1,1)$ we may assume that each element u_k of the minimising sequence satisfies (3.3). The rest of the proof is on the same line as that of Theorem 3.11. ☐

Proceeding as in the proof of Proposition 3.12, one can show that the energy is strictly decreasing.

Proposition 3.19. *Let $\alpha > 0$, $\beta \geq 0$ and $\alpha\beta < 1$. Then, $M_{\widetilde{\alpha},\beta} > M_{\alpha,\beta}$ for all $\widetilde{\alpha} \in (0,\alpha)$.*

Also in this case, we can prove an additional qualitative information on our solution of (1.4) constructed in Theorem 3.18, namely that $u' < 0$ in $(0,1)$. This property is expected but here, it is slightly more involved to prove it when compared with the dual case $\alpha\beta > 1$. It will prove to be helpful also for the constructions in the case $\beta < 0$.

Lemma 3.20. *Let u be a solution of* (1.4) *minimising the hyperbolic Willmore energy in $N_{\alpha,\beta}$ as constructed in the proof of Theorem 3.18. Then, u satisfies $u' < 0$ in $(0,1)$.*

Proof. We assume by contradiction that there exists $x_0 \in (0,1)$ such that $u'(x_0) = 0$. This zero of u' is isolated because otherwise, by reflection and uniqueness for the initial value problem for (2.5), u were even about x_0. In view of $u' \leq 0$ on $[0,1]$ this would imply that $u'(x) = 0$ for x close to x_0. This, however, is impossible since constants do not solve (2.5).

Then there exist $a, b \in (0,1)$ such that $a < x_0 < b$, $u'(a) = u'(b)$, $u'(x) > u'(a)$ for all $x \in (a,b)$. Finally, by choosing a, b close enough to x_0 and $|u'(a)|$ small enough we may achieve that $(u(b) + u'(b)(a-b))(-u'(b)) \leq a$ which will be used to insert a piece of a solution according to Theorem 3.18 on $[-a,a]$.

We construct a function $v \in N_{\alpha,\beta}$ with lower Willmore energy than u and with non-zero derivative in x_0 as follows. $v|_{[b,1]}$ is equal to $u|_{[b,1]}$. Then $v|_{[a,b)}$ equals the line starting at $(b,u(b))$ with derivative $u'(b)$ and ending at $(a, u(b) + u'(b)(a-b))$. It remains to define v on $[0,a)$. Here v equals a solution of (1.4) in the interval $[-a,a]$ with boundary values $w(\pm a) = v(a)$ and $w'(a) = u'(a)$ obtained by a rescaled version of Theorem 3.18. Here we use that, by construction, $v(a)(-u'(a)) \leq a$. See Figure 4.

It remains to show that v has strictly lower Willmore energy than u. We first compare the energies in $[-a,a]$. Since $v(a) > u(a)$ and $v'(a) = u'(a)$ by a rescaled version of Proposition 3.19 we see that the Willmore energy of $v|_{[-a,a]}$ is strictly lower than the Willmore energy of $u|_{[-a,a]}$.

Now we compare the energies in $[a,b]$. From the definition of v and since $u'(a)=u'(b)$ we have

$$
\begin{aligned}
& 2\int_a^b \kappa_h[u]^2 ds[u] - 2\int_a^b \kappa_h[v]^2 ds[v] \\
= \; & 2\int_a^b \frac{u''^2 u}{(1+u'^2)^{\frac{5}{2}}}\,dx + 2\int_a^b \frac{1}{u\sqrt{1+u'^2}}\,dx + 4\int_a^b \frac{u''}{(1+u'^2)^{\frac{3}{2}}}\,dx - 2\int_a^b \frac{1}{v\sqrt{1+v'^2}}\,dx \\
\geq \; & 2\int_a^b \frac{1}{u\sqrt{1+u'^2}}\,dx - 2\int_a^b \frac{1}{v\sqrt{1+v'^2}}\,dx \geq 0
\end{aligned}
$$

where in the last step we used that $v(x)\geq u(x)$ in $[-1,1]$ and $|v'|\geq|u'|$ in $[a,b]$. Comparing the total Willmore energies we then have $\mathcal{W}_h(u)>\mathcal{W}_h(v)$. A contradiction since u is the minimiser for $M_{\alpha,\beta}$ in $N_{\alpha,\beta}$. □

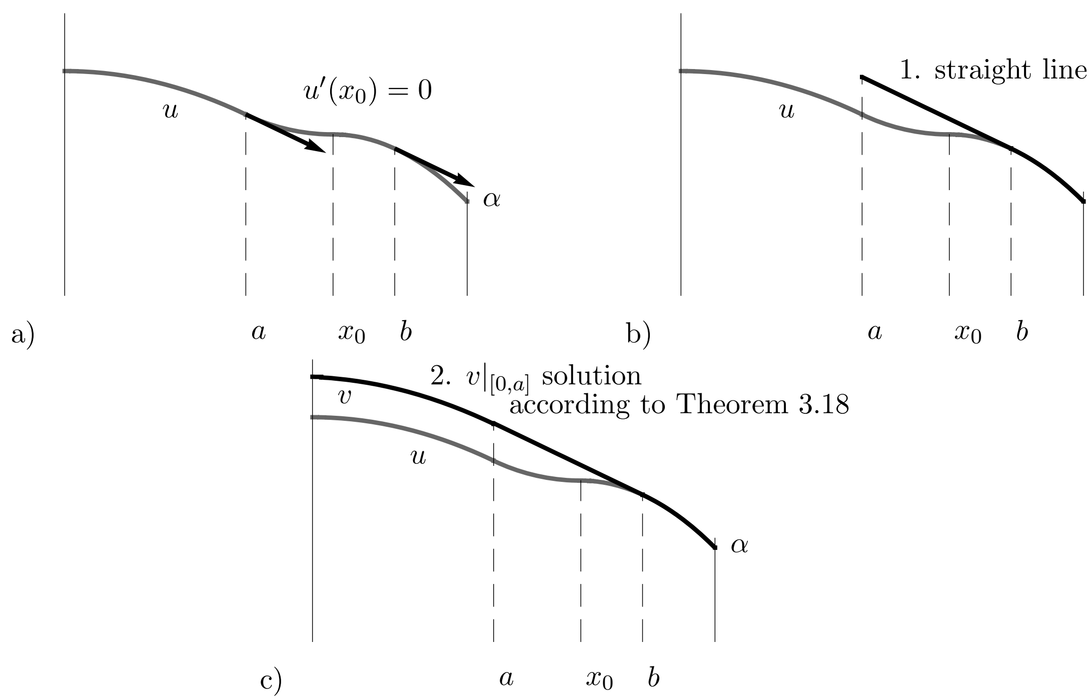


Figure 4: Proof of Lemma 3.20.

4 Existence result: The case $\beta<0$

In this section we consider $\beta<0$ fixed, while α varies in the positive real numbers.

The case $\beta<0$ is quite different from $\beta\geq 0$. In the latter, our constructions were based on inserting parts of geodesic circles. Here, also catenoids will play an important role. Each of these minimal surfaces is generated by the graph of $u(x):=\cosh(bx)/b$, $x\in[-1,1]$, for some $b>0$. They are solutions of (1.4) for particular values of α and β. Given $\beta<0$ we denote

$$\alpha_\beta := \frac{\cosh(b)}{b} \quad \text{with} \quad b=\operatorname{arsinh}(-\beta). \tag{4.1}$$

Notice that $\alpha_\beta \operatorname{arsinh}(-\beta) = \sqrt{1+\beta^2}$. We comment on these particular solutions in some more detail in the next subsection. Then, the cases $\alpha > \alpha_\beta$ and $\alpha < \alpha_\beta$ have to be treated separately. In the first case the energy is increasing for α increasing, while in the second case it is decreasing for α increasing. Moreover, the behaviour of the solution we construct is different in the two cases. If $\alpha > \alpha_\beta$ the solution satisfies $u' > 0$ in $(0, 1]$ while for $\alpha < \alpha_\beta$ a further critical point could in principle appear in $(0, 1)$. An intuition for this is given by looking for a function of the kind $v(x) = \cosh(\lambda(x-d))/\lambda$ choosing λ and d suitably such that v satisfies $v(1) = \alpha$ and $v'(1) = -\beta$. If $\alpha > \alpha_\beta$, then $d < 0$. This tell us that, in some sense, there is not enough space for a catenoid. On the other hand, if $\alpha < \alpha_\beta$, then $d > 0$ so there is too much space for a catenoid. One could think that a further critical point should show up in $(0, 1)$ together with a solution for $\beta = 0$ in the inner part. By Lemma 5.2 this will certainly happen for α close enough to 0. However, we are not able to determine the precise range of $\alpha \in (0, \alpha_\beta)$ where this extra local minimum may be observed. The function $u_{Cl}(x) = 2 - \sqrt{2 - x^2}$ for $x \in [-1, 1]$ (part of the – projected – *Clifford torus*) solves the Willmore equation (1.4) for $\alpha = 1$ and $\beta = -1$ ($\alpha < \alpha_\beta$) and has no critical point in $(0, 1)$.

4.1 The case $\alpha = \alpha_\beta$: The catenoid

We summarise the main properties of the catenoids as explicit minimal surface solutions.

Lemma 4.1. *For $\beta < 0$ and α such that $\alpha = \cosh(b)/b$ with $b = \operatorname{arsinh}(-\beta)$, the part of the catenoid $\Gamma \subset \mathbb{R}^3$ generated by the function $u(x) = \cosh(bx)/b$, $x \in [-1, 1]$, solves the Dirichlet problem* (1.4).

Moreover, the corresponding surface of revolution is the minimiser of the Willmore functional (1.1) *among all axially symmetric surfaces generated by graphs of symmetric positive functions in $C^{1,1}([-1, 1], (0, \infty))$ with $v(\pm 1) = \alpha$ and $v'(1) = -\beta$.*

Proof. Rotating the graph of u around the x-axis generates a minimal surface, i.e. a surface such that $H \equiv 0$. Moreover, by the choice of b the function u satisfies the boundary conditions $u(\pm 1) = \alpha_\beta$ and $u'(1) = -\beta$. For any $v \in N_{\alpha,\beta}$ we have

$$\begin{aligned}
\mathcal{W}_h(v) &= 2\int_0^1 \left(\frac{v''}{(1+v'^2)^{\frac{3}{2}}} - \frac{1}{v(x)\sqrt{1+v'(x)^2}} \right)^2 v(x)\sqrt{1+v'(x)^2}\, dx + 8\int_0^1 \frac{v''}{(1+v'^2)^{\frac{3}{2}}}\, dx \\
&\geq -8\frac{\beta}{\sqrt{1+\beta^2}} = \mathcal{W}_h(u). \qquad (4.2)
\end{aligned}$$

This shows that u minimises $M_{\alpha,\beta}$ and, by Lemma 2.1, that the axially symmetric surface generated by u minimises the Willmore functional among axially symmetric surfaces generated by graphs of symmetric functions satisfying the prescribed boundary conditions. ☐

Remark 4.2. *Notice that given $\beta < 0$, there exist unique associated b and α_β defined as in* (4.1). *When β varies in the negative real numbers, α_β is bounded from below. Indeed, the function $b \mapsto \frac{1}{b}\cosh(b)$ has precisely one minimum at $b^* > 0$ which is the solution of the equation*

$$\cosh(b^*) = b^* \sinh(b^*), \quad b^* = 1.1996786\ldots.$$

The value α^* defined in (1.5) *denotes the minimal value of $(0, \infty) \ni b \mapsto \cosh(b)/b$. For $\alpha < \alpha^*$, there are no minimal surfaces of revolution solving* (1.4). *If $\alpha = \alpha^*$, then $\frac{\cosh(b^* x)}{b^*}$ is a minimal* *surface solution for the boundary datum* $\beta = -\sinh(b^*)$. *In the case* $\alpha > \alpha^*$, *there are two positive real numbers* $b_1(\alpha), b_2(\alpha)$ *such that*

$$b_1(\alpha) < b^* < b_2(\alpha) \quad \text{and} \quad \frac{\cosh(b_1)}{b_1} = \alpha = \frac{\cosh(b_2)}{b_2}. \tag{4.3}$$

Two different minimal surfaces with the same height α *in* 1 *and different boundary slopes correspond to these two values. These two catenoids play an important role in what follows.*

4.2 The case $\alpha > \alpha_\beta$

In this case the height prescribed at the boundary is bigger than the height of the catenoid centered at 0 and having derivative $-\beta$ at $x = 1$. As observed in Remark 4.2, there are two catenoids that in 1 have the height α. These are $\cosh(b_1 x)/b_1$ and $\cosh(b_2 x)/b_2$ with $b_1 = b_1(\alpha)$ and $b_2 = b_2(\alpha)$ defined in (4.3). Since $\alpha = \cosh(b_1)/b_1 = \cosh(b_2)/b_2 > \alpha_\beta = \cosh(b)/b$, it follows that $b_1 < b < b_2$ and $\sinh(b_1) < -\beta = \sinh(b) < \sinh(b_2)$. So, close to $x = 1$, the graph of $u \in N_{\alpha,\beta}$ is between the graphs of the two catenoids (see Figure 5). In the following we use this observation to characterise functions in $N_{\alpha,\beta}$ with low Willmore energy.

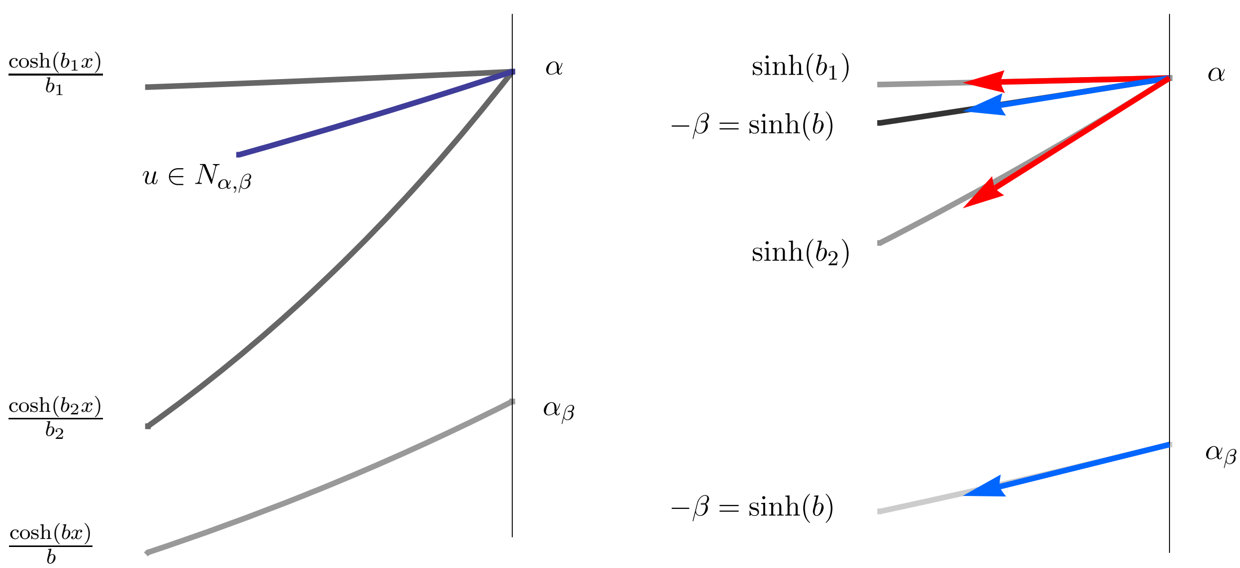


Figure 5: Comparison between $u \in N_{\alpha,\beta}$ and the catenoids $\cosh(b_1 x)/b_1$ and $\cosh(b_2 x)/b_2$.

We explain first how to lower the Willmore energy by inserting $C^{1,1}$-smoothly suitable parts of catenoids. This construction also yields that we may restrict ourselves to functions increasing in $[0, 1]$. To proceed we have to distinguish between $\alpha \leq -\beta$ and $\alpha > -\beta$. The line $y \mapsto \alpha y$ is crucial for rescaling and the different positions of curves in $N_{\alpha,\beta}$ relative to this line close to $x = 1$ require different geometric constructions. If $-\beta \geq \alpha$, these constructions allow for suitably modifying minimising sequences so that strong enough a priori bounds are available. If $-\beta < \alpha$, we need to pass to a smaller class of admissible functions instead of $N_{\alpha,\beta}$ in order to avoid a possible loss of compactness.

4.2.1 First observations

In this subsection we introduce some geometric constructions which lower the Willmore energy and will be used repeatedly in the rest of this section. In the next lemma we formulate a criterion which allows for inserting a piece of a catenoid in a $C^{1,1}$-smooth way. This criterion is dual to the condition $0 = x_0 + v(x_0)v'(x_0)$ which allows for inserting $C^{1,1}$-smoothly a part of a geodesic circle on $[-x_0, x_0]$.

Lemma 4.3. *Fix $a > 0$. Let $f \in C^{1,1}([0,a],(0,+\infty))$ be such that $f'(0) = 0$. Furthermore assume that there is $x_0 \in (0,a)$ such that $f'(x_0) > 0$ and*

$$1 - \frac{1}{\sqrt{1+f'(x_0)^2}} \cosh\left(\frac{\sqrt{1+f'(x_0)^2}}{f(x_0)} x_0\right) = 0. \tag{4.4}$$

Then, the function

$$v(x) := \begin{cases} \frac{1}{\gamma}\cosh(\gamma x) & \text{for } x \in [0,x_0] \\ f(x) & \text{for } x \in [x_0,a] \end{cases} \qquad \text{with } \gamma := \frac{\sqrt{1+f'(x_0)^2}}{f(x_0)}$$

is in $C^{1,1}([0,a],(0,+\infty))$, and it satisfies $v'(0) = 0$.

Proof. It is sufficient to study the behaviour in x_0. We see that

$$\lim_{x \nearrow x_0} v(x) = \frac{f(x_0)}{\sqrt{1+f'(x_0)^2}} \cosh\left(\frac{\sqrt{1+f'(x_0)^2}}{f(x_0)} x_0\right) = f(x_0),$$

using (4.4). For the derivative we find

$$\lim_{x \nearrow x_0} v'(x) = \sinh\left(\frac{\sqrt{1+f'(x_0)^2}}{f(x_0)} x_0\right) = \sqrt{\cosh^2\left(\frac{\sqrt{1+f'(x_0)^2}}{f(x_0)} x_0\right) - 1} = f'(x_0),$$

using (4.4) again and the fact that $f'(x_0) > 0$. □

Remark 4.4. *Notice that, by the convexity of* cosh, *if $f'(x) \le \delta$ for all $x \in [0,a]$ then also $v'(x) \le \delta$ for all $x \in [0,a]$.*

In the case $\beta \ge 0$ we could without loss of generality consider only functions satisfying $x + u(x)u'(x) \ge 0$ (or ≤ 0). In the next lemma we deduce a dual condition in the case $\beta < 0$ and $\alpha > \alpha_\beta$. Here we use that an arc of catenoid gives the lowest Willmore energy when connecting one point with prescribed positive derivative to another with prescribed and bigger positive derivative. As a consequence we see that without loss of generality it is sufficient to consider functions $u \in N_{\alpha,\beta}$ such that $u' > 0$ in $(0,1]$.

Lemma 4.5. *For each $u \in N_{\alpha,\beta}$ there exists $v \in N_{\alpha,\beta}$ such that $\mathcal{W}_h(v) \le \mathcal{W}_h(u)$, $v' > 0$ in $(0,1]$ and v satisfies*

$$1 - \frac{1}{\sqrt{1+v'(x)^2}} \cosh\left(\frac{\sqrt{1+v'(x)^2}}{v(x)} x\right) \ge 0 \quad \text{in } [0,1]. \tag{4.5}$$

Proof. Let $u \in N_{\alpha,\beta}$ be arbitrary. For easy reference we here denote by $g(x)$ the function on the left hand side of inequality (4.5) with v replaced by u. Obviously, $g(0) = 0$. Since $b = \operatorname{arsinh}(-\beta)$, we find in $x = 1$:

$$\begin{aligned} g(1) &= 1 - \frac{1}{\sqrt{1+\beta^2}} \cosh\left(\frac{\sqrt{1+\beta^2}}{\alpha}\right) = 1 - \frac{1}{\cosh(b)} \cosh\left(\frac{\cosh(b)}{\alpha}\right) \\ &= \frac{1}{\alpha_\beta}\left(\alpha_\beta - \frac{1}{b}\cosh\left(\frac{\alpha_\beta}{\alpha} b\right)\right) = \frac{1}{b\alpha_\beta}\left(\cosh(b) - \cosh\left(\frac{\alpha_\beta}{\alpha} b\right)\right) > 0, \end{aligned}$$

using (4.1) and that $\alpha > \alpha_\beta$. If $g(x)$ is negative at some point in $(0,1)$, there exists a largest $x_0 \in (0,1)$ such that $g(x_0) = 0$ and $g(x) > 0$ in $(x_0, 1]$. We first observe that $u'(x_0) > 0$. This follows from $u'(1) > 0$, the continuity of u' and the fact that $u'(x) \neq 0$ for $x > 0$ where $g(x) \geq 0$. Then by Lemma 4.3 with $a = 1$ and $f = u$ we can define a new function v that coincides with u on $[x_0, 1]$ and with a cosh on $[0, x_0]$ (see Figure 6, a)). Since $v'(0) = 0$ we may extend it by symmetry to a $C^{1,1}$-function on $[-1,1]$. For this new function (4.5) is always satisfied. Moreover v has lower Willmore energy than u. Indeed, we have

$$\begin{aligned}
\mathcal{W}_h(u) &= 2\int_{x_0}^{1} \kappa_h[u]^2 ds_h[u] + 2\int_0^{x_0} \left(\frac{u''(x)}{(1+u'(x)^2)^{\frac{3}{2}}} - \frac{1}{u(x)\sqrt{1+u'(x)^2}} \right)^2 u(x)\sqrt{1+u'(x)^2}dx \\
&\quad +8\int_0^{x_0} \frac{u''(x)}{(1+u'(x)^2)^{\frac{3}{2}}} dx \geq 2\int_{x_0}^{1} \kappa_h[u]^2 ds_h[u] + 8\frac{u'(x_0)}{\sqrt{1+u'(x_0)^2}} = \mathcal{W}_h(v),
\end{aligned}$$

by definition of v and since $x \mapsto \cosh(bx)/b$ satisfies $H(x) \equiv 0$.

Finally, $v'(x) > 0$ in $(0,1)$ since v satisfies (4.5) in $[0,1]$ and $v'(1) = -\beta > 0$. □

Remark 4.6. *Notice that if $u'(x) \leq \delta$ for all $x \in [0,1]$ then also $v'(x) \leq \delta$ for all $x \in [0,1]$. This is due to the convexity of* cosh.

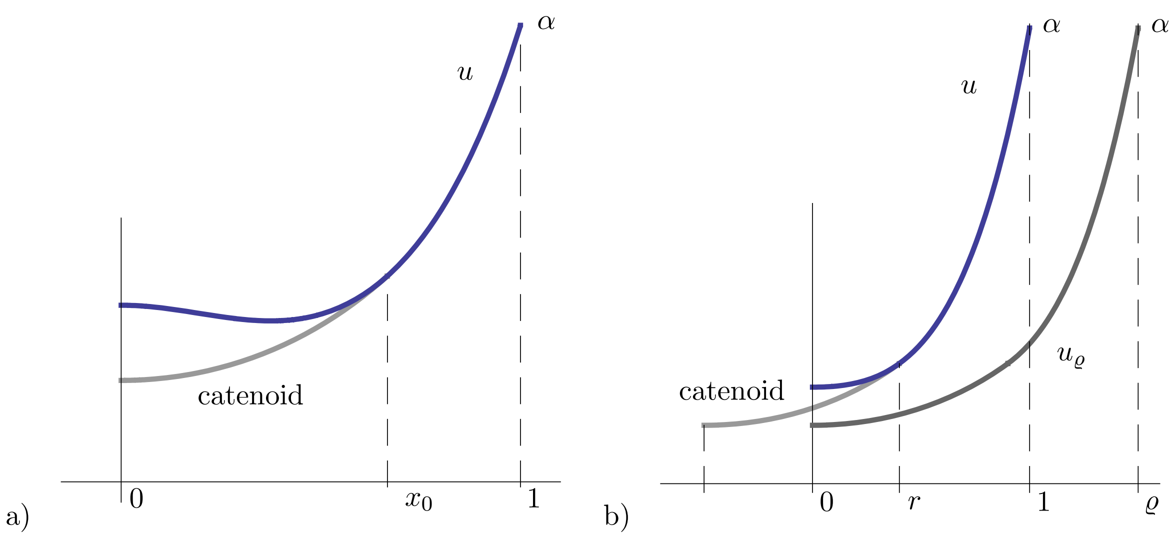


Figure 6: Proof of Lemma 4.5 (left) and of Lemma 4.11 (right).

In what follows we consider functions having the following property:

$$u \text{ satisfies: } 1 - \frac{1}{\sqrt{1+u'(x)^2}} \cosh\left(\frac{\sqrt{1+u'(x)^2}}{u(x)} x \right) \geq 0 \text{ in } [0,1] \text{ and } u' > 0 \text{ in } (0,1]. \tag{4.6}$$

We first remark that this condition is scaling invariant, i.e. it is also satisfied for $u_r(x) = \frac{1}{r}u(rx)$, $x \in [-\frac{1}{r}, \frac{1}{r}]$. The fact that $u \in N_{\alpha,\beta}$ satisfies (4.6) gives us information on the behaviour of the graph of u with respect to the two catenoids going through the point $(1, \alpha)$ and centered at the origin. We recall that these are the functions

$$\frac{\cosh(b_1 x)}{b_1} \text{ and } \frac{\cosh(b_2 x)}{b_2} \text{ with } b_1 < b^* < b_2 \text{ such that } \frac{\cosh(b_1)}{b_1} = \alpha = \frac{\cosh(b_2)}{b_2}. \tag{4.7}$$

Here b^* is the unique solution of $\cosh(b^*) = b^* \sinh(b^*)$, $b^* = 1.1996786\ldots$. We recall that also $b_1 < b < b_2$.

One might expect that $x \mapsto \frac{1}{b_1}\cosh(b_1 x)$ and $x \mapsto \frac{1}{b_2}\cosh(b_2 x)$ could serve as comparison functions. Unfortunately this works out only partially.

Lemma 4.7. *Let $u \in N_{\alpha,\beta}$ satisfy (4.6). For $x \in [0,1)$ we have:*

$$u(x) = \frac{1}{b_1}\cosh(b_1 x) \quad \Rightarrow \quad u'(x) \geq \sinh(b_1 x).$$

More restrictively, if $x \in [b^*/b_2, 1]$, then

$$u(x) = \frac{1}{b_2}\cosh(b_2 x) \quad \Rightarrow \quad u'(x) \leq \sinh(b_2 x).$$

Proof. It is convenient to rewrite the inequality (4.6) by means of $\cosh(\operatorname{arsinh}(y)) = \sqrt{1+y^2}$ as follows

$$\operatorname{arsinh}(u'(x)) \geq \cosh(\operatorname{arsinh}(u'(x)))\frac{x}{u(x)} \text{ in } [0,1],$$

or

$$\frac{u(x)}{x} \geq \frac{\cosh(\operatorname{arsinh}(u'(x)))}{\operatorname{arsinh}(u'(x))} \text{ in } (0,1].$$

We already know – see Figure 5 – that in a left neighbourhood of 1 we have $\cosh(b_1 x)/b_1 > u(x) > \cosh(b_2 x)/b_2$. Let $x \in (0,1)$ be such that $u(x) = \cosh(b_i x)/b_i$, $i = 1$ or 2. Then from (4.6) it follows that

$$\frac{\cosh(b_i x)}{b_i x} \geq \frac{\cosh(\operatorname{arsinh}(u'(x)))}{\operatorname{arsinh}(u'(x))}. \tag{4.8}$$

We consider first $i = 1$. Since $x \in (0,1)$, $b_1 < b^*$ which is the minimum of $g(b) = \frac{1}{b}\cosh(b)$, it follows that $b_1 x$ is left from this minimum. Hence, an argument with a smaller g-value than $b_1 x$ must be right from $b_1 x$, i.e. $\operatorname{arsinh}(u'(x)) \geq b_1 x$, $u'(x) \geq \sinh(b_1 x)$.

For $i = 2$ and $x \geq b^*/b_2$ we have that $b_2 x$ is right of the g-minimum b^*. Smaller g-values than $g(b_2 x)$ are attained at most left from $b_2 x$, i.e. if $\operatorname{arsinh}(u'(x)) \leq b_2 x$, $u'(x) \leq \sinh(b_2 x)$. □

Remark 4.8. 1. *If a function $u \in N_{\alpha,\beta}$ satisfying (4.6) intersects $x \mapsto \frac{1}{b_1}\cosh(b_1 x)$ in a largest point $x_0 \in (0,1)$, then left of x_0, it is below the* cosh *so that $u'(x_0) \leq \sinh(b_1 x_0)$. The previous lemma shows that, on the other hand, $u'(x_0) \geq \sinh(b_1 x_0)$ so that $u'(x_0) = \sinh(b_1 x_0)$. The function u is in x_0 tangent to $x \mapsto \frac{1}{b_1}\cosh(b_1 x)$ so that the latter may replace $C^{1,1}$-smoothly $u|_{[-x_0,x_0]}$. This new function v is again in $N_{\alpha,\beta}$, has lower Willmore energy, satisfies (4.6) and in addition*

$$v(x) \leq \frac{\cosh(b_1 x)}{b_1} \quad in \ [0,1]. \tag{4.9}$$

2. *Analogously we may achieve on minimising sequences that*

$$u(x) \geq \frac{\cosh(b_2 x)}{b_2} \quad in \ [b^*/b_2, 1].$$

Unfortunately there is no obvious mechanism to achieve a lower bound also on $[-b^*/b_2, b^*/b_2]$.

3. *Analogously one may also achieve on minimising sequences that $v(x) \geq \alpha^*|x|$. Again, this bound is not sufficient in order to ensure compactness.*

In order to prove strong enough lower bounds on suitable minimising sequences, we first achieve uniform derivative bounds. Then, the following lemma will prove to be useful.

Lemma 4.9. *Let $\alpha > 0$ and $\beta < 0$ be arbitrary and $u \in N_{\alpha,\beta}$ such that there exists $x_0 \in [0,1)$ so that $u'(x_0) = 0$, $u' > 0$ in $(x_0, 1]$ and $u' \leq 0$ in $[0, x_0]$. Let $\gamma := \max_{x\in[x_0,1]} u'(x)$. Then it holds that*

$$\min_{x\in[0,1]} u(x) = u(x_0) \geq \gamma \frac{1-x_0}{e^C - 1},$$

where $C > 0$ a constant depending monotonically on $\mathcal{W}_h(u), \gamma$ and β.

Proof. We estimate the Willmore energy from below as follows

$$\begin{aligned}
\mathcal{W}_h(u) &\geq 2\int_{x_0}^{1} \left(\frac{u'' u}{(1+u'^2)^{\frac{3}{2}}} + \frac{1}{\sqrt{1+u'(x)^2}} \right)^2 \frac{\sqrt{1+u'(x)^2}}{u(x)}\, dx \\
&\geq 2\int_{x_0}^{1} \frac{1}{u\sqrt{1+u'(x)^2}}\, dx + 4\int_{x_0}^{1} \frac{u''}{(1+u'^2)^{\frac{3}{2}}}\, dx \\
&= 2\int_{x_0}^{1} \frac{1}{u\sqrt{1+u'(x)^2}}\, dx - 4\frac{\beta}{\sqrt{1+\beta^2}}.
\end{aligned}$$

We recall here that from (4.2) it follows that $\mathcal{W}_h(v) \geq -8\beta/\sqrt{1+\beta^2}$ for all $v \in N_{\alpha,\beta}$. Since $u' \leq \gamma$ and, hence, $u(x) \leq u(x_0) + \gamma(x - x_0)$ for $x \in [x_0, 1]$ we get

$$\begin{aligned}
\mathcal{W}_h(u) &\geq \frac{2}{\sqrt{1+\gamma^2}} \int_{x_0}^{1} \frac{1}{u(x_0) + \gamma(x - x_0)}\, dx - 4\frac{\beta}{\sqrt{1+\beta^2}} \\
&= \frac{2}{\gamma\sqrt{1+\gamma^2}} \log\left(1 + \frac{\gamma(1-x_0)}{u(x_0)}\right) - 4\frac{\beta}{\sqrt{1+\beta^2}}
\end{aligned}$$

that gives

$$1 + \frac{\gamma(1-x_0)}{u(x_0)} \leq e^C$$

with C depending monotonically (increasing) on $\mathcal{W}_h(u), \beta$ and γ. The claim follows. □

Later we show by possibly inserting a rescaled solution with zero boundary slope that the assumption just made on $u \in N_{\alpha,\beta}$ is not restrictive.

In the following remark we collect some conclusions which can be drawn for bounds on the derivatives of functions satisfying (4.6).

Remark 4.10. *Let $u \in N_{\alpha,\beta}$ satisfy (4.6) in $[0,1]$. Let $b_1 = b_1(\alpha)$ and $b_2 = b_2(\alpha)$ be as defined in (4.7). Then, one has the following inequalities:*

1. *$u'(x) = -\beta$ implies $u(x) \geq \alpha_\beta x$ with α_β defined in (4.1);*
2. *$u'(x) = \sinh(b_i)$, $i = 1, 2$, implies $u(x) \geq \alpha x$;*
3. *$u(x) \leq \alpha x$ implies $\sinh(b_1) \leq u'(x) \leq \sinh(b_2)$. (In general $u(x) \leq \gamma x$, $\gamma > \alpha^*$, implies bounds for the value of the derivative).*

As explained at the beginning of this section we proceed now by discussing the cases $\alpha \leq -\beta$ and $\alpha > -\beta$ separately. This distinction requires to study the minimisation process in different classes of admissible functions.

4.2.2 The case $-\beta \geq \alpha$

We first prove that the energy is monotonically increasing in α. Then, using that u satisfies (4.6), we get a priori bounds on the derivative leading to an existence theorem.

Monotonicity of the optimal energy

For $\beta \geq 0$, when studying monotonicity of the energy we constructed new functions with lower Willmore energy by inserting a suitable arc of a circle. Here we do an analogous construction inserting arcs of catenoids.

Lemma 4.11. *Assume that $u \in N_{\alpha,\beta}$ satisfies* (4.6). *Then for each $\varrho \in (1, \alpha/\alpha_\beta)$ there exists $u_\varrho \in C^{1,1}([-\varrho,\varrho],(0,\infty))$ positive, symmetric and such that $u_\varrho(\pm\varrho) = \alpha$, $u_\varrho'(\varrho) = -\beta$,* (4.5) *is satisfied in $[0,\varrho]$ and $u_\varrho' > 0$ in $(0,\varrho]$ as well as*

$$\int_{-\varrho}^{\varrho} \kappa_h[u_\varrho]^2 \, ds_h[u_\varrho] \leq \mathcal{W}_h(u).$$

Proof. The idea of the construction is to change the graph of $u|_{[0,r]}$ for some $r > 0$ by inserting $C^{1,1}$-smoothly an arc of a catenoid, see Figure 6, b). Then, translating and extending it by symmetry we find an even function. Choosing r appropriately depending on ϱ, we obtain a function defined in the bigger interval $[-\varrho,\varrho]$ and satisfying (4.5) in $[0,\varrho]$. We give now the technical details of the construction.

For $\varrho \in (1,\alpha/\alpha_\beta)$ let $r \in (0,1)$ be the biggest element in $(0,1)$ such that $\varphi(r) = 0$ where φ is defined by

$$\varphi(x) = x - 1 + \varrho - \operatorname{arsinh}(u'(x)) \frac{u(x)}{\sqrt{1+u'(x)^2}} \qquad \text{for} \qquad x \in [0,1]. \tag{4.10}$$

Such an element exists since we have $\varphi(0) > 0$ and, by recalling $\operatorname{arsinh}(-\beta)/\sqrt{1+\beta^2} = 1/\alpha_\beta$, that $\varphi(1) < 0$. Let λ be defined by $\lambda = \sqrt{1+u'(r)^2}/u(r)$. Then the function u_ϱ defined in $[0,1]$ by

$$u_\varrho(x) := \begin{cases} u(x+1-\varrho) & \text{if } r-1+\varrho \leq x \leq \varrho, \\ \frac{1}{\lambda}\cosh(\lambda x) & \text{if } 0 \leq x < r-1+\varrho, \end{cases}$$

and symmetrically extended to $[-1,1]$ is in $C^{1,1}([-1,1],(0,\infty))$. It satisfies $u_\varrho(\pm\varrho) = \alpha$, $u_\varrho'(\varrho) = -\beta$, $u_\varrho' > 0$ in $(0,\varrho]$ and has a smaller curvature integral than u.

It remains to prove that u_ϱ satisfies (4.5) in $[0,\varrho]$. For easy notation let consider ψ defined by

$$\psi(x) = \frac{1}{\sqrt{1+u_\varrho'(x)^2}} \cosh\left(\frac{\sqrt{1+u_\varrho'(x)^2}}{u_\varrho(x)} x\right) \qquad \text{for} \qquad x \in [0,\varrho].$$

We need to show that $\psi(x) \leq 1$ in $[0,\varrho]$. By construction, $\psi(x) \equiv 1$ in $[0, r-1+\varrho]$ and from $\sqrt{1+\beta^2}/\alpha_\beta = \operatorname{arsinh}(-\beta)$ we conclude that $\psi(\varrho) < 1$. The claim follows since, by choice of r, the biggest point in $[0,\varrho]$ such that $\psi(x) = 1$ is $x = r-1+\varrho$. $\square$

By rescaling we obtain:

Corollary 4.12. *For each $u \in N_{\alpha,\beta}$ such that u satisfies* (4.6) *and for each $\gamma \in [\alpha_\beta, \alpha)$ there exists a positive symmetric $v \in C^{1,1}([-1,1],(0,\infty))$ such that v satisfies* (4.6), *$v(\pm 1) = \gamma$, $v'(1) = -\beta$ and $\mathcal{W}_h(v) \leq \mathcal{W}_h(u)$.*

Proof. If $\gamma = \alpha_\beta$ the claim follows choosing $v(x) = \cosh(bx)/b$ with $b = -\operatorname{arsinh}(-\beta)$. If $\gamma \in (\alpha_\beta, \alpha)$ the claim follows from Lemma 4.11 by rescaling. □

Proposition 4.13. *Let $M_{\alpha,\beta}$ be defined as in* (2.7). *Then for $\tilde\alpha \geq \alpha \geq \alpha_\beta$ we have $M_{\tilde\alpha,\beta} \geq M_{\alpha,\beta}$.*

Proof. Let $(u_k)_{k\in\mathbb{N}}$ be a minimising sequence for $M_{\tilde\alpha,\beta}$ in $N_{\tilde\alpha,\beta}$. By Lemma 4.5 for all $k \in \mathbb{N}$ there exists $v_k \in N_{\tilde\alpha,\beta}$ such that $\mathcal{W}_h(v_k) \leq \mathcal{W}_h(u_k)$ and v_k satisfies (4.6). Then Corollary 4.12 yields the claim. □

Properties of minimising sequences

In the next two lemmas we achieve bounds on the derivative. We first observe that we can assume that when the graph of u is above the line $y \mapsto \alpha y$ the derivative cannot be equal to $-\beta$. On the other hand, condition (4.6) (in particular (4.5)) gives bounds on the derivatives when the graph of u is below the line $y \mapsto \alpha y$.

Lemma 4.14. *Let $u \in N_{\alpha,\beta}$ satisfy* (4.6)*. Then, there exists $v \in N_{\alpha,\beta}$ with lower Willmore energy than u satisfying* (4.6) *and $v(x) < \alpha x$ for all $x \in (0,1)$ with $v'(x) = -\beta$.*

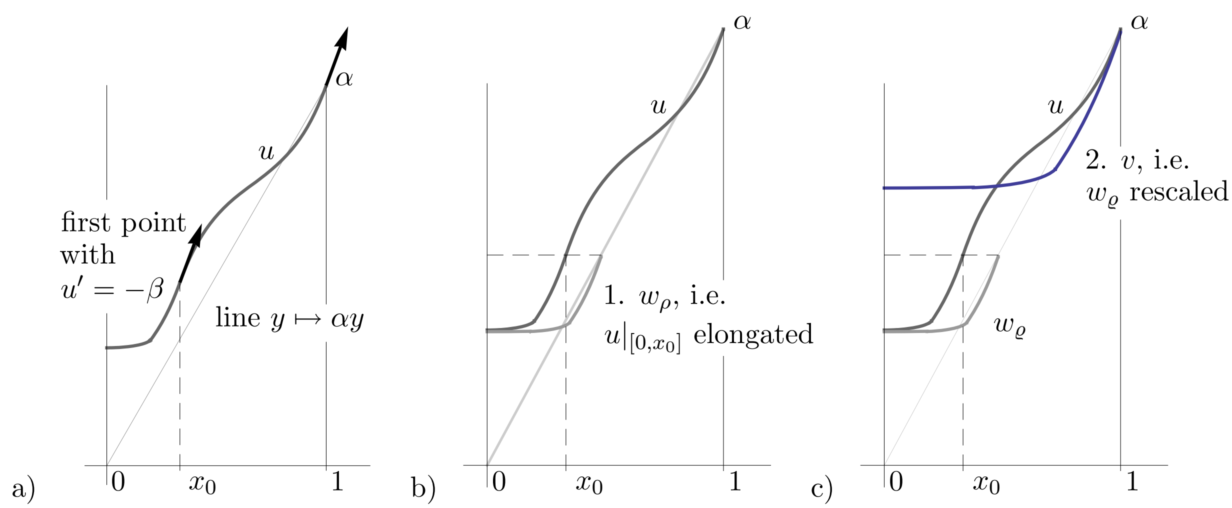


Figure 7: Proof of Lemma 4.14.

Proof. Let x_0 be the smallest element in $[0,1]$ such that $u'(x_0) = -\beta$ and $u(x_0) \geq \alpha x_0$. If $x_0 = 1$ the claim follows with $v = u$. If $x_0 < 1$ and $u(x_0) = \alpha x_0$ the function $v(x) = u(x_0 x)/x_0$, $x \in [-1,1]$, yields the claim. On the other hand, if $x_0 < 1$ and $u(x_0) > \alpha x_0$ by using a scaled version of Lemma 4.11 we "extend" the function $u|_{[-x_0,x_0]}$ by inserting a cosh (see Figure 7). For each $\varrho \in (x_0, u(x_0)/\alpha_\beta)$ there exists $w_\varrho \in C^{1,1}([-\varrho,\varrho],(0,\infty))$ with lower Willmore energy than $u|_{[-x_0,x_0]}$ such that $w_\varrho(\pm\varrho) = u(x_0)$ and $w_\varrho'(\varrho) = -\beta$. We then choose $\varrho = u(x_0)/\alpha$ and v to be equal to the function w_ϱ rescaled to the interval $[-1,1]$. The choice of ϱ is such that we extend $u|_{[0,x_0]}$ until we touch the line $y \mapsto \alpha y$. Notice that $v \in N_{\alpha,\beta}$ and that v satisfies (4.6). It remains to check that if $v'(x) = -\beta$ for some $x \in (0,1)$ then $v(x) < \alpha x$. By construction, the function w_ϱ is given by

$$w_\varrho(x) := \begin{cases} u(x + x_0 - \varrho) & \text{if } r - x_0 + \varrho \leq x \leq \varrho, \\ \dfrac{1}{\lambda}\cosh(\lambda x) & \text{if } 0 \leq x < r - x_0 + \varrho, \end{cases}$$

for some $r \in (0, x_0)$ and $\lambda = \lambda(r) > 0$. If there exists $x \in (0,1)$ such that $v'(x) = -\beta$ then $w'_\varrho(\varrho x) = -\beta$. If $\varrho x \in [0, r - x_0 + \varrho]$ then $w'_\varrho(\varrho x) = -\beta$ implies $\lambda \varrho x = b$ and hence

$$\frac{v(x)}{x} = \frac{w_\varrho(\varrho x)}{\varrho x} = \frac{\cosh(\lambda \varrho x)}{\lambda \varrho x} = \alpha_\beta < \alpha.$$

If instead $\varrho x \in (r + \varrho - x_0, \varrho]$ then $u'(\varrho x + x_0 - \varrho) = -\beta$ and hence $u(\varrho x + x_0 - \varrho) < \alpha(\varrho x + x_0 - \varrho)$ from which it follows

$$\frac{v(x)}{x} = \frac{u(\varrho x + x_0 - \varrho)}{\varrho x} = \frac{u(\varrho x + x_0 - \varrho)}{\varrho x + x_0 - \varrho} \frac{\varrho x + x_0 - \varrho}{\varrho x} < \alpha.$$

The claim follows. ∎

In the proof we use only that $\alpha > \alpha_\beta$.

We recall the definition (4.7) of the positive real numbers $b_2 = b_2(\alpha)$ and $b_1 = b_1(\alpha)$ such that $\cosh(b_2)/b_2 = \alpha = \cosh(b_1)/b_1$ and $b_2 > b^* > b_1$, with b^* being the solution of $\cosh(b^*) = b^* \sinh(b^*)$.

Lemma 4.15. *Let $u \in N_{\alpha,\beta}$ satisfy* (4.6) *and $u'(x) \neq -\beta$ for all $x \in (0,1)$ with $u(x) \geq \alpha x$. Then, $u'(x) \leq \sinh(b_2)$ in* $[0,1]$.

Proof. We assume first in addition that there exists a left neighbourhood of 1 such that there we have $u(x) \leq \alpha x$. Such a neighbourhood always exists if $-\beta > \alpha$. By 3) in Remark 4.10 we have that $u'(x) \leq \sinh(b_2)$ for all x such that $u(x) \leq \alpha x$. Hence, when the graph of u is below the line $y \mapsto \alpha y$ we have a bound for the derivative. Let now $x \in (0,1)$ be such that $u(x) > \alpha x$. We show that $u'(x) < -\beta$. Let x_0 be the smallest element in $(x, 1)$ such that $u(x_0) = \alpha x_0$. Then $u'(x_0) \leq \alpha \leq -\beta$. If we assume that $u'(x) \geq -\beta$ then, by continuity, there exists $y \in [x, x_0]$ such that $u'(y) = -\beta$. A contradiction. Hence $u'(x) < -\beta < \sinh(b_2)$.

It remains to consider the case where there is no left neighbourhood of 1 such that there we have $u(x) \leq \alpha x$. Then, necessarily $-\beta = \alpha$, and we have a sequence $x_k \nearrow 1$ with $u(x_k) > \alpha x_k$. Looking at the first point right from x_k, where u reaches $y \mapsto \alpha y$ shows that $u(x) > \alpha x$ on $[0, x_k]$. Otherwise the mean value theorem would yield a point $\xi \in (0,1)$ with $u(\xi) \geq \alpha \xi$ and $u'(\xi) = \alpha = -\beta$, a contradiction. Letting $k \to \infty$ yields $u(x) > \alpha x$ on $[0,1)$. By $u'(0) = 0$ we conclude that $0 \leq u'(x) < -\beta < \sinh(b_2)$ on $[0,1)$ in this case. ∎

The following proposition characterises suitably modified minimising sequences.

Proposition 4.16. *Let $(u_k)_{k\in\mathbb{N}}$ be a minimising sequence for $M_{\alpha,\beta}$ in $N_{\alpha,\beta}$ such that $\mathcal{W}_h(u_k) \leq M_{\alpha,\beta} + 1$ for all $k \in \mathbb{N}$. Let $b_2 = b_2(\alpha)$ and $b_1 = b_1(\alpha)$ be as defined in* (4.7). *Then, there exists a minimising sequence $(v_k)_{k\in\mathbb{N}} \subset N_{\alpha,\beta}$ such that for all $k \in \mathbb{N}$ the function v_k satisfies* (4.6), *$\mathcal{W}_h(v_k) \leq \mathcal{W}_h(u_k)$,*

$$\sinh(b_2) \geq v_k'(x) > 0 \ \text{ for all } x \in (0,1] \ \text{ and } \ C_{\alpha,\beta} \leq v_k(x) \leq \frac{1}{b_1}\cosh(b_1 x) \ \text{ in } [-1,1], \tag{4.11}$$

with a constant $C_{\alpha,\beta} > 0$ depending on $M_{\alpha,\beta}$, $\sinh(b_2)$ and $-\beta$.

Proof. By Lemmas 4.5, 4.14 and 4.15 for each u_k there exists $v_k \in N_{\alpha,\beta}$ with lower Willmore energy than u_k such that v_k satisfies (4.6) and $\sinh(b_2) \geq v_k' > 0$ in $(0,1]$. According to Remark 4.8 we may also achieve that $v_k(x) \leq \frac{1}{b_1}\cosh(b_1 x)$. The estimate from below for v_k follows from Lemma 4.9. The constant $C_{\alpha,\beta}$ denotes the term on the right hand side of Lemma 4.9 with $\gamma = \sinh(b_2)$ and $x_0 = 0$. Notice that by the assumption $\mathcal{W}_h(u_k) \leq M_{\alpha,\beta} + 1$ the constant $C_{\alpha,\beta}$ depends only on $M_{\alpha,\beta}$, $\sinh(b_2)$ and $-\beta$. ∎

Proof of the existence theorem

The real numbers $b_2 = b_2(\alpha)$ and $b_1 = b_1(\alpha)$ are defined in (4.7) and such that $\cosh(b_2)/b_2 = \alpha = \cosh(b_1)/b_1$ and $b_2 \geq b^* \geq b_1$, with b^* the solution of $\cosh(b^*) = b^* \sinh(b^*)$.

Theorem 4.17 (Existence and regularity)**.** *For $\beta < 0$ and α such that $\alpha > \alpha_\beta$ and $-\beta \geq \alpha$ there exists a function $u \in C^\infty([-1,1],(0,\infty))$ such that the corresponding surface of revolution $\Gamma \subset \mathbb{R}^3$ solves the Dirichlet problem* (1.4)*. This solution is positive and symmetric, and it has the following properties:*

$$\sinh(b_2) \geq u'(x) > 0 \text{ in } (0,1] \quad \text{and} \quad \frac{1}{b_1}\cosh(b_1 x) \geq u(x) \geq C_{\alpha,\beta} \text{ in } [-1,1]$$

with a constant $C_{\alpha,\beta} > 0$ depending on $M_{\alpha,\beta}$, $\sinh(b_2)$ and $-\beta$.

Proof. Let $(u_k)_{k\in\mathbb{N}} \in N_{\alpha,\beta}$ be a minimising sequence for $M_{\alpha,\beta}$ such that $\mathcal{W}_h(u_k) \leq M_{\alpha,\beta} + 1$ for all $k \in \mathbb{N}$. By Proposition 4.16 we may assume that each element u_k of the minimising sequence satisfies (4.6) and (4.11). The rest of the proof is on the same line as that of Theorem 3.11. Notice that since u_k satisfies (4.6) for all $k \in \mathbb{N}$ then also u satisfies (4.6) and so $u' > 0$ in $(0,1]$. □

We can improve Proposition 4.13 by showing that the energy is strictly increasing in α.

Proposition 4.18. *Let $M_{\alpha,\beta}$ be defined as in* (2.7) *and $\alpha > \alpha_\beta$. Then, for $-\beta \geq \tilde{\alpha} > \alpha$ we have $M_{\tilde{\alpha},\beta} > M_{\alpha,\beta}$.*

Proof. Let $u \in N_{\widetilde{\alpha},\beta}$ be a solution of (1.4) with boundary values $\widetilde{\alpha}$, β as constructed in Theorem 4.17. Then $\mathcal{W}_h(u) = M_{\widetilde{\alpha},\beta}$ and u satisfies (4.6). We first notice that u satisfies (4.6) with a strict inequality. Indeed, if there exists $x_0 \in (0,1)$ such that

$$1 - \frac{1}{\sqrt{1+u'(x_0)^2}} \cosh\left(\frac{\sqrt{1+u'(x_0)^2}}{u(x_0)} x_0\right) = 0,$$

reasoning as in Lemma 4.5 and using that u is the minimiser in $N_{\widetilde{\alpha},\beta}$, it follows that $u|_{[-x_0,x_0]}$ is equal to a catenoid. Then, u being a solution of (2.5), it follows that u is a catenoid in $[-1,1]$. This is not possible since $\alpha > \alpha_\beta$. Hence, applying the procedure of Corollary 4.12 to a minimiser $u \in N_{\widetilde{\alpha},\beta}$ yields a $v \in N_{\alpha,\beta}$ with strictly lower energy $\mathcal{W}_h(u) > \mathcal{W}_h(v)$. Since $\mathcal{W}_h(v) \geq M_{\alpha,\beta}$ the claim follows. Notice that the same reasoning shows that also this last inequality is strict. □

4.2.3 The case $-\beta < \alpha$

In this case we are not able to obtain a bound from above for the derivative for minimising sequences in $N_{\alpha,\beta}$. Possibly, a loss of compactness could occur. To avoid this problem we restrict the set on which we minimise by adding a constraint. We require the derivative to be bounded by α.

We consider

$$\widetilde{N}_{\alpha,\beta} = \{u \in N_{\alpha,\beta} : \ u'(x) \leq \alpha \text{ for all } x \in [0,1]\},$$

and

$$\widetilde{M}_{\alpha,\beta} = \inf_{u \in \widetilde{N}_{\alpha,\beta}} \mathcal{W}_h(u). \tag{4.12}$$

The assumption $-\beta < \alpha$ ensures that $\widetilde{N}_{\alpha,\beta}$ is not empty.

Also in this case, by Lemma 4.5 and the subsequent remark, it is sufficient to consider functions $u \in \widetilde{N}_{\alpha,\beta}$ satisfying (4.6).

Monotonicity of the optimal energy

Proceeding as in the previous section we find:

Lemma 4.19. *Assume that $u \in \widetilde{N}_{\alpha,\beta}$ satisfies* (4.6). *Then for each $\varrho \in (1, \alpha/\alpha_\beta)$ there exists $u_\varrho \in C^{1,1}([-\varrho,\varrho],(0,\infty))$ positive and symmetric such that $u_\varrho(\pm\varrho) = \alpha$, $u'_\varrho(\varrho) = -\beta$,* (4.5) *is satisfied in $[0,\varrho]$ and $\alpha \geq u'_\varrho > 0$ in $(0,\varrho]$ as well as*

$$\int_{-\varrho}^{\varrho} \kappa_h[u_\varrho]^2 \, ds_h[u_\varrho] \leq \mathcal{W}_h(u).$$

Proof. The proof is exactly as in Lemma 4.11. By the explicit expression of u_ϱ and the convexity of cosh, we see that $u' \leq \alpha$ implies $u'_\varrho \leq \alpha$. □

Corollary 4.20. *For each $u \in \widetilde{N}_{\alpha,\beta}$ such that u satisfies* (4.6) *and for each $\gamma \in [\alpha_\beta, \alpha)$ there exists a positive symmetric $v \in C^{1,1}([-1,1],(0,\infty))$ such that v satisfies* (4.6)*, $v(\pm 1) = \gamma$, $v'(1) = -\beta$, $\alpha \geq v'(x) > 0$ for $x \in (0,1]$ and $\mathcal{W}_h(v) \leq \mathcal{W}_h(u)$.*

Proposition 4.21. *Let $\widetilde{M}_{\alpha,\beta}$ be defined as in* (4.12). *Then for $\tilde{\alpha} \geq \alpha$ we have $\widetilde{M}_{\tilde{\alpha},\beta} \geq \widetilde{M}_{\alpha,\beta}$.*

Properties of minimising sequences

The following lemma is the analogue of Lemma 4.14 in the case $\alpha \leq -\beta$.

Lemma 4.22. *Let $u \in \widetilde{N}_{\alpha,\beta}$ satisfy* (4.6). *Then there exists $v \in \widetilde{N}_{\alpha,\beta}$ with lower Willmore energy than u satisfying* (4.6) *and $v(x) > \alpha x$ as well as $v'(x) < -\beta$ in $(0,1)$.*

Proof. We first notice that $u(x) > \alpha x$ in $(0,1)$. If $u'(x) < -\beta$ in $(0,1)$ then the claim follows with $v = u$. Otherwise let $x_0 \in (0,1)$ be the smallest element in $(0,1)$ such that $u'(x_0) = -\beta$. We repeat then the construction in Lemma 4.14. By using a scaled version of Lemma 4.19 we elongate the function $u|_{[-x_0,x_0]}$ by inserting a cosh. For each $\varrho \in (x_0, u(x_0)/\alpha_\beta)$ there exists $w_\varrho \in C^{1,1}([-\varrho,\varrho],(0,\infty))$ with lower Willmore energy than $u|_{[-x_0,x_0]}$ such that $w_\varrho(\pm\varrho) = u(x_0)$ and $w'_\varrho(\varrho) = -\beta$. We then choose $\varrho = u(x_0)/\alpha$ and v to be equal to the function w_ϱ rescaled to the interval $[-1,1]$. The choice of ϱ is such that we extend $u|_{[0,x_0]}$ until we touch the line $y \mapsto \alpha y$. Notice that $v \in N_{\alpha,\beta}$, v satisfies (4.6) and that by convexity of cosh we have $v'(x) < -\beta$ in $[0,1)$. In particular $v \in \widetilde{N}_{\alpha,\beta}$. Compared with Lemma 4.14, the proof in this case is simpler since we are always above the line $y \mapsto \alpha y$. In $[0,x_0)$ there are no points with derivative $\geq -\beta$. With this construction we do not add such points. □

The following proposition characterises suitably modified minimising sequences.

Proposition 4.23. *Let $(u_k)_{k\in\mathbb{N}}$ be a minimising sequence for $\widetilde{M}_{\alpha,\beta}$ in $\widetilde{N}_{\alpha,\beta}$ such that $\mathcal{W}_h(u_k) \leq \widetilde{M}_{\alpha,\beta}+1$ for all $k \in \mathbb{N}$. Let $b_1 = b_1(\alpha)$ as defined in* (4.7). *Then, there exists a minimising sequence $(v_k)_{k\in\mathbb{N}} \subset \widetilde{N}_{\alpha,\beta}$ such that for all $k \in \mathbb{N}$, v_k satisfies* (4.6)*, $\mathcal{W}_h(v_k) \leq \mathcal{W}_h(u_k)$ and*

$$-\beta \geq v'_k(x) > 0 \text{ for all } x \in (0,1] \quad \text{and} \quad 0 < \alpha+\beta \leq v_k(x) \leq \frac{1}{b_1}\cosh(b_1 x) \text{ in } [-1,1]. \quad (4.13)$$

Proof. By Lemmas 4.5 and 4.22 for each u_k there exists $v_k \in \widetilde{N}_{\alpha,\beta}$ with lower Willmore energy than u_k such that v_k satisfies (4.6) and $-\beta \geq v'_k > 0$ in $(0,1]$. According to Remark 4.8 we may also achieve that $v_k(x) \leq \frac{1}{b_1}\cosh(b_1 x)$. The estimate from below of v_k follows directly. □

Proof of the existence theorem

We recall that $b_1 = b_1(\alpha)$ is defined in (4.7) and it is such that $\cosh(b_1)/b_1 = \alpha$ and $b_1 \le b^*$, with b^* solution of $\cosh(b^*) = b^* \sinh(b^*)$.

Theorem 4.24 (Existence and regularity)**.** *For $\beta < 0$ and α such that $\alpha > \alpha_\beta$ and $\alpha > -\beta$ there exists a function $u \in C^\infty([-1,1],(0,\infty))$ such that the corresponding surface of revolution $\Gamma \subset \mathbb{R}^3$ solves the Dirichlet problem* (1.4)*. This solution is positive and symmetric, and it has the following properties:*

$$-\beta \ge u'(x) > 0 \text{ in } (0,1] \quad \text{and} \quad \frac{1}{b_1}\cosh(b_1 x) \ge u(x) \ge \alpha + \beta \text{ in } [-1,1]. \tag{4.14}$$

Proof. As in the proof of Theorem 3.11 we find a minimiser $u \in \widetilde{N}_{\alpha,\beta}$ of $\mathcal{W}_h$. This means that u minimises $\mathcal{W}_h$ in the class of all positive and symmetric $H^2(-1,1)$-functions v satisfying $v(\pm 1) = \alpha$, $v'(+1) = -\beta$, and having first derivative bounded pointwise by α. Moreover, since the elements of the minimising sequence satisfy (4.6) and (4.13) then u satisfies also (4.6) and hence (4.14). Since $u'(x) \le -\beta < \alpha$ for $x \in [0,1]$, then for $|t|$ sufficiently small $u + t\varphi \in \widetilde{N}_{\alpha,\beta}$ for $\varphi \in H^2(-1,1)$ with $\varphi(\pm 1) = 0 = \varphi'(\pm 1)$. Therefore, u is an interior point of $\widetilde{N}_{\alpha,\beta}$ in $H^2(-1,1)$ and u weakly solves (2.5).

The proof of smoothness of the solution is as in [4, Theorem 3.9, Step 2]. □

Proceeding as in the proof of Proposition 4.18 one can show that the energy also in this case is strictly increasing in α.

Proposition 4.25. *Let $-\beta < \alpha$ and $\alpha > \alpha_\beta$. Let $\widetilde{M}_{\alpha,\beta}$ be as defined in* (4.12)*. Then $\widetilde{M}_{\widetilde{\alpha},\beta} > \widetilde{M}_{\alpha,\beta}$ for all $\widetilde{\alpha}$ such that $\widetilde{\alpha} > \alpha$.*

4.3 The case $\alpha < \alpha_\beta$

In this case the height prescribed at the boundary is smaller than the height of the catenoid centered at 0 and having derivative $-\beta$ at $x = 1$. This case is not simply the dual of the case $\alpha > \alpha_\beta$. The function $b \mapsto \cosh(b)/b$ has a unique minimum at $b^* = 1.1996786\ldots$ and its minimal value is $\alpha^* = 1.5088795\ldots$ (see (1.5)). Hence, when considering $\alpha < \alpha_\beta$ we have to consider two different cases: when $\alpha \ge \alpha^*$ and when $\alpha < \alpha^*$. The first case is, in some sense, the dual to the case $\alpha > \alpha_\beta$. The constructions and the methods of proof are similar. On the other hand, the case $\alpha < \alpha^*$ is completely different. Here, only parts of the functions $u \in N_{\alpha,\beta}$ close to $x = 1$ can be compared with catenoids.

It is useful to restrict further the functions we consider. This restriction is technically important for the case $\alpha < \alpha^*$ but, for the sake of a uniform presentation, we use it in the entire section. We restrict our study to, what we call, admissible functions. These admissible functions are, however, dense in the space of all symmetric $H^2((-1,1),(0,\infty))$-functions and so, one can stick to them in minimising the Willmore functional without any loss of generality.

Definition 4.26 (*Admissible functions*)**.** *A function $u \in C^{1,1}([-a,a],(0,\infty))$, $a > 0$, is called admissible if it is positive, symmetric and if there exist finitely many points $0 = x_0 < x_1 < x_2 < \cdots < x_m = a$ such that $u|_{[x_j,x_{j+1}]}$, $j = 0,\ldots,m-1$, is a polynomial of degree at least two, or equal to $\cosh(\lambda(x-d))/\lambda$ for some $\lambda \in (0,\infty)$, $d \in \mathbb{R}$, or an arc of a circle with centre on the x-axis or an arc of a solution of* (1.4) *with $\beta = 0$ as constructed in Theorem 3.18.*

In what follows, we only perform constructions for admissible functions which yield again admissible functions. In most cases the starting point will be polynomials.

In this section we first show that it is sufficient to consider functions having at most one critical point in $(0,1)$ and satisfying a condition dual to (4.6). Moreover, we employ the catenoids as comparison functions. We then show that the energy is monotonically decreasing in α. To proceed we need to distinguish the cases $\alpha \geq \alpha^*$ and $\alpha < \alpha^*$. We explain later the strategy of proof in the two cases.

4.3.1 First observations

The next two lemmas correspond to Lemma 4.5 for $\alpha > \alpha_\beta$. There we could restrict ourselves to functions satisfying $u' > 0$ in $(0,1)$. Here we show that we can restrict ourselves to functions having at most one critical point in $(0,1)$.

Lemma 4.27. *Let $u \in N_{\alpha,\beta}$ be an admissible function in the sense of Definition 4.26. Then, there exists an admissible function $v \in N_{\alpha,\beta}$ with lower Willmore energy than u and having at most one critical point in $(0,1)$, i.e. either $v' > 0$ in $(0,1]$ or there exists $x_0 \in (0,1)$ such that $v'(x_0) = 0$, $v' > 0$ in $(x_0, 1]$ and $v' < 0$ in $(0, x_0)$.*

Proof. If u does not satisfy $u' > 0$ in $(0,1]$ there exists $x_0 \in (0,1)$ such that $u'(x_0) = 0$ and $u'(x) > 0$ in $(x_0, 1]$. We then replace $u|_{[-x_0,x_0]}$ with an appropriately rescaled solution of (1.4) with boundary data $u(x_0)$ and 0 as constructed in Theorem 3.18. This rescaled function has strictly negative derivative in $(0, x_0)$ by Lemma 3.20. The obtained function v yields the claim. □

In the next result we give a condition corresponding to (4.5) in this case. Here we use both catenoids and geodesic circles. The condition $x + u(x)u'(x) \geq 0$ was a consequence of (4.5) for $\alpha > \alpha_\beta$ but this is not the case here.

Lemma 4.28. *Let $u \in N_{\alpha,\beta}$ be an admissible function in the sense of Definition 4.26. Then, there exists an admissible function $v \in N_{\alpha,\beta}$ and $x_0 \in [0,1)$ with $v' < 0$ in $(0, x_0)$, $v'(x_0) = 0$, $v' > 0$ in $(x_0, 1]$ and $\mathcal{W}_h(v) \leq \mathcal{W}_h(u)$. Moreover, v satisfies*

$$1 - \frac{1}{\sqrt{1+v'(x)^2}} \cosh\left(\frac{\sqrt{1+v'(x)^2}}{v(x)} x\right) \leq 0 \ \ \text{in } [x_0, 1] \tag{4.15}$$

and

$$x + v(x)v'(x) \geq 0 \ \ \text{in } [0,1]. \tag{4.16}$$

Proof. Let $w \in N_{\alpha,\beta}$ be the function constructed in Lemma 4.27. One has $\mathcal{W}_h(w) \leq \mathcal{W}_h(u)$. We denote by $x_1 \in [0,1)$ the point such that $w' > 0$ in $(x_1, 1]$, $w'(x_1) = 0$ and $w' < 0$ in $(0, x_1)$.

This function w satisfies (4.15) in $x = 1$ and in x_1. Indeed, in $x = 1$ we find

$$1 - \frac{1}{\sqrt{1+\beta^2}} \cosh\left(\frac{\sqrt{1+\beta^2}}{\alpha}\right) = \frac{1}{\alpha_\beta}\left(\alpha_\beta - \frac{1}{b}\cosh\left(\frac{\alpha_\beta}{\alpha} b\right)\right) < 0$$

since $\beta = -\sinh(b)$, $\alpha_\beta = \frac{1}{b}\cosh(b)$, using (4.1) and $\alpha < \alpha_\beta$. In x_1 we get $1 - \cosh(x_1/w(x_1)) \leq 0$ and equality holds only if $x_1 = 0$. If w satisfies (4.15) in $[x_1, 1]$ we define in $[0,1]$ the function $h(x) := x + w(x)w'(x)$. The function h is strictly positive in $[x_1, 1]$ since $w' \geq 0$ in $[x_1, 1]$. Moreover, $h(0) = 0$. If $h > 0$ in $(0, x_1]$ the claim follows with $v = w$ and $x_0 = x_1$. Otherwise there exists a biggest element $\bar{x} \in (0, x_1)$ with $h(\bar{x}) = 0$. Then we may substitute w in $[-\bar{x}, \bar{x}]$ in a $C^{1,1}$-smooth way by an arc of a circle lowering the Willmore energy. This new function gives the claim.

It remains to treat the case when w does not satisfy (4.15) in $[x_1, 1]$. For easy reference we denote here by g the function on the left hand side of (4.15) with v replaced by w. Let x_2 be the biggest element in $[x_1, 1]$ such that $g(x_2) = 0$ and $g(x) \le 0$ in $[x_2, 1]$. By Lemma 4.3 with $a = 1$ and $f = w$ we can define a new function v coinciding with u on $[x_2, 1]$ and being a cosh on $[0, x_2]$. Since $v'(0) = 0$ we may extend it by symmetry to a $C^{1,1}$-function on $[-1, 1]$. This new function always satisfies (4.15) and has lower Willmore energy. Notice that in this case $x_0 = 0$ and hence, (4.16) is certainly satisfied in $[0, 1]$. □

In what follows we consider only admissible functions $u \in N_{\alpha,\beta}$ satisfying the following conditions.

$$\begin{gathered}\text{There exists } x_0 \in [0,1) \text{ such that } u' > 0 \text{ in } (x_0, 1],\ u'(x_0) = 0,\ u' < 0 \text{ in } (0, x_0),\\ 1 - \frac{1}{\sqrt{1+u'(x)^2}} \cosh\left(\frac{\sqrt{1+u'(x)^2}}{u(x)} x\right) \le 0 \text{ in } [x_0, 1],\\ \text{and } x + u(x)u'(x) \ge 0 \ \text{ in } [0,1].\end{gathered} \tag{4.17}$$

Before proceeding by proving monotonicity of the energy, we first compare functions in $N_{\alpha,\beta}$ with arcs of catenoids. In the next lemma we show that without loss of generality we may assume that functions satisfying (4.17) with $x_0 > 0$ satisfies also an uniform bound from below for $u(x_0)/x_0$.

Lemma 4.29. *Let $u \in N_{\alpha,\beta}$ be an admissible function in the sense of Definition 4.26 satisfying (4.17) for some $x_0 > 0$. Then, there exists an admissible function $v \in N_{\alpha,\beta}$ such that $\mathcal{W}_h(u) \ge \mathcal{W}_h(v)$, v satisfies (4.17) for some $x_1 > 0$ and $v(x_1) \ge \frac{\alpha}{\operatorname{arsinh}(-\beta)(\alpha_\beta - \alpha)} x_1$.*

Proof. We recall that $b = \operatorname{arsinh}(-\beta)$. If $u(x_0) \ge \frac{\alpha}{b(\alpha_\beta - \alpha)} x_0$ the claim follows with $v = u$. Otherwise we can construct a function satisfying the claim and with lower Willmore energy than u. We consider, starting from 1 and going towards 0, the arc of the catenoid going through $(1, \alpha)$ and having derivative $-\beta$ in 1. This is $x \mapsto \alpha \cosh(b\alpha_\beta(x - 1 + \alpha/\alpha_\beta)/\alpha)/b\alpha_\beta$. We follow the catenoid up to its minimum. Since $\alpha < \alpha_\beta$, the minimum is achieved in the point $1 - \alpha/\alpha_\beta \in (0, 1)$. In this point, we attach to this catenoid a suitably rescaled solution of (1.4) as constructed in Theorem 3.18 with boundary data $\alpha b/\alpha_\beta$ and 0. Finally, extending the graph by symmetry, we obtain a function v. Notice that v satisfies (4.17) with $x_1 = 1 - \alpha/\alpha_\beta$ and that $v(x_1) = \frac{\alpha}{b(\alpha_\beta - \alpha)} x_1$. By the monotonicity property of the energy in the case $\beta = 0$ (see Proposition 3.19) one sees that v has lower Willmore energy than u. Notice that the cosh-part has the lowest possible energy among all curves connecting the boundary point α with slope $-\beta$ and any point with horizontal tangent. □

The next lemma corresponds to Remark 4.10 in the case $\alpha > \alpha_\beta$. We recall here that for $\alpha' \ge \alpha^*$, the real numbers $b_2 = b_2(\alpha')$ and $b_1 = b_1(\alpha')$ are defined in (4.7) by $\cosh(b_2)/b_2 = \alpha' = \cosh(b_1)/b_1$ and $b_2 \ge b^* \ge b_1$, where b^* is the solution of $\cosh(b^*) = b^* \sinh(b^*)$.

Lemma 4.30. *Let $u \in N_{\alpha,\beta}$ be an admissible function in the sense of Definition 4.26 and let u satisfy (4.17) for some $x_0 \in [0, 1)$. Consider $\alpha' \ge \alpha^*$. Then for all $x \in (x_0, 1]$ such that $u(x) > \alpha' x$ we have that either $u'(x) < \sinh(b_1(\alpha'))$ or $u'(x) > \sinh(b_2(\alpha'))$.*

Proof. The claim follows directly using that u satisfies in particular (4.15). □

The previous lemma shows that when the graph of $u \in N_{\alpha,\beta}$ is above the line $y \mapsto \alpha' y$, $\alpha' > \alpha^*$, we have a bound on the derivative. For this reason it is natural to distinguish below the cases $\alpha \ge \alpha^*$ and $\alpha < \alpha^*$.

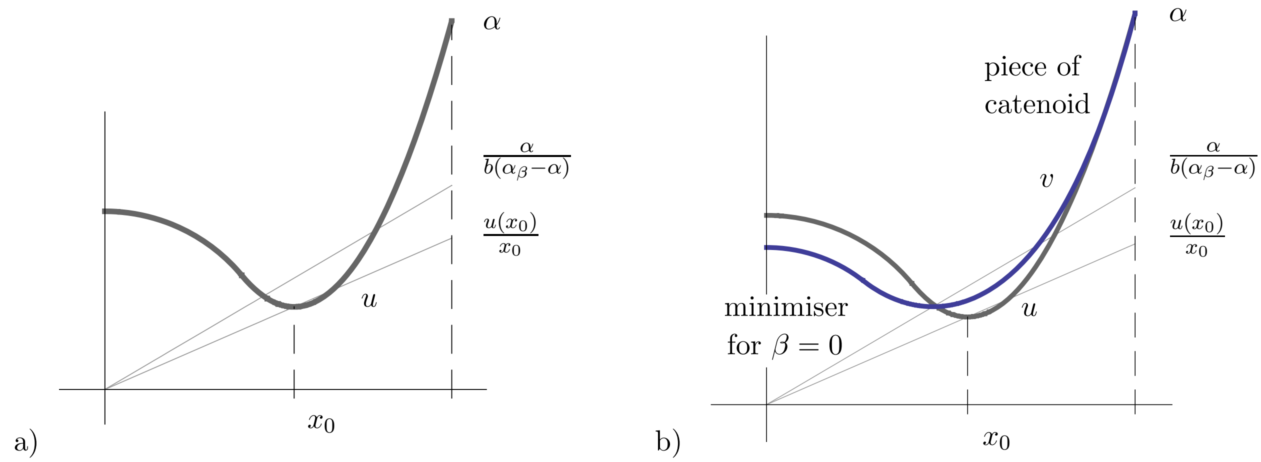


Figure 8: The construction in Lemma 4.29. On the left: a function $u \in N_{\alpha,\beta}$ with $u(x_0) < \alpha x_0/(b(\alpha_\beta - \alpha))$. On the right: a function $v \in N_{\alpha,\beta}$ with lower Willmore energy than u satisfying $v(x_1) = \alpha x_1/(b(\alpha_\beta - \alpha))$ with $x_1 = 1 - \alpha/\alpha_\beta$.

4.3.2 Monotonicity of the optimal energy

We prove here that $M_{\alpha,\beta}$ decreases when α increases to α_β. For later use we work in a more general setting.

We start by showing that we can construct functions defined in a smaller interval, with the same boundary values and with lower Willmore energy. We first prove the result for functions satisfying (4.17) with $x_0 = 0$ and then extend it to the general case.

Lemma 4.31. *Fix $t < 0$. Assume that $u \in C^{1,1}([-1,1],(0,\infty))$ is an admissible function in the sense of Definition 4.26 satisfying $u(1) < \alpha_t$, $u'(1) = -t$ and (4.17) with $x_0 = 0$. Then for each $\varrho \in (u(1)/\alpha_t, 1)$ there exists an admissible function $u_\varrho \in C^{1,1}([-\varrho,\varrho],(0,\infty))$ such that $u_\varrho(\pm\varrho) = u(1)$, $u_\varrho'(\varrho) = -t$, $u_\varrho' > 0$ in $(0,\varrho]$, u_ϱ satisfies (4.15) in $[0,\varrho]$ (with $x_0 = 0$) as well as*

$$\int_{-\varrho}^{\varrho} \kappa_h[u_\varrho]^2 \, ds_h[u_\varrho] \le \mathcal{W}_h(u).$$

Proof. One uses the same construction as in Lemma 4.11. Since $\alpha < \alpha_\beta$, this procedure now shortens the original function. □

Lemma 4.32. *Fix $t < 0$. Assume that $u \in C^{1,1}([-1,1],(0,\infty))$ is an admissible function in the sense of Definition 4.26 satisfying $u'(1) = -t$, $u(1) < \alpha_t$ and (4.17) for some $x_0 \in [0,1)$.*

Then for each $\varrho \in (u(1)/\alpha_t, 1)$ there exists an admissible function $u_\varrho \in C^{1,1}([-\varrho,\varrho],(0,\infty))$ such that $u_\varrho(\pm\varrho) = u(1)$, $u_\varrho'(\varrho) = -t$. Moreover, there exists an $x_1 \in [0,\varrho)$ with $u_\varrho'(x_1) = 0$, $u' > 0$ in $(x_1,\varrho]$ and $u_\varrho' < 0$ in $(0,x_1)$, u_ϱ satisfies (4.15) in $[x_1,\varrho]$, $x + u_\varrho(x)u_\varrho'(x) \ge 0$ in $[0,\varrho]$ as well as

$$\int_{-\varrho}^{\varrho} \kappa_h[u_\varrho]^2 \, ds_h[u_\varrho] \le \mathcal{W}_h(u).$$

Proof. It combines the constructions of Lemmas 3.3 and 3.16 (inserting circular arcs) and those of Lemma 4.31 (inserting catenoidal parts). See Figure 9. We emphasise that these constructions preserve the strict inequalities for the derivatives. The additional properties of u_ϱ are ensured by possibly inserting once more a circular arc or a cosh, respectively, into the shortened function. Observe that (4.15) is certainly satisfied in $x = \varrho$ for any shortened function. $\square$

Notice that if $u(x_0) \geq \mu x_0$ then also $u_\varrho(x_1) \geq \mu x_1$.

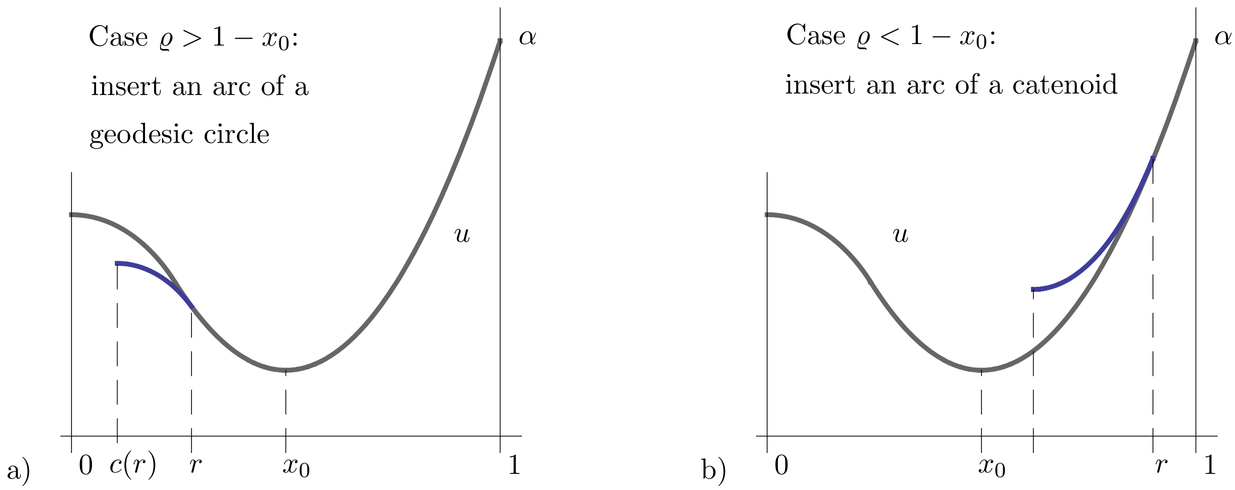


Figure 9: Proof of Lemma 4.32.

Corollary 4.33. *Assume that $u \in N_{\alpha,\beta}$ satisfies (4.17) for some $x_0 \in [0, 1)$ and that u is an admissible function in the sense of Definition 4.26. Then for all $\gamma \in (\alpha, \alpha_\beta]$ we find an admissible function $v \in C^{1,1}([-1, 1], (0, \infty))$ satisfying (4.17) for some $x_1 \in [0, 1)$, $v(\pm 1) = \gamma$, $v'(1) = -\beta$ as well as $\mathcal{W}_h(v) \leq \mathcal{W}_h(u)$.*

Proof. The claim follows from Lemma 4.32 by rescaling and taking $t = \beta$ and $u(1) = \alpha$. $\square$

Before showing monotonicity of the optimal Willmore energy, we prove a result being dual to Lemma 4.14.

Lemma 4.34. *Let $u \in N_{\alpha,\beta}$ be an admissible function in the sense of Definition 4.26 satisfying (4.17) for some $x_0 \in [0, 1)$. Then, there exists an admissible function $v \in N_{\alpha,\beta}$ with lower Willmore energy than u satisfying (4.17) for some $x_1 \in [0, 1)$ and $v(x) > \alpha x$ for all $x \in (0, 1)$ with $v'(x) = -\beta$.*

Proof. Let $\bar{x}$ be the smallest element in $[0, 1]$ such that $u'(\bar{x}) = -\beta$ and $u(\bar{x}) \leq \alpha\bar{x}$. If $\bar{x} = 1$ the claim follows with $v = u$ and $x_1 = x_0$. If $\bar{x} < 1$ and $u(\bar{x}) = \alpha\bar{x}$ the function $v(x) = u(\bar{x}x)/\bar{x}$, $x \in [-1, 1]$, yields the claim with $x_1 = x_0/\bar{x}$. Finally, if $\bar{x} < 1$ and $u(\bar{x}) < \alpha\bar{x}$ by using a scaled version of Lemma 4.32 we shorten the function $u|_{[-\bar{x},\bar{x}]}$ by inserting a cosh or an arc of a circle. For each $\varrho \in (u(\bar{x})/\alpha_\beta, \bar{x})$ there exists $w_\varrho \in C^{1,1}([-\varrho, \varrho], (0, \infty))$ with lower Willmore energy than $u|_{[-\bar{x},\bar{x}]}$ such that $w_\varrho(\pm\varrho) = u(\bar{x})$ and $w_\varrho'(\varrho) = -\beta$. We then choose $\varrho = u(\bar{x})/\alpha$ such that the graph of $u|_{[-\bar{x},\bar{x}]}$ is shortened until we touch the line $y \mapsto \alpha y$. We define v to be equal to the function w_ϱ rescaled to the interval $[-1, 1]$. Notice that $v \in N_{\alpha,\beta}$ is an admissible function and satisfies (4.17) for some $x_1 \in [0, 1)$. It remains to check that if $v'(x) = -\beta$ for some $x \in (0, 1)$ then $v(x) > \alpha x$. The function w_ϱ is given by

$$w_\varrho(x) := \begin{cases} u(x + \bar{x} - \varrho) & \text{if } r \leq x \leq \varrho, \\ g(x) & \text{if } 0 \leq x < r, \end{cases}$$

for some $r \in (0, \varrho)$, and either $g(x) = \cosh(\lambda x)/\lambda$ for some $\lambda > 0$ or g is an arc of a geodesic circle and $g' \leq 0$. If there exists $x \in (0, 1)$ such that $v'(x) = -\beta$ then $w_\varrho'(\varrho x) = -\beta$. Then, either

$\varrho x \in [r, \varrho)$ and $w_\varrho(\varrho x) = u(\varrho x + \bar{x} - \varrho)$, or $\varrho x \in [0, r)$ and $w_\varrho(\varrho x) = \cosh(\lambda \varrho x)/\lambda$. In the first case, since $\varrho x + \bar{x} - \varrho < \bar{x}$ and $\bar{x}$ is the smallest element such that $u'(\bar{x}) = -\beta$ and $u(\bar{x}) \leq \alpha \bar{x}$, then $w_\varrho(\varrho x) = u(\varrho x + \bar{x} - \varrho) > \alpha(\varrho x + \bar{x} - \varrho)$ and so, by $\varrho < \bar{x}$

$$\frac{v(x)}{x} = \frac{w_\varrho(\varrho x)}{\varrho x} = \frac{u(\varrho x + \bar{x} - \varrho)}{\varrho x} > \frac{\alpha(\varrho x + \bar{x} - \varrho)}{\varrho x} > \alpha.$$

In the second case, if $w_\varrho'(\varrho x) = -\beta$ then necessarily $\varrho \lambda x = b$ and so

$$\frac{v(x)}{x} = \frac{w_\varrho(\varrho x)}{\varrho x} = \frac{\cosh(\lambda \varrho x)}{\lambda \varrho x} = \alpha_\beta > \alpha.$$

The claim follows. ☐

Note that $u(x_0) \geq \mu x_0$ implies that $v(x_1) \geq \mu x_1$.

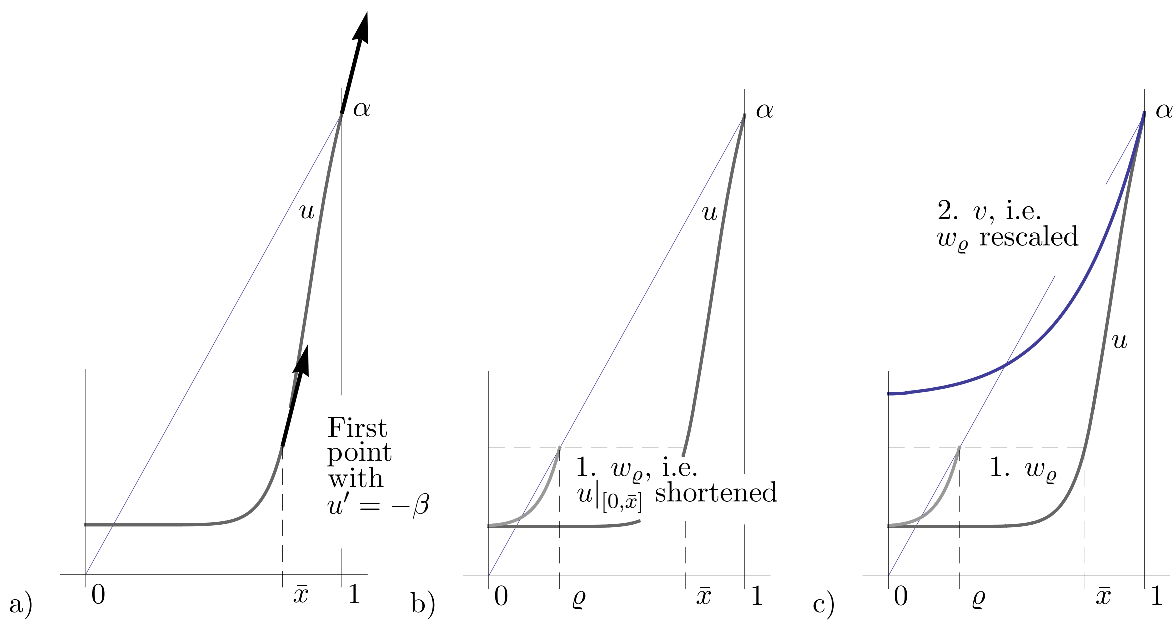


Figure 10: The three main steps of the proof of Lemma 4.34.

Proposition 4.35. *Let $M_{\alpha,\beta}$ be defined as in* (2.7) *and $\alpha < \alpha_\beta$. Then, for $\tilde{\alpha} \leq \alpha$ we have $M_{\tilde{\alpha},\beta} \geq M_{\alpha,\beta}$.*

Proof. By density, we may choose a minimising sequence $(u_k)_{k\in\mathbb{N}} \subset N_{\alpha,\beta}$ for $M_{\tilde{\alpha},\beta}$ consisting of positive symmetric polynomials of degree at least two. These functions are in particular admissible in the sense of Definition 4.26. Then, by Lemma 4.28 there exists a sequence $(v_k)_{k\in\mathbb{N}} \subset N_{\tilde{\alpha},\beta}$ of admissible functions such that v_k satisfies (4.17) for some $x_k \in [0,1)$ and $\mathcal{W}_h(v_k) \leq \mathcal{W}_h(u_k)$. Corollary 4.33 then yields the claim. ☐

4.3.3 The case $\alpha \geq \alpha^*$

In this case we can compare $u \in N_{\alpha,\beta}$ with the catenoids centered at 0 and going through $(1,\alpha)$. As observed in Remark 4.2, these are the functions $x \mapsto \cosh(b_1 x)/b_1$ and $x \mapsto \cosh(b_2 x)/b_2$ with $b_1 = b_1(\alpha)$ and $b_2 = b_2(\alpha)$ the positive real numbers such that $b_1 \leq b^* \leq b_2$ and $\cosh(b_1)/b_1 = \alpha = \cosh(b_2)/b_2$, with b^* the solution of $\cosh(b^*) = b^* \sinh(b^*)$. Since $\alpha < \alpha_\beta$ one sees that or

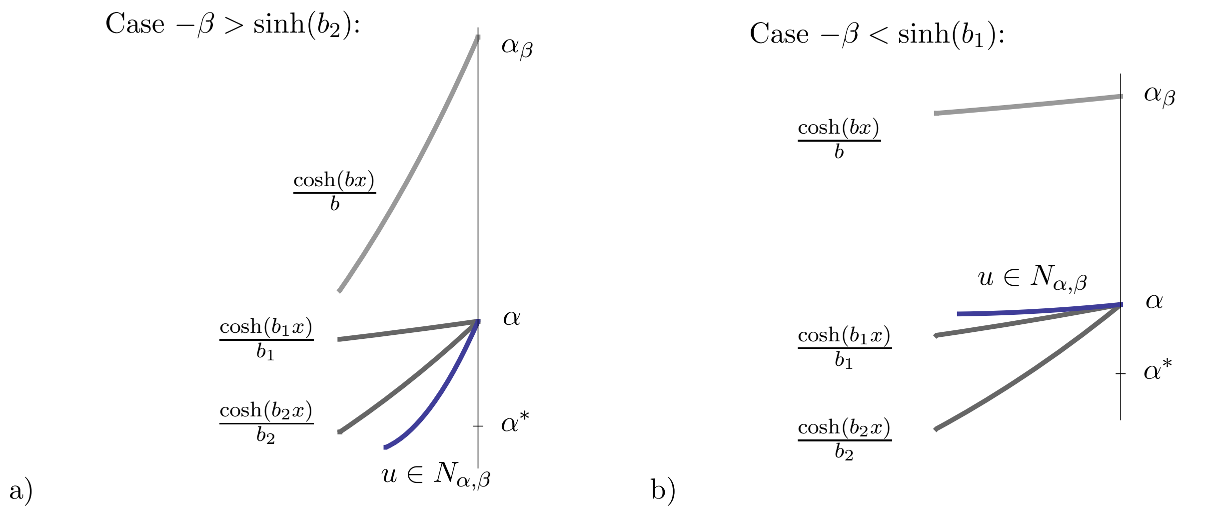


Figure 11: Two possibilities for the behaviour near 1 of the graph of $u \in N_{\alpha,\beta}$ when $\alpha^* \le \alpha < \alpha_\beta$. Compare with Figure 5.

$-\beta < \sinh(b_1)$ or $-\beta > \sinh(b_2)$ (see Figure 11). Notice that since $\sinh(b_1) \le \alpha \le \sinh(b_2)$, these two cases correspond to the two cases $-\beta < \alpha$ and $-\beta \ge \alpha$ that we have treated separately also in the case $\alpha > \alpha_\beta$.

By comparing $u \in N_{\alpha,\beta}$ with the catenoids we show that in the case $-\beta < \sinh(b_1) \le \alpha$ it is sufficient to consider functions $u \in N_{\alpha,\beta}$ such that $u(x) \ge \cosh(b_1x)/b_1$, i.e. remaining above the larger of the two catenoids. This in particular implies $u(x) \ge \alpha x$. This together with Lemma 4.30 gives bounds on the derivative. In the case $-\beta > \sinh(b_2) \ge \alpha$ we first prove bounds on the derivative using Lemmas 4.30 and 4.34. Then, by Lemma 4.9 we get a bound from below for the function.

Properties of minimising sequences

In the next lemmas it is convenient to distinguish the cases $-\beta < \sinh(b_1)$ and $-\beta > \sinh(b_2)$ because of the different behaviour with respect to the line $y \mapsto \alpha y$. Recall that $b_1 = b_1(\alpha)$ and $b_2 = b_2(\alpha)$ are the positive real numbers such that $b_1 \le b^* \le b_2$ and $\cosh(b_1)/b_1 = \alpha = \cosh(b_2)/b_2$, with b^* being the solution of $\cosh(b^*) = b^* \sinh(b^*)$.

Lemma 4.36. *We assume in addition that $-\beta < \sinh(b_1)$. Let $u \in N_{\alpha,\beta}$ be an admissible function in the sense of Definition 4.26. Assume furthermore that (4.17) is satisfied for some $x_0 \in [0,1)$ and that $u'(x) \ne -\beta$ for all $x \in [0,1)$ with $u(x) \le \alpha x$. Then, $u(x) \ge \cosh(b_1x)/b_1$ and $u'(x) \le \sinh(b_1x)$ in $[0,1)$.*

Proof. Since $-\beta < \sinh(b_1) \le \alpha$, $u(x) > \cosh(b_1x)/b_1$ in a left neighbourhood of 1. Moreover, since u satisfies (4.17) (in particular (4.15) in $[x_0,1]$) one sees as long as $u(x) \ge \cosh(b_1x)/b_1$ in $[x_0,1]$ that

$$\frac{\cosh(b_1x)}{b_1x} \le \frac{u(x)}{x} \le \frac{\cosh(\operatorname{arsinh}(u'(x)))}{\operatorname{arsinh}(u'(x))}.$$

Since $\operatorname{arsinh}(u'(1)) < b_1 \le b^*$, we conclude by continuity that $u'(x) \le \sinh(b_1x)$. Hence, $u(x) > \frac{1}{b_1}\cosh(b_1x)$ on $[x_0,1)$ and so, also in $[0,1)$. □

Lemma 4.37. *We assume in addition that $-\beta > \sinh(b_2)$. Let $u \in N_{\alpha,\beta}$ be an admissible function in the sense of Definition 4.26. Assume furthermore that (4.17) is satisfied for some $x_0 \in [0,1)$ and that $u'(x) \ne -\beta$ for all x with $u(x) \le \alpha x$. Then, there exists an admissible function $v \in N_{\alpha,\beta}$*

with lower Willmore energy than u, which satisfies (4.17) *for some $x_1 \in [0, x_0]$ and $v'(x) \le -\beta$ in* $[0, 1]$.

Proof. Since $-\beta > \sinh(b_2) \ge \frac{\cosh(b_2)}{b_2} = \alpha$, $u(x) < \alpha x$ in a left neighbourhood of 1. Let x_1 be the biggest element in $(0, 1)$ such that $u(x_1) = \alpha x_1$ and $u'(x_1) \le \alpha$. Such an element exists since $u(0) > 0$. Since $u'(x_1) \le \alpha < -\beta$ and $u' \ne -\beta$ in $(x_1, 1)$ we have $u' \le -\beta$ in $[x_1, 1]$.

If $u'(x_1) < \alpha$ then $u'(x) < \alpha$ also in a left neighbourhood of x_1 and $u(x) > \alpha x$ in this neighbourhood. Hence by Lemma 4.30 for these points $u'(x) < \sinh(b_1)$. Since $\sinh(b_1) \le \frac{\cosh(b_1)}{b_1} = \alpha$, then, by continuity, $u(x) > \alpha x$ and $u'(x) \le \sinh(b_1) \le -\beta$ for all $x \in [0, x_1]$.

From Lemma 4.30 it follows also that $u'(x_1) = \alpha$ can hold only if $\alpha = \alpha^*$ since $\sinh(b_1) < \alpha < \sinh(b_2)$ for $\alpha \ne \alpha^*$. Hence for $\alpha > \alpha^*$ the claim is proved with $u = v$. If $\alpha = \alpha^*$ and $u'(x_1) = \alpha^*$ then we substitute u in $[-x_1, x_1]$ by the function $\cosh(\lambda x)/\lambda$ with $\lambda = b^*/x_1$ and b^* defined in (1.5). We get a new function $v \in N_{\alpha,\beta}$ with lower Willmore energy than u and such that v satisfies (4.17) with $x_1 = 0$, $v'(x) \le \alpha^*$ and $v(x) \ge \alpha^* x$ in $[0, x_1]$. □

The following proposition characterises suitably modified minimising sequences.

Proposition 4.38. *Let $(u_k)_{k\in\mathbb{N}}$ be a minimising sequence for $M_{\alpha,\beta}$ of admissible functions in the sense of Definition 4.26 in $N_{\alpha,\beta}$ such that $\mathcal{W}_h(u_k) \le M_{\alpha,\beta} + 1$ for all $k \in \mathbb{N}$. Then, there exists a minimising sequence $(v_k)_{k\in\mathbb{N}} \subset N_{\alpha,\beta}$ of admissible functions satisfying* (4.17), *$\mathcal{W}_h(v_k) \le \mathcal{W}_h(u_k)$ and*

$$\max\big\{-\beta, \sinh(b_1)\big\} \ge v_k'(x) \ge -\frac{\operatorname{arsinh}(-\beta)}{\alpha}(\alpha_\beta - \alpha) \quad \textit{and} \quad C_{\alpha,\beta} \le v_k(x) \le \sqrt{1 + \alpha^2 - x^2}, \tag{4.18}$$

in $[0, 1]$ with a constant $C_{\alpha,\beta} > 0$ depending on α, $-\beta$ and $M_{\alpha,\beta}$.

Proof. By Lemmas 4.28, 4.34, 4.36 if $-\beta < \sinh(b_1)$ or 4.37 if $-\beta > \sinh(b_2)$, and Lemma 4.29 for each u_k there exists $v_k \in N_{\alpha,\beta}$ with lower Willmore energy than u_k such that v_k satisfies (4.17) for some $x_k \in [0, 1)$ and

$$v_k'(x) \le \max\{-\beta, \sinh(b_1)\} \qquad \text{and} \qquad v_k(x_k) \ge \frac{\alpha}{\operatorname{arsinh}(-\beta)(\alpha_\beta - \alpha)} x_k. \tag{4.19}$$

Since v_k satisfies (4.16) we get $v_k(x) \le \sqrt{1 + \alpha^2 - x^2}$ in $[0, 1]$ and

$$v_k'(x) \ge -\frac{x}{v_k(x)} \ge -\frac{x_k}{v_k(x_k)} \ge -\operatorname{arsinh}(-\beta)\frac{\alpha_\beta - \alpha}{\alpha} \qquad \text{for } x \in [0, x_k],$$

while $v_k' \ge 0$ in $[x_k, 1]$. The estimate from below for v_k follows from the second estimate in (4.19) if $x_k \ge 1/2$ and from Lemma 4.9 if $x_k \le 1/2$. □

Proof of the existence theorem

We recall here that for $\alpha \ge \alpha^*$, $b_1 = b_1(\alpha)$ denotes the positive real number such that $\cosh(b_1)/b_1 = \alpha$ and $b_1 \le b^*$ with b^* being the solution of $\cosh(b^*) = b^* \sinh(b^*)$.

Theorem 4.39 (Existence and regularity). *For $\beta < 0$ and α such that $\alpha^* \le \alpha < \alpha_\beta$ there exists a function $u \in C^\infty([-1, 1], (0, \infty))$ such that the corresponding surface of revolution $\Gamma \subset \mathbb{R}^3$ solves the Dirichlet problem* (1.4). *This solution is positive and symmetric, has at most one critical point in* $(0, 1)$, *and satisfies*

$$\max\big\{\sinh(b_1), -\beta\big\} \ge u'(x) \ge -(\alpha - \alpha_\beta)\frac{\operatorname{arsinh}(-\beta)}{\alpha} \ \textit{ in } (0, 1)$$
$$\textit{and} \quad \sqrt{1 + \alpha^2 - x^2} \ge u(x) \ge C_{\alpha,\beta} \ \textit{ in } [-1, 1],$$

with a constant $C_{\alpha,\beta} > 0$ depending on $M_{\alpha,\beta}$, α and $-\beta$.

Proof. By density of polynomials in $H^2(-1,1)$ a minimising sequence $(u_k)_{k\in\mathbb{N}}$ for $M_{\alpha,\beta}$ may be chosen in $N_{\alpha,\beta}$ which consists of positive symmetric polynomials of degree at least two and such that $\mathcal{W}_h(u_k) \le M_{\alpha,\beta}+1$ for all $k \in \mathbb{N}$. By Proposition 4.38 we may assume that each element u_k of the minimising sequence satisfies (4.18). The rest of the proof is along the lines of Theorem 3.11. Moreover, with the construction of Lemma 4.27 one can prove that u has at most one critical point in $(0,1)$. □

Reasoning as in the proof of Propositions 3.12 and 4.18, one can prove that the energy is strictly decreasing in α.

Proposition 4.40. *Let $M_{\alpha,\beta}$ be as defined in* (2.7) *and $\alpha^* \le \alpha < \alpha_\beta$. Then $M_{\widetilde{\alpha},\beta} > M_{\alpha,\beta}$ for all $\widetilde{\alpha} \in (\alpha^*, \alpha)$.*

4.3.4 The case $\alpha < \alpha^*$

In this case no catenoid is going through the points $(\pm 1, \alpha)$ which $u \in N_{\alpha,\beta}$ can be compared with. However, the results from the previous subsection will be useful also here. Since $u \in N_{\alpha,\beta}$ is strictly positive, going from the right to the left, there exists certainly a first point $\bar{x}$ where $u(\bar{x}) = \alpha^*\bar{x}$. From here on, we may refer to the geometric constructions which led to suitable minimising sequences as described in Proposition 4.38.

The difficulty is now to understand how the graph of a suitable function $u \in N_{\alpha,\beta}$ should behave or should be suitably modified before reaching the line $y \mapsto \alpha^* y$. By Lemma 4.34 it is sufficient to consider functions where $u' \ne -\beta$ when we are below the line $y \mapsto \alpha y$. This result gives a bound on the derivative when the graph of u is below the line $y \mapsto \alpha y$. Hence, it remains to get an estimate on u' on the set $\{x : \alpha x < u(x) < \alpha^* x\}$. To this end we study the function $u(x)/x$. In order to ensure that $u(x)/x$ has only finitely many oscillations in $[0,1]$ we restrict ourselves to admissible functions as defined in Definition 4.26. Going from the left to the right, we prove that the function $u(x)/x$ is decreasing from the first and only point where the graph of u crosses the line $y \mapsto \alpha^* y$ to the point where it crosses or touches the line $y \mapsto \alpha y$. This leads to bounds for the derivative on suitably modified minimising sequences.

Properties of minimising sequences

We start by showing that, going from the right to the left, once the graph of u reaches the line $y \mapsto \alpha^* y$, then one may achieve that it remains above this line.

Lemma 4.41. *Let $u \in N_{\alpha,\beta}$ be an admissible function in the sense of Definition 4.26 satisfying* (4.17) *for some $x_0 \in [0,1)$. Let $\bar{x}$ be such that $u(\bar{x}) = \alpha^*\bar{x}$ and $u(x) < \alpha^* x$ in $(\bar{x}, 1]$.*

Then there exists an admissible function $v \in N_{\alpha,\beta}$ with $\mathcal{W}_h(u) \ge \mathcal{W}_h(v)$ and satisfying (4.17) *for some $x_1 \in [0,1)$. Moreover, $v(\bar{x}) = \alpha^*\bar{x}$, $v(x) < \alpha^* x$ in $(\bar{x}, 1]$ and $v(x) \ge \cosh(b^* x/\bar{x})\bar{x}/b^* > \alpha^* x$ as well as $v'(x) < \alpha^*$ in $[0, \bar{x})$.*

Proof. We have $u'(\bar{x}) \le \alpha^*$. If $u'(\bar{x}) < \alpha^*$ then $u(x) > \cosh(b^* x/\bar{x})\bar{x}/b^*$ in a left neighbourhood of $\bar{x}$. Since u satisfies (4.17) one sees as in the proof of Lemma 4.36 that $u(x) > \cosh(b^* x/\bar{x})\bar{x}/b^* > \alpha^* x$ and $u'(x) < \alpha^*$ for all $x \in [0, \bar{x}]$. The claim then follows with $v = u$.

If instead $u'(\bar{x}) = \alpha^*$ then we substitute u in $[-\bar{x}, \bar{x}]$ by $\cosh(b^* x/\bar{x})\bar{x}/b^*$. We get a new admissible function $v \in N_{\alpha,\beta}$ with lower Willmore energy than u and $v(x) > \alpha^* x$ as well as $v'(x) < \alpha^*$ in $(0, \bar{x})$. □

Notice that in the previous lemma if $u(x) \ge \alpha x$ then also $v(x) \ge \alpha x$. Moreover, if $u(x_0) \ge \mu x_0$ then also $v(x_1) \ge \mu x_1$.

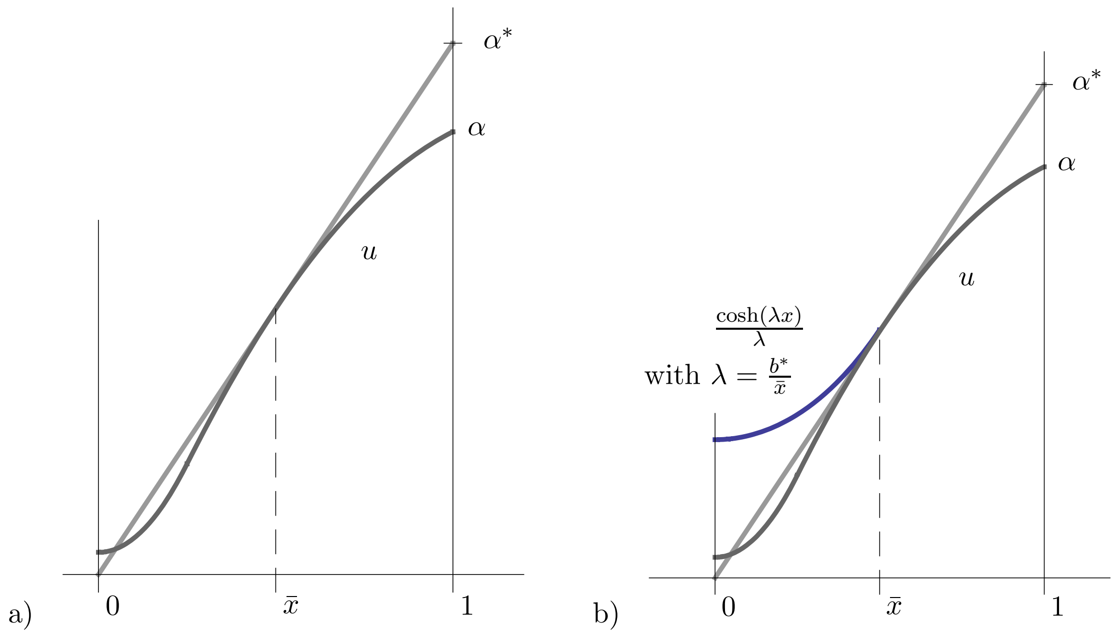


Figure 12: Proof of Lemma 4.41 in the case where $u \in N_{\alpha,\beta}$ is tangent in $\bar{x}$ to the line $y \mapsto \alpha^* y$.

The aim of the next constructions is to show for functions u as in Lemma 4.41 one may achieve that $u(x)/x$ is decreasing for $x \in (0,1)$ where $\alpha x < u(x) < \alpha^* x$. As in Lemma 4.32, they are based on inserting parts of geodesic circles and catenoids to shorten the intervals and decrease the Willmore energy. Assuming $u(1) < \alpha^*$ we study now additional properties inherited by the shortened function u_ϱ.

In the next result we prove that if $u(x)/x$ is decreasing in $\{x \in (0,1) : u(1)x \le u(x) \le \alpha^* x\}$ and $u(x) \ge u(1)x$ then, when $\varrho \ge u(1)/\alpha^*$, also $u_\varrho(x)/x$ is decreasing in $\{x \in (0,\varrho) : u(1)x \le u_\varrho(x) \le \alpha^* x\}$ and $u_\varrho(x) \ge u(1)x/\varrho$. Notice that the result holds when we shorten the graph of u until we reach the line $y \mapsto \alpha^* y$ but not until $y \mapsto \alpha_\beta y$.

Proposition 4.42. *Fix $t < 0$. Let $u \in C^{1,1}([-1,1],(0,\infty))$ be an admissible function in the sense of Definition 4.26 satisfying (4.17) for some $x_0 \in [0,1)$, $u(x) \ge u(1)x$ in $[0,1]$, $u'(1) = -t$ and $u(1) < \alpha^*$. Moreover, for $\varrho \in [u(1)/\alpha^*, 1]$, let u_ϱ be the function constructed in Lemma 4.32. Then*

$$u_\varrho(x) \ge \frac{u(1)}{\varrho} x \quad \textit{for all} \quad x \in [0,\varrho]$$

and u_ϱ satisfies (4.17) on $[0,\varrho)$ for some $\hat{x} \in [0,\varrho)$.

Furthermore, if there exists $\bar{x} \in (0,1)$ such that $u(x) \ge \alpha^* x$ for all $x \in [0,\bar{x}]$, $u(x) < \alpha^* x$ for all $x \in (\bar{x},1]$ and $u(x)/x$ is decreasing in $[\bar{x},1]$, then there exists $\widetilde{x} \in (0,\varrho)$ such that $u_\varrho(x) \ge \alpha^* x$ for all $x \in [0,\widetilde{x}]$, $u_\varrho(x) < \alpha^* x$ for all $x \in (\widetilde{x},\varrho]$ and $u_\varrho(x)/x$ is decreasing in $[\widetilde{x},\varrho]$.

Proof. For $\varrho \in [u(1)/\alpha^*, 1]$ there exists $r' \in [0,\varrho)$ such that u_ϱ is given in $[0,\varrho]$ by

$$u_\varrho(x) = \begin{cases} u(1+x-\varrho) & \text{if } r' \le x \le \varrho, \\ f(x) & \text{if } 0 \le x < r', \end{cases}$$

where f is either an arc of a circle (and $u_\varrho'(r') \le 0$) or a $\cosh(\lambda x)/\lambda$ for $\lambda \in \mathbb{R}^+$. The first claim is satisfied in $[0,r']$ since if f is a cosh then $u_\varrho(x) \ge \alpha^* x$ and $\alpha^* x \ge u(1)x/\varrho$ by assumption. On the other hand if f is a circular arc then

$$\frac{u_\varrho(x)}{x} = \frac{f(x)}{x} \ge \frac{f(r')}{r'} = \frac{u(r'+1-\varrho)}{r'} \ge u(1)\frac{r'+1-\varrho}{r'} \ge \frac{u(1)}{\varrho}.$$

For $x \in [r', \varrho]$ we have

$$\frac{u_\varrho(x)}{x} = \frac{u(x+1-\varrho)}{x} \geq u(1)\frac{x+1-\varrho}{x} \geq \frac{u(1)}{\varrho}.$$

For the second claim let $\widetilde{x}$ be the biggest element in $[0, \varrho]$ such that $u_\varrho(x) \geq \alpha^* x$ in $[0, \widetilde{x}]$. We first treat the case when $f(x) = \cosh(\lambda x)/\lambda$. Since $\cosh(\lambda x)/\lambda \geq \alpha^* x$ then $\widetilde{x} \geq r'$. Moreover, since $u(\widetilde{x} + 1 - \varrho) = u_\varrho(\widetilde{x}) = \alpha^* \widetilde{x} < \alpha^*(\widetilde{x} + 1 - \varrho)$ we necessarily have $\widetilde{x} + 1 - \varrho > \bar{x}$. So, for $x > \widetilde{x}$ we have

$$u_\varrho(x) = \frac{u(x+1-\varrho)}{x+1-\varrho}(x+1-\varrho) \leq \frac{u(\widetilde{x}+1-\varrho)}{\widetilde{x}+1-\varrho}(x+1-\varrho) = \frac{\alpha^*\widetilde{x}}{\widetilde{x}+1-\varrho}(x+1-\varrho) < \alpha^* x, \quad (4.20)$$

giving $u_\varrho(x) < \alpha^* x$ in $(\widetilde{x}, \varrho]$. Since $u(x)/x$ is decreasing in $(\bar{x}, 1]$ then $u'(x) \leq u(x)/x$ in $(\bar{x}, 1]$. Using that $\bar{x} < \widetilde{x} + 1 - \varrho$ we find for $x \in (\widetilde{x}, \varrho]$

$$u'_\varrho(x) = u'(x+1-\varrho) \leq \frac{u(x+1-\varrho)}{x+1-\varrho} = \frac{u_\varrho(x)}{x}\frac{x}{x+1-\varrho} < \frac{u_\varrho(x)}{x}, \quad (4.21)$$

showing that $u_\varrho(x)/x$ is decreasing in $[\widetilde{x}, \varrho]$.

If instead $f(x)$ is a circular arc of a circle we need to distinguish two cases. If $\widetilde{x} \geq r'$ then we reason as in (4.20) and (4.21). If instead $\widetilde{x} < r'$ then $u_\varrho(x) < \alpha^* x$ and $u_\varrho(x)/x$ is decreasing in $(\widetilde{x}, r']$ since $u'_\varrho \leq 0$ in $[0, r']$. In particular $u(r' + 1 - \varrho) = u_\varrho(r') < \alpha^* r'$ and so $r' + 1 - \varrho > \bar{x}$. It then follows for $x \in [r', \varrho]$ that

$$u_\varrho(x) = \frac{u(x+1-\varrho)}{x+1-\varrho}(x+1-\varrho) \leq \frac{u(r'+1-\varrho)}{r'+1-\varrho}(x+1-\varrho) < \alpha^* \frac{r'(x+1-\varrho)}{r'+1-\varrho} \leq \alpha^* x,$$

and proceeding as in (4.21) one shows that $u_\varrho(x)/x$ is decreasing also in $[r', \varrho]$. $\square$

Thanks to the previous proposition we may now show that if $u(x) \geq u(1)x$ in $[0, 1]$ and $u(1) < \alpha^*$, then we can also assume that $u(x)/x$ is decreasing on the set $\{x \in (0, 1] : u(x) \leq \alpha^* x\}$.

Proposition 4.43. *Let $u \in C^{1,1}([-1, 1], (0, \infty))$ be a admissible function in the sense of Definition 4.26 satisfying (4.17) for some $x_0 \in [0, 1)$, $u'(1) > 0$ and $u(1) < \alpha^*$. We assume further that $u(x) > u(1)x$ in $(0, 1)$ and that there exists $\bar{x} \in (0, 1)$ with $u(x) \geq \alpha^* x$ in $[0, \bar{x}]$ and $u(x) < \alpha^* x$ in $(\bar{x}, 1]$.*

Then, there exists a admissible function $v \in C^{1,1}([-1, 1], (0, \infty))$ with $v'(1) = u'(1)$, $u(1) = v(1)$, $\mathcal{W}_h(u) \geq \mathcal{W}_h(v)$ and satisfying (4.17) for some $\hat{x} \in [0, 1)$. Moreover, there exists $\widetilde{x} \in (0, 1)$ so that $v(x) \geq \alpha^* x$ in $[0, \widetilde{x}]$ and $v(x) < \alpha^* x$ for all $x \in (\widetilde{x}, 1]$ and $v(x)/x$ is decreasing in $[\widetilde{x}, 1]$.

Proof. By assumption $u(x)/x < u(\bar{x})/\bar{x}$ in a right neighbourhood of $\bar{x}$ and $u(x)/x > u(1)/1$ in a left neighbourhood of 1. If $u(x)/x$ is decreasing in $[\bar{x}, 1]$ the claim follows with $v = u$. Otherwise there exists a first local minimum x_1 of $u(x)/x$ in $[\bar{x}, 1]$. By our definition of admissibility this minimum is strict. For easy notation let α' denote $u(x_1)/x_1$. Notice that $u(1) < \alpha' < \alpha^*$ and that $u'(x_1) = \alpha'$. Let x_3 be the smallest element in $(x_1, 1]$ with $u(x_3) = \alpha' x_3$ and x_2 be the largest element in (x_1, x_3) with $u'(x_2) = \alpha'$. Then $u(x) > \alpha' x$ for $x \in (x_1, x_3)$. For $x \in (x_2, x_3)$ we see that $x^2(\frac{u}{x})' = xu' - u < x\alpha' - x\alpha' = 0$, i.e. $x \mapsto \frac{u}{x}$ is strictly decreasing on (x_2, x_3) so that it has a local maximum on (x_1, x_2).

The idea is to replace $u|_{[-x_2, x_2]}$ by the appropriately shortened and rescaled $u|_{[-x_1, x_1]}$ according to Proposition 4.42. For this new function v the number of local extrema of $x \mapsto v(x)/x$ below the line $y \mapsto \alpha^* y$ has decreased by at least two. Since $x \mapsto u(x)/x$ has only finitely many local

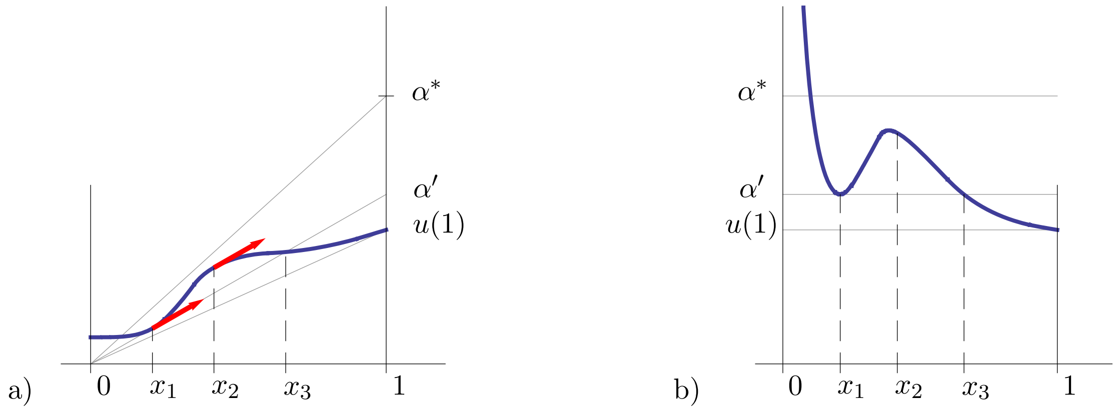


Figure 13: Proof of Proposition 4.43. In x_1 and x_2 the tangents are parallel. $u|_{[-x_1,x_1]}$ is shortened and rescaled. So, we avoid oscillations of $x \mapsto u(x)/x$ decreasing the Willmore energy.

extrema, after finitely many iterations we obtain the claim. We present this argument now in detail.

By using a scaled version of Proposition 4.42 we shorten the function $u|_{[-x_1,x_1]}$ by inserting a cosh or an arc of a circle. For each $\varrho \in [u(x_1)/\alpha^*, x_1]$ there exists a symmetric admissible $w_\varrho \in C^{1,1}([-\varrho,\varrho],(0,\infty))$ with $w_\varrho(\pm\varrho) = u(x_1)$, $w_\varrho'(\varrho) = \alpha' = u'(x_1)$ and lower Willmore energy than $u|_{[-x_1,x_1]}$. We choose $\varrho = u(x_1)x_2/u(x_2)$ so that we shorten the graph of $u|_{[-x_1,x_1]}$ until the line $y \mapsto u(x_2)y/x_2$ is reached. By $\frac{u(x_2)}{x_2} > \frac{u(x_1)}{x_1}$ and $u(x_2) < \alpha^* x_2$ we see that indeed $\varrho \in [u(x_1)/\alpha^*, x_1]$. Moreover, since $u(x) \geq \alpha^* x$ in $[0,\bar{x}]$ and $u(x)/x$ is decreasing in $[\bar{x}, x_1]$ then by Proposition 4.42, there exists x' such that $w_\varrho(x) \geq \alpha^* x$ in $[0, x']$ and $w_\varrho(x)/x$ is decreasing in $[x', \varrho]$. The function v equal to u in $[x_2, 1]$ and to the rescaled w_ϱ in $[0, x_2]$ is admissible and has the same boundary values as u. Finally, v satisfies (4.17) for some $\hat{x} \in [0,1)$ and there exists $\widetilde{x}$ such that $v(x) \geq \alpha^* x$ in $[0,\widetilde{x}]$ and $v(x) < \alpha^* x$ in $[\widetilde{x}, 1]$ and $v(x)/x$ has on $[\widetilde{x}, 1]$ at least two local extrema less than $u(x)/x$ in $[\bar{x}, 1]$.

Since $u(x)/x$ has only finitely many local extrema, the claim is proved by finitely many iterations. □

Notice that if $u(x_0) \geq \mu x_0$ then also $v(\hat{x}) \geq \mu \hat{x}$.

The previous proposition is the main ingredient which allows us to pass to functions with uniformly bounded derivatives. For this purpose, we distinguish again the cases $\alpha \geq -\beta$ and $\alpha < -\beta$.

The case $\alpha \geq -\beta$

In the next lemma we prove that in the case $\alpha \geq -\beta$ it is sufficient to consider functions satisfying $u(x) \geq \alpha x$ in $[0,1]$.

Lemma 4.44. *We assume in addition that $\alpha \geq -\beta$. Let $u \in N_{\alpha,\beta}$ be an admissible function in the sense of Definition 4.26 satisfying* (4.17) *for some $x_0 \in [0,1)$ and $u'(x) \neq -\beta$ for all $x \in [0,1)$ with $u(x) \leq \alpha x$.*

Then, there exists an admissible function $v \in N_{\alpha,\beta}$ with lower Willmore energy than u, satisfying $v(x) > \alpha x$ for all $x \in [0,1)$ and (4.17) *for some $x' \in [0,1)$.*

Proof. We assume first that even $\alpha > -\beta$ so that $u(x) > \alpha x$ in a left neighbourhood of 1. If $u(x) \leq \alpha x$ for some $x \in (0,1)$ then there exists a smallest element x_1 in $[0,1]$ such that $u(x_1) = \alpha x_1$. Let $x_2 \geq x_1$ be the smallest element such that $u'(x_2) = \alpha$ and $u(x_2) \leq \alpha x_2$. If $u(x)/x \geq u(x_2)/x_2$

for all $x \in (0, x_2]$ we denote x_2 by $\bar{x}$. Otherwise, $\bar{x}$ denotes the largest element in $(0, x_2)$ such that $u(x)/x \geq u(\bar{x})/\bar{x}$ for all $x \in (0, \bar{x}]$. Then $u(\bar{x}) \leq \alpha\bar{x}$, $u'(\bar{x}) \leq \alpha$ and, by assumption, $u'(\bar{x}) > -\beta$. Let $\widetilde{x} \in [x_2, 1]$ be the biggest element such that $u'(\widetilde{x}) = u'(\bar{x})$ and $u(\widetilde{x}) > \alpha\widetilde{x}$. Such an element exists since $-\beta < \alpha$.

We notice first that $u(\widetilde{x}) < \alpha^*\widetilde{x}$. Indeed, if $u(\widetilde{x}) \geq \alpha^*\widetilde{x}$ since $u'(\widetilde{x}) \leq \alpha < \alpha^*$ then $u(x) > \alpha^* x$ in a left neighbourhood of $\widetilde{x}$ and by Lemma 4.30 for these points $u'(x) < \alpha^*$ and by continuity of u and of its derivative then $u(x) \geq \alpha^* x$ for all $x \in [0, \tilde{x}]$. This contradicts the assumption that $u(x) < \alpha x$ in some interval.

The construction is now done similarly to Proposition 4.43. By using a scaled version of Proposition 4.42 we shorten the function $u|_{[-\bar{x},\bar{x}]}$ by inserting a cosh or an arc of a circle. We shorten it until we reach the line $y \mapsto u(\widetilde{x})y/\widetilde{x}$. That is, we consider the function w_ϱ with $\varrho = u(\bar{x})\widetilde{x}/u(\widetilde{x})$ constructed by a rescaled version of Proposition 4.42 applied to $u|_{[-\bar{x},\bar{x}]}$. Since $u(x)/x \geq u(\bar{x})/\bar{x}$ in $(0, \bar{x}]$ then by the first claim in Proposition 4.42, we have $w_\varrho(x) \geq w_\varrho(\varrho)x/\varrho$ in $(0, \varrho]$. Hence, the function v which is equal to u in $[\widetilde{x}, 1]$ and equal to the rescaled w_ϱ in $[0, \widetilde{x}]$ yields the claim.

If $\alpha = -\beta$, let $\bar{x} \in (0, 1]$ be the smallest element such that $v(\bar{x}) = \alpha\bar{x}$. By the assumptions it follows that $\bar{x} = 1$. Indeed, if $\bar{x} < 1$ then, $u'(\bar{x}) \leq \alpha = -\beta$ and the assumption gives $u'(\bar{x}) < -\beta = \alpha$. But there exists then $x' > \bar{x}$ such that $v'(x') = \alpha = -\beta$ and $v(x') < \alpha x'$, a contradiction. □

We may now assume that $u(x) \geq \alpha x$ in $[0, 1]$. In the next corollary, we first observe that the set $\{x \in [0, 1] : \alpha x \leq u(x) \leq \alpha^* x\}$ is an interval and then, by using Proposition 4.43, we show that we may assume that in this interval $u(x)/x$ is decreasing. This yields suitable a priori bounds.

Corollary 4.45. *Let α be such that $\alpha \geq -\beta$. Let $u \in N_{\alpha,\beta}$ be an admissible function in the sense of Definition 4.26 satisfying* (4.17) *for some $x_0 \in [0, 1)$, $u'(x) \neq -\beta$ for all $x \in [0, 1)$ with $u(x) \leq \alpha x$.*

Then, there exists an admissible function $v \in N_{\alpha,\beta}$ with lower Willmore energy than u and satisfying $v'(x) \leq \alpha^*$ in $[0, 1]$ and $v(x) > \alpha x$ in $[0, 1)$ as well as (4.17) *for some $x_1 \in [0, 1)$.*

Proof. By Lemmas 4.44 and 4.41 and the following remark, there exists $w \in N_{\alpha,\beta}$ with lower Willmore energy than u such that $w(x) > \alpha x$ in $[0, 1)$, w satisfies (4.17) for some $x' \in [0, 1)$ and so that there exists $\bar{x} \in (0, 1)$ such that $w(x) \geq \alpha^* x$ in $[0, \bar{x}]$ and $w(x) < \alpha^* x$ in $(\bar{x}, 1]$. By Proposition 4.43 there exists $v \in N_{\alpha,\beta}$ with lower Willmore energy than w such that v satisfies (4.17) for some $x_1 \in [0, 1)$ and so that there exists $x_2 \in (0, 1)$ such that $v(x) \geq \alpha^* x$ in $[0, x_2]$ and $v(x)/x$ is decreasing in $[x_2, 1]$. This shows in particular that $v(x) > \alpha x$ in $[0, 1)$. Since $v'(x) \leq v(x)/x$ in $[x_2, 1]$ we find $v'(x) \leq \alpha^*$ in $[x_2, 1]$. Reasoning as in Lemma 4.41 we get $v'(x) \leq \alpha^*$ in $[0, 1]$. □

The case $\alpha < -\beta$

The next result corresponds to Corollary 4.45. We first observe that we have a bound on the derivative when the graph of u is below the line $y \mapsto \alpha y$. Then, when the graph of u crosses this line, we are back in the previous case.

Corollary 4.46. *We assume in addition that $-\beta > \alpha$. Let $u \in N_{\alpha,\beta}$ be an admissible function in the sense of Definition 4.26 satisfying* (4.17) *for some $x_0 \in [0, 1)$ and $u'(x) \neq -\beta$ for all $x \in [0, 1)$ with $u(x) \leq \alpha x$.*

Then, there exists an admissible function $v \in N_{\alpha,\beta}$ with lower Willmore energy than u, satisfying (4.17) *for some $x_1 \in [0, 1)$ and $v'(x) \leq \max\{-\beta, \alpha^*\}$ on $[0, 1]$.*

Proof. Let $w \in N_{\alpha,\beta}$ be the function constructed in Lemma 4.41 such that $\mathcal{W}_h(w) \leq \mathcal{W}_h(u)$, w satisfies (4.17) for some $\widetilde{x} \in [0, 1)$ and there exists $\bar{x} \in (0, 1)$ with $w(x) \geq \alpha^* x$ in $[0, \bar{x}]$ and

$w(x) < \alpha^* x$ in $(\bar{x}, 1]$. Notice that by the construction also w satisfies that $w'(x) \neq -\beta$ for all $x \in [0,1)$ with $w(x) < \alpha x$. Let x_2 be the biggest element in $(0,1)$ such that $w(x_2) = \alpha x_2$. Then for all $x \in (x_2, 1)$ we have $w(x) < \alpha x$ and $w'(x) < -\beta$.

If $\widetilde{x} \geq x_2$ the claim follows with $v = w$ and $x_1 = \widetilde{x}$. Otherwise, since $w(x_2) = \alpha x_2 < \alpha^* x_2$ and $w'(x_2) \leq \alpha$ then $w(x_2)/x_2 \geq w'(x_2)$. Hence, applying a rescaled version of Lemma 4.44 and of Corollary 4.45 to $w|_{[-x_2, x_2]}$ we find an admissible function $v \in C^{1,1}([-x_2, x_2], (0, \infty))$ with lower Willmore energy than $w|_{[-x_2, x_2]}$ with the same boundary values and such that $v(x) > \alpha x$ in $[0, x_2)$ and $v'(x) \leq \alpha^*$ in $[0, x_2)$. Defining $v(x) = w(x)$ for $x \in [x_2, 1]$ and extending v by symmetry to the interval $[-1, 1]$ yields the claim. □

Characterisation of suitable minimising sequences

The following proposition characterises suitably modified minimising sequences. We do not need to distinguish the cases $\alpha \geq -\beta$ and $\alpha < -\beta$.

Proposition 4.47. *Let $(u_k)_{k\in\mathbb{N}}$ be a minimising sequence for $M_{\alpha,\beta}$ in $N_{\alpha,\beta}$ of admissible functions in the sense of Definition 4.26 such that $\mathcal{W}_h(u_k) \leq M_{\alpha,\beta} + 1$ for all $k \in \mathbb{N}$. Then, there exists a minimising sequence $(v_k)_{k\in\mathbb{N}} \subset N_{\alpha,\beta}$ of admissible functions having lower Willmore energy and satisfying* (4.17) *as well as*

$$\max\{-\beta, \alpha^*\} \geq v_k'(x) \geq -\frac{\operatorname{arsinh}(-\beta)}{\alpha}(\alpha_\beta - \alpha) \quad \text{and} \quad C_{\alpha,\beta} \leq v_k(x) \leq \sqrt{1 + \alpha^2 - x^2}, \tag{4.22}$$

in $[0,1]$ *with a constant $C_{\alpha,\beta} > 0$ depending on α, $-\beta$ and $M_{\alpha,\beta}$.*

Proof. By Lemmas 4.28, 4.29, 4.34, 4.44 and Corollary 4.45 if $-\beta \leq \alpha$ or Corollary 4.46 if $-\beta > \alpha$, for each u_k there exists an admissible $v_k \in N_{\alpha,\beta}$ with lower Willmore energy than u_k satisfying (4.17) for some $x_k \in [0, 1)$ and

$$v_k'(x) \leq \max\{-\beta, \alpha^*\} \quad \text{and} \quad v_k(x_k) \geq \frac{\alpha}{\operatorname{arsinh}(-\beta)(\alpha_\beta - \alpha)} x_k. \tag{4.23}$$

Since v_k satisfies (4.16) we get $v_k(x) \leq \sqrt{1 + \alpha^2 - x^2}$ for $x \in [0,1]$ and

$$v_k'(x) \geq -\frac{x}{v_k(x)} \geq -\frac{x_k}{v_k(x_k)} \geq -\operatorname{arsinh}(-\beta)\frac{\alpha_\beta - \alpha}{\alpha} \text{ for } x \in [0, x_k],$$

while $v_k' \geq 0$ in $[x_k, 1]$. The estimate from below for v_k follows from the second estimate in (4.23) if $x_k \geq 1/2$ and from Lemma 4.9 if $x_k \leq 1/2$. □

Proof of the existence theorem

Theorem 4.48 (Existence and regularity)**.** *For $\beta < 0$ and $\alpha < \alpha^*$ there exists a symmetric function $u \in C^\infty([-1,1], (0, \infty))$ such that the corresponding surface of revolution $\Gamma \subset \mathbb{R}^3$ solves the Dirichlet problem* (1.4)*. This solution u has at most one critical point in* $(0,1)$ *and obeys the following estimates:*

$$\begin{gathered} \max\left\{\alpha^*, -\beta\right\} \geq u'(x) \geq -(\alpha - \alpha_\beta)\frac{\operatorname{arsinh}(-\beta)}{\alpha} \text{ in } (0,1] \\ \text{and} \quad \sqrt{1 + \alpha^2 - x^2} \geq u(x) \geq C_{\alpha,\beta} \text{ in } [-1, 1], \end{gathered}$$

with a constant $C_{\alpha,\beta} > 0$ depending on $M_{\alpha,\beta}$, α and $-\beta$.

Proof. By density of polynomials in $H^2(-1,1)$ a minimising sequence $(u_k)_{k\in\mathbb{N}}$ for $M_{\alpha,\beta}$ may be chosen in $N_{\alpha,\beta}$ which consists of positive symmetric polynomials of degree at least 2 and obeys $\mathcal{W}_h(u_k) \le M_{\alpha,\beta}+1$ for all $k \in \mathbb{N}$. By Proposition 4.47, there exists a minimising sequence $(v_k)_{k\in\mathbb{N}} \subset N_{\alpha,\beta}$ such that $\mathcal{W}_h(v_k) \le \mathcal{W}_h(u_k)$ and each element v_k of the minimising sequence satisfies (4.22). The rest of the proof is along the lines of Theorem 3.11. Moreover, Lemma 3.20 shows that u has at most one critical point in $(0,1)$. $\square$

Reasoning as in the proof of Propositions 3.12 and 4.18, one can prove that also in this case the energy is strictly decreasing in α.

Proposition 4.49. *Let $M_{\alpha,\beta}$ be as defined in (2.7) and $\alpha < \alpha^*$. Then $M_{\widetilde{\alpha},\beta} > M_{\alpha,\beta}$ for all $\widetilde{\alpha} < \alpha$.*

5 Convergence to the sphere for $\alpha \searrow 0$

In this section, we choose any $\beta \in \mathbb{R}$, keep it fixed and study the singular limit $\alpha \searrow 0$, where the "holes" $\{\pm 1\} \times B_\alpha(0)$ in the cylindrical surfaces of revolution disappear.

The aim of this chapter is to show that if $u_\alpha \in N_{\alpha,\beta}$ is an energy minimising solution to (1.4), i.e. $\mathcal{W}_h(u_\alpha) = M_{\alpha,\beta}$, then u_α converges for $\alpha \searrow 0$ to the semicircle $\sqrt{1-x^2}$. So, the surface of revolution generated by the graph of u_α converges to the sphere, which shows up as a limit irrespective of the prescribed boundary slope $\pm\beta$.

We first show that for α small, any minimiser $u_\alpha \in N_{\alpha,\beta}$ of $\mathcal{W}_h$, i.e. $\mathcal{W}_h(u_\alpha) = M_{\alpha,\beta}$, has the same qualitative properties as the solution we have constructed.

Lemma 5.1. *We assume that $\alpha < \min\{\alpha^*, 1/\beta\}$ if $\beta > 0$ and $\alpha < \alpha^*$ if $\beta \le 0$. Let $u \in N_{\alpha,\beta}$ be such that $\mathcal{W}_h(u) = M_{\alpha,\beta}$. Then, $u \in C^\infty([-1,1],(0,\infty))$ and u has the following additional properties:*

1. *If $\beta \ge 0$, then $u' < 0$ in $(0,1)$ and*

$$\alpha \le u(x) \le \sqrt{1+\alpha^2-x^2} \text{ in } [-1,1],\ x + u(x)u'(x) > 0 \text{ in } (0,1).$$

2. *If $\beta < 0$, then u has at most one critical point in $(0,1)$, i.e. there exists $x_0 \in [0,1)$ such that $u' > 0$ in $(x_0,1]$, $u'(x_0) = 0$ and $u' < 0$ in $(0,x_0)$. Moreover,*

$$\begin{aligned} &x + u(x)u'(x) > 0 \text{ in } (0,1], \quad u'(x) \le \gamma := \max\{-\beta,\alpha^*\} \text{ in } [x_0,1] \\ &\text{and } u(x) \ge \min\left\{\frac{1}{2}\frac{\alpha}{\operatorname{arsinh}(-\beta)(\alpha_\beta-\alpha)}, \frac{1}{2}\frac{\gamma}{e^C-1}\right\} \text{ in } [-1,1], \end{aligned}$$

with $C = \frac{\gamma\sqrt{1+\gamma^2}}{2}\left(M_{\alpha,\beta} + \frac{4\beta}{\sqrt{1+\beta^2}}\right) > 0$.

Proof. Since u minimises $\mathcal{W}_h$ and hence, weakly solves the Euler-Lagrange equation (2.5), the argument in [4, Theorem 3.9, Step 2] yields $u \in C^\infty([-1,1],(0,\infty))$. Whenever $x_0 \in (0,1)$ is a critical point of u one may insert on $[-x_0,x_0]$ a rescaled energy minimising solution v according to Theorem 3.18 and Lemma 3.20 satisfying $v' < 0$ on $(0,x_0)$. Putting together v and $u|_{[-1,1]\setminus[-x_0,x_0]}$ yields a further minimiser in $N_{\alpha,\beta}$ and so, a solution to (2.5). By uniqueness of the initial value problem, this new solution coincides with the original u. This shows that u has at most one critical point. Exploiting this observation, one proves that u satisfies the estimate in the claim by the same constructions as in the proof of the respective existence theorems. $\square$

The assumption on α excludes in particular the case $0 < -\beta < \alpha$ and $\alpha > \alpha_\beta$, where "our" solution was constructed in a much smaller set than $N_{\alpha,\beta}$.

In what follows, when considering minimisers u of $\mathcal{W}_h$ in $N_{\alpha,\beta}$, we make use of the qualitative properties of u stated in Lemma 5.1 without further notice. In particular, we restrict ourselves always to the case $\alpha < \min\{\alpha^*, 1/|\beta|\}$.

5.1 An upper bound for the energy as $\alpha \searrow 0$

For α small we first construct a function $f_\alpha \in N_{\alpha,\beta}$ such that its Willmore energy converges to the one of the sphere for $\alpha \searrow 0$. We consider the symmetric function:

$$f_\alpha(x) = \begin{cases} \frac{\alpha}{\sqrt{1+\beta^2}} \cosh\left(\frac{\sqrt{1+\beta^2}}{\alpha}(x - x_1)\right) & \text{if } x_0 \le x \le 1, \\ \sqrt{r^2 - x^2} & \text{if } -x_0 < x < x_0, \\ \frac{\alpha}{\sqrt{1+\beta^2}} \cosh\left(\frac{\sqrt{1+\beta^2}}{\alpha}(x + x_1)\right) & \text{if } -1 \le x \le -x_0, \end{cases} \tag{5.1}$$

where $x_1 = 1 - \alpha \operatorname{arsinh}(-\beta)/\sqrt{1+\beta^2}$, $r^2 = x_0^2 + f_\alpha(x_0)^2$ and, for α small enough, $x_0 \in (0,1)$ is solution of

$$-x_0 = \frac{\alpha}{2\sqrt{1+\beta^2}} \sinh\left(2\frac{\sqrt{1+\beta^2}}{\alpha}(x_0 - x_1)\right). \tag{5.2}$$

Assuming α to be small enough ensures the existence of $x_0 \in (0,1)$. We remark that this x_0 should not be mixed with the one in Condition (4.17). The function f_α has Willmore energy

$$\begin{aligned} \mathcal{W}_h(f_\alpha) &= 2\int_{x_0}^{1} \kappa_h[f_\alpha]^2 \frac{\sqrt{1+f_\alpha'^2(x)}}{f_\alpha(x)}\,dx = 8\int_{x_0}^{1} \frac{1}{\cosh^2(\frac{\sqrt{1+\beta^2}}{\alpha}(x-x_1))} \frac{\sqrt{1+\beta^2}}{\alpha}\,dx \\ &= 8\tanh(\operatorname{arsinh}(-\beta)) - 8\tanh\left(\frac{\sqrt{1+\beta^2}(x_0-x_1)}{\alpha}\right) \\ &= -8\frac{\beta}{\sqrt{1+\beta^2}} + 8\tanh\left(\frac{\sqrt{1+\beta^2}(x_1-x_0)}{\alpha}\right) \le -8\frac{\beta}{\sqrt{1+\beta^2}} + 8. \end{aligned}$$

This particular function shows that $M_{\alpha,\beta}$ is uniformly bounded for α going to 0 . Since $M_{\alpha,\beta}$ is increasing for $\alpha \searrow 0$ for all $\beta \in \mathbb{R}$, it follows that

$$\lim_{\alpha\searrow 0} M_{\alpha,\beta} \le 8 - 8\frac{\beta}{\sqrt{1+\beta^2}}. \tag{5.3}$$

5.2 The limit of the energy

In this section we prove that the limit of the energy is equal to the upper bound given in the previous section.

We start by proving that when $\beta < 0$ and α is small the minimiser has precisely one critical point in $(0,1)$ and this point approaches 1 for α going to 0.

Lemma 5.2. *Let $\beta < 0$. We assume that $u_\alpha \in N_{\alpha,\beta}$ minimises the Willmore energy, i.e. $\mathcal{W}_h(u_\alpha) = M_{\alpha,\beta}$. Let $x_\alpha \in [0,1)$ be such that $u_\alpha'(x_\alpha) = 0$ and $u_\alpha' > 0$ in $(x_\alpha, 1]$. Then,*

$$\lim_{\alpha\searrow 0} x_\alpha = 1.$$

Proof. Let us assume that there exist a sequence $\alpha_k \searrow 0$ and $\delta > 0$ such that $x_{\alpha_k} \le 1-\delta$ for all $k \in \mathbb{N}$. For each $\alpha > 0$, the measure of the set $A := \{x \in [1-\delta, 1] : u'_\alpha(x) \ge 2\alpha/\delta\}$ is bounded by $\delta/2$, since u_α is strictly positive. Then looking at the energy we find

$$\begin{aligned} M_{\alpha_k,\beta} = \mathcal{W}_h(u_{\alpha_k}) &\ge \int_{x_{\alpha_k}}^{1} \frac{1}{u_{\alpha_k}(x)\sqrt{1+u'^2_{\alpha_k}(x)}}\,dx + 2\,\frac{u'_{\alpha_k}(x)}{\sqrt{1+u'_{\alpha_k}(x)^2}}\Big|_{-1}^{1} \\ &\ge \int_{[1-\delta,1]\setminus A} \frac{1}{\alpha_k\sqrt{1+u'_{\alpha_k}(x)^2}}\,dx - 4\frac{\beta}{\sqrt{1+\beta^2}} \\ &\ge \frac{\delta}{2\alpha_k\sqrt{1+\frac{4\alpha_k^2}{\delta^2}}} - 4\frac{\beta}{\sqrt{1+\beta^2}} \to \infty \quad \text{for} \quad k \to \infty, \end{aligned}$$

a contradiction to (5.3). □

We show that the gradient of any minimiser is unbounded near $x = -1$ in the limit $\alpha \searrow 0$. From now on, β is a fixed element of $\mathbb{R}$.

Lemma 5.3. *We fix $\delta_0 \in (0,1)$. For $\alpha > 0$, let $u_\alpha \in N_{\alpha,\beta}$ be a minimiser of the Willmore energy, i.e. $\mathcal{W}_h(u_\alpha) = M_{\alpha,\beta}$. Then,*

$$\lim_{\alpha\searrow 0} \max_{x\in[-1,-1+\delta_0]} u'_\alpha(x) = +\infty.$$

Proof. We assume by contradiction that there exist a sequence $\alpha_k \searrow 0$ and a positive constant K such that

$$\max_{x\in[-1,-1+\delta_0]} u'_{\alpha_k}(x) \le K \quad \text{for all } k \in \mathbb{N}. \tag{5.4}$$

Let $x_{\alpha_k} = 1$ if $\beta \ge 0$. If $\beta < 0$, let $x_{\alpha_k} \in [0,1)$ be the element such that $u'_{\alpha_k}(x_{\alpha_k}) = 0$ and $u'_{\alpha_k} > 0$ in $(x_{\alpha_k}, 1]$. By Lemma 5.2 we have $1 - x_{\alpha_k} \to 0$ for $k \to \infty$. Notice that $u_{\alpha_k}(x_{\alpha_k}) \le \alpha_k$. Then, we estimate the Willmore energy from below as follows

$$\begin{aligned} \mathcal{W}_h(u_{\alpha_k}) &\ge \int_{-1}^{1} \frac{1}{u_{\alpha_k}(x)(1+u'_{\alpha_k}(x)^2)^{\frac12}}\,dx - 4\frac{\beta}{\sqrt{1+\beta^2}} \\ &\ge 2\int_{-x_{\alpha_k}}^{-1+\delta_0} \frac{1}{u_{\alpha_k}(x)(1+u'_{\alpha_k}(x)^2)^{\frac12}}\,dx - 4\,\frac{\beta}{\sqrt{1+\beta^2}}\,. \end{aligned} \tag{5.5}$$

By (5.4) we have $u_{\alpha_k}(x) \le u_{\alpha_k}(x_{\alpha_k}) + K(x+1)$ for $x \in [-x_{\alpha_k}, -1+\delta_0]$ and hence from (5.5) we conclude for k large enough

$$\begin{aligned} \mathcal{W}_h(u_{\alpha_k}) &\ge \frac{2}{\sqrt{1+K^2}} \int_{-x_{\alpha_k}}^{-1+\delta_0} \frac{1}{u_{\alpha_k}(x_{\alpha_k}) + K(x+1)}\,dx - 4\,\frac{\beta}{\sqrt{1+\beta^2}} \\ &= \frac{2}{K\sqrt{1+K^2}} \log\left(1 + K\frac{\delta_0 - 1 + x_{\alpha_k}}{u_{\alpha_k}(x_{\alpha_k}) + K(1-x_{\alpha_k})}\right) - 4\,\frac{\beta}{\sqrt{1+\beta^2}} \\ &\ge \frac{2}{K\sqrt{1+K^2}} \log\left(1 + \frac{K}{2}\,\frac{\delta_0}{u_{\alpha_k}(x_{\alpha_k}) + K(1-x_{\alpha_k})}\right) - 4\,\frac{\beta}{\sqrt{1+\beta^2}}\,. \end{aligned}$$

Since $u_{\alpha_k}(x_{\alpha_k}) \le \alpha_k \searrow 0$ and $x_{\alpha_k} \to 1$ for $k \to \infty$, the energy $\mathcal{W}_h(u_{\alpha_k})$ diverges to $+\infty$, thereby contradicting estimate (5.3). □

Theorem 5.4 (Limit of the energy for $\alpha \searrow 0$)**.** *For $\alpha > 0$ let $u_\alpha \in N_{\alpha,\beta}$ be such that $\mathcal{W}_h(u_\alpha) = M_{\alpha,\beta}$. Then, it holds that*

$$\lim_{\alpha\searrow 0} \mathcal{W}_h(u_\alpha) = \lim_{\alpha\searrow 0} M_{\alpha,\beta} = 8 - \frac{8\beta}{\sqrt{1+\beta^2}}\,.$$

Proof. For any $u \in N_{\alpha,\beta}$ and $\delta_0 > 0$ to be chosen we have

$$\begin{aligned}
\frac{1}{2}\,\mathcal{W}_h(u) &= \int_{-1}^{-1+\delta_0} \left(\frac{u''(x)}{(1+u'(x)^2)^{\frac{3}{2}}} - \frac{1}{u(x)(1+u'(x)^2)^{\frac{1}{2}}} \right)^2 u(x)\sqrt{1+u'(x)^2}\,dx \\
&\quad + 4 \int_{-1}^{-1+\delta_0} \frac{u''(x)}{(1+u'(x)^2)^{\frac{3}{2}}}\,dx + \int_{-1+\delta_0}^{0} \kappa_h[u]^2 \frac{\sqrt{1+u'(x)^2}}{u(x)}\,dx \\
&\geq 4 \int_{-1}^{-1+\delta_0} \frac{u''(x)}{(1+u'(x)^2)^{\frac{3}{2}}}\,dx \;=\; 4\,\frac{u'(x)}{\sqrt{1+u'(x)^2}}\bigg|_{-1}^{-1+\delta_0} \\
&= 4\,\frac{u'(-1+\delta_0)}{\sqrt{1+u'(-1+\delta_0)^2}} - 4\,\frac{\beta}{\sqrt{1+\beta^2}}\,.
\end{aligned} \tag{5.6}$$

Let $\alpha_k \searrow 0$ be any sequence. By Lemma 5.3 we find $\delta_{\alpha_k} \in [0, 1/2]$ with $\lim_{k\to\infty} u'_{\alpha_k}(-1+\delta_{\alpha_k}) = \infty$. From (5.6) it follows with $\delta_0 = \delta_{\alpha_k}$

$$\mathcal{W}_h(u_{\alpha_k}) \geq 8\,\frac{u'_{\alpha_k}(-1+\delta_{\alpha_k})}{\sqrt{1+u'_{\alpha_k}(-1+\delta_{\alpha_k})^2}} - 8\,\frac{\beta}{\sqrt{1+\beta^2}}\,,$$

and hence

$$\lim_{k\to\infty} \mathcal{W}_h(u_{\alpha_k}) \geq 8 - 8\,\frac{\beta}{\sqrt{1+\beta^2}}\,.$$

This estimate together with (5.3) yields the claim. □

Corollary 5.5. *For $\alpha > 0$ let $u_\alpha \in N_{\alpha,\beta}$ be such that $\mathcal{W}_h(u_\alpha) = M_{\alpha,\beta}$. Then,*

$$\lim_{\alpha\searrow 0} \int_{-1+\delta_0}^{1-\delta_0} \kappa_h[u_\alpha]^2\,\frac{\sqrt{1+u'_\alpha(x)^2}}{u_\alpha(x)}\,dx = 0 \qquad \textit{for all } \delta_0 \in (0,1).$$

Proof. For any sequence $\alpha_k \searrow 0$, by Lemma 5.3 there exist $\delta_{\alpha_k} \in [0, \delta_0]$ with

$$\lim_{k\to\infty} u'_{\alpha_k}(-1+\delta_{\alpha_k}) = +\infty. \tag{5.7}$$

Proceeding similarly as in the proof of Theorem 5.4 we have

$$\mathcal{W}_h(u_{\alpha_k}) \geq \int_{-1+\delta_{\alpha_k}}^{1-\delta_{\alpha_k}} \kappa_h[u_{\alpha_k}]^2\,\frac{\sqrt{1+u'_{\alpha_k}(x)^2}}{u_{\alpha_k}(x)}\,dx + 8\,\frac{u'_{\alpha_k}(-1+\delta_{\alpha_k})}{\sqrt{1+u'_{\alpha_k}(-1+\delta_{\alpha_k})^2}} - 8\,\frac{\beta}{\sqrt{1+\beta^2}}\,.$$

Since

$$0 \leq \int_{-1+\delta_0}^{1-\delta_0} \kappa_h[u_{\alpha_k}]^2\,\frac{\sqrt{1+u'_{\alpha_k}(x)^2}}{u_{\alpha_k}(x)}\,dx \leq \int_{-1+\delta_{\alpha_k}}^{1-\delta_{\alpha_k}} \kappa_h[u_{\alpha_k}]^2\,\frac{\sqrt{1+u'_{\alpha_k}(x)^2}}{u_{\alpha_k}(x)}\,dx$$

the claim follows from the inequalities above, Theorem 5.4 and (5.7). □

5.3 The minimiser converges to the sphere

Lemma 5.6. *Fix $\delta_0 \in (0,1)$. For $\alpha > 0$ let $u_\alpha \in N_{\alpha,\beta}$ solve $\mathcal{W}_h(u_\alpha) = M_{\alpha,\beta}$. Then, there exists $\varepsilon > 0$ such that $u_\alpha(x) \geq \varepsilon$ in $[-1+\delta_0, 1-\delta_0]$ for all $\alpha \leq 1$.*

Proof. We assume by contradiction that there is a sequence $1 \geq \alpha_k \searrow 0$ and that there are points $x_k \in [0, 1-\delta_0]$ with $1 \geq u_{\alpha_k}(x_k) = \min_{x\in[0,1-\delta_0]} u_{\alpha_k}(x) =: m_k \searrow 0$. The energy of this sequence of minimisers is bounded from below as follows

$$\begin{aligned}
\mathcal{W}_h(u_{\alpha_k}) &\geq \int_{-1}^{1} \frac{1}{u_{\alpha_k}(x)\sqrt{1+u'_{\alpha_k}(x)^2}}\, dx - 4\frac{\beta}{\sqrt{1+\beta^2}} \\
&\geq 2\int_{1-\delta_0}^{1} \frac{1}{u_{\alpha_k}(x)\sqrt{1+u'_{\alpha_k}(x)^2}}\, dx - 4\frac{\beta}{\sqrt{1+\beta^2}} \\
&\geq \frac{2}{\max\{m_k,\alpha_k\}} \int_{1-\delta_0}^{1} \frac{1}{\sqrt{1+u'_{\alpha_k}(x)^2}}\, dx - 4\frac{\beta}{\sqrt{1+\beta^2}}\,.
\end{aligned} \tag{5.8}$$

In order to estimate the integral in (5.8), we apply the Cauchy-Schwarz inequality

$$\begin{aligned}
\delta_0 &= \int_{1-\delta_0}^{1} \frac{1}{(1+u'_{\alpha_k}(x)^2)^{\frac14}} (1+u'_{\alpha_k}(x)^2)^{\frac14}\, dx \\
&\leq \left(\int_{1-\delta_0}^{1} \frac{1}{\sqrt{1+u'_{\alpha_k}(x)^2}}\, dx\right)^{\frac12} \left(\int_{1-\delta_0}^{1} \sqrt{1+u'_{\alpha_k}(x)^2}\, dx\right)^{\frac12},
\end{aligned}$$

which implies

$$\delta_0^2 \leq \left(\delta_0 + \int_{1-\delta_0}^{1} |u'_{\alpha_k}(x)|\, dx\right) \int_{1-\delta_0}^{1} \frac{1}{\sqrt{1+u'_{\alpha_k}(x)^2}}\, dx. \tag{5.9}$$

We estimate the first integral. Let $x_{\alpha_k} = 1$ if $\beta \geq 0$ and if $\beta < 0$ let $x_{\alpha_k} \in [0,1)$ be the element such that $u'_{\alpha_k}(x_{\alpha_k}) = 0$ and $u'_{\alpha_k} > 0$ in $(x_{\alpha_k}, 1]$. Lemma 5.2 shows that $x_{\alpha_k} \geq 1-\delta_0$ for sufficiently large k. Splitting the integral we find

$$\int_{1-\delta_0}^{1} |u'_{\alpha_k}(x)|\, dx \leq \int_{x_k}^{x_{\alpha_k}} |u'_{\alpha_k}(x)|\, dx + \int_{x_{\alpha_k}}^{1} |u'_{\alpha_k}(x)|\, dx = \begin{cases} m_k - \alpha_k & \text{if } \beta \geq 0, \\ m_k - 2u_{\alpha_k}(x_{\alpha_k}) + \alpha_k & \text{if } \beta < 0. \end{cases}$$

Estimating the right hand side in the inequality above by $m_k + \alpha_k$, we then conclude from (5.9) that

$$\delta_0^2 \leq (\delta_0 + m_k + \alpha_k) \int_{1-\delta_0}^{1} \frac{1}{\sqrt{1+u'_{\alpha_k}(x)^2}}\, dx.$$

Inserting this into (5.8) yields for k sufficiently large

$$\begin{aligned}
\mathcal{W}_h(u_{\alpha_k}) &\geq \frac{2\delta_0^2}{\max\{m_k,\alpha_k\}\,(\delta_0 + m_k + \alpha_k)} - 4\frac{\beta}{\sqrt{1+\beta^2}} \\
&\geq \frac{2\delta_0^2}{\max\{m_k,\alpha_k\}\,(\delta_0 + 2)} - 4\frac{\beta}{\sqrt{1+\beta^2}} \longrightarrow \infty \quad \text{for } k \to \infty,
\end{aligned}$$

contradicting Theorem 5.4. ☐

Corollary 5.7. *Fix $\delta_0 \in (0,1)$. For $\alpha > 0$ small enough let $u_\alpha \in N_{\alpha,\beta}$ solve $\mathcal{W}_h(u_\alpha) = M_{\alpha,\beta}$. Then, there exists $\varepsilon > 0$ such that*

$$-\frac{1}{\varepsilon} \leq u'_\alpha(x) \leq \max\{\alpha^*, -\beta\} \quad \textit{for all} \quad x \in [0, 1-\delta_0],$$

where $\alpha^* = \min\{\cosh(b)/b : b > 0\}$.

Proof. The first inequality is a consequence of Lemma 5.6 and the inequality $0 \leq x + u(x)u'(x)$ in $[0,1]$. The second one follows from the estimates on the minimiser in Lemma 5.1. ☐

Theorem 5.8 (Convergence to the sphere)**.** *For $\alpha > 0$ sufficiently small let $u_\alpha \in N_{\alpha,\beta}$ be a minimiser of the Willmore energy, i.e. $\mathcal{W}_h(u_\alpha) = M_{\alpha,\beta}$. Let u_0 denote the semicircle $u_0(x) := \sqrt{1-x^2}$, $x \in [-1,1]$. Then, for any $m \in \mathbb{N}$,*

$$\lim_{\alpha \searrow 0} u_\alpha = u_0 \quad \textit{in } C^m_{loc}(-1,1).$$

Proof. We choose any $\delta_0 \in (0,1)$. Let $(\alpha_k)_{k\in\mathbb{N}}$ be any sequence with $\alpha_k \searrow 0$. By Lemma 5.6 and Corollary 5.7 there exists a $\varepsilon > 0$ such that

$$\varepsilon \leq u_{\alpha_k}(x) \leq \sqrt{1+\alpha_k^2 - x^2} \quad \text{and} \quad -\frac{1}{\varepsilon} \leq u'_{\alpha_k}(x) \leq \frac{1}{\varepsilon},$$

for $x \in [-1+\delta_0, 1-\delta_0]$ and k sufficiently large. By these uniform bounds, the monotonicity in α of the energy, and Theorem 5.4 we find

$$\begin{aligned}
8 - 8\frac{\beta}{\sqrt{1+\beta^2}} &\geq \mathcal{W}_h(u_{\alpha_k}) \\
&\geq \int_{-1+\delta_0}^{1-\delta_0} \frac{u''_{\alpha_k}(x)^2 u_{\alpha_k}(x)}{(1+u'_{\alpha_k}(x)^2)^{\frac{5}{2}}}\, dx + \int_{-1+\delta_0}^{1-\delta_0} \frac{1}{u_{\alpha_k}(x)\sqrt{1+u'_{\alpha_k}(x)^2}}\, dx - 4\frac{\beta}{\sqrt{1+\beta^2}} \\
&\geq \frac{\varepsilon}{(1+\frac{1}{\varepsilon^2})^{\frac{5}{2}}} \int_{-1+\delta_0}^{1-\delta_0} u''^2_{\alpha_k}\, dx + \frac{2}{\sqrt{1+\alpha_k^2}} \frac{1}{(1+\frac{1}{\varepsilon^2})^{\frac{1}{2}}} - 4\frac{\beta}{\sqrt{1+\beta^2}}.
\end{aligned}$$

Hence, $(u_{\alpha_k})_{k\in\mathbb{N}}$ is uniformly bounded in $H^2(-1+\delta_0, 1-\delta_0)$. So, there exists a subsequence $(\alpha_{k_j})_{j\in\mathbb{N}}$ and a function $\tilde{u}_0 \in H^2(-1+\delta_0, 1-\delta_0)$ such that

$$u''_{\alpha_{k_j}} \rightharpoonup \tilde{u}''_0 \quad \text{in } L^2(-1+\delta_0, 1-\delta_0) \ \text{ and } \ u_{\alpha_{k_j}} \to \tilde{u}_0 \quad \text{in } C^1([-1+\delta_0, 1-\delta_0], (0,\infty)).$$

Moreover, $\tilde{u}_0$ satisfies: $\varepsilon \leq \tilde{u}_0(x) \leq \sqrt{1-x^2}$, $|\tilde{u}'_0(x)| \leq \frac{1}{\varepsilon}$ for all $x \in [-1+\delta_0, 1-\delta_0]$ and by Corollary 5.5

$$0 = \liminf_{j\to\infty} \int_{-1+\delta_0}^{1-\delta_0} \kappa_h[u_{\alpha_{k_j}}]^2 \frac{\sqrt{1+u'_{\alpha_{k_j}}(x)^2}}{u_{\alpha_{k_j}}(x)}\, dx \geq \int_{-1+\delta_0}^{1-\delta_0} \kappa_h[\tilde{u}_0]^2 \frac{\sqrt{1+\tilde{u}'_0(x)^2}}{\tilde{u}_0(x)}\, dx.$$

Hence, $\kappa_h[\tilde{u}_0] \equiv 0$ on $[-1+\delta_0, 1-\delta_0]$ and, therefore, $\tilde{u}_0|_{[-1+\delta_0,1-\delta_0]}$ is an arc of a geodesic circle, i.e., since $\tilde{u}_0$ is also symmetric around 0, it exists a radius $r > 0$ such that $\tilde{u}_0(x) = \sqrt{r^2-x^2}$ in

$[-1+\delta_0, 1-\delta_0]$. Necessarily $r \geq 1-\delta_0$ and by the arbitrariness of δ_0 we have $r \geq 1$. On the other hand, since $\tilde{u}_0(x) \leq \sqrt{1-x^2}$ we have $r \leq 1$. Hence, $r=1$ and $\tilde{u}_0 = u_0$.

Since for any sequence $(\alpha_k)_{k\in\mathbb{N}}$ there exists a subsequence $(\alpha_{k_j})_{j\in\mathbb{N}}$ such that $u_{\alpha_{k_j}}$ converges to u_0, we have that also u_{α_k} converges to u_0. The sequence being arbitrary, convergence in $C^1 \cap H^2([-1+\delta_0, 1-\delta_0])$ follows. Proceeding as in the proof of regularity in [4, Theorem 3.9] we conclude from the weak form of the differential equation (2.5) that $u_\alpha \to u_0$ for $\alpha \searrow 0$ also in $C^m_{loc}(-1,1)$ for any $m \in \mathbb{N}$. □

6 Qualitative properties of minimisers and estimates of the energy

In this section we give upper and lower bounds of the energy and we study the sign of the hyperbolic curvature of our minimiser. We have to distinguish the cases as in the proof of existence. We remark that any minimiser in the respective class of admissible functions has the qualitative properties mentioned in the existence theorems, since our geometric constructions apply also to these minimisers.

6.1 The case $\alpha\beta > 1$

6.1.1 Bounds on the energy

Proposition 6.1 (Upper bound of the energy)**.** *We have*

$$M_{\alpha,\beta} \leq \frac{2(\alpha\beta-1)}{\sqrt{1+\beta^2}} \arcsin \frac{\beta}{\sqrt{1+\beta^2}}.$$

Proof. We consider the arc $w \in N_{\alpha,\beta}$ of the circle with centre in $(0, \alpha - 1/\beta)$ and radius $\sqrt{1+\frac{1}{\beta^2}}$ which is given by

$$w(x) := \alpha - \frac{1}{\beta} + \sqrt{1+\frac{1}{\beta^2} - x^2} \quad \text{for } x \in [-1,1]. \tag{6.1}$$

Its hyperbolic curvature is

$$\kappa_h[w](x) = -\frac{\alpha\beta-1}{\sqrt{1+\beta^2}} \quad \text{for all } x \in [-1,1].$$

The previous identity for $\kappa_h[w]$ implies

$$\begin{aligned}
\mathcal{W}_h(w) &= \frac{\alpha\beta-1}{\sqrt{1+\beta^2}} \int_{-1}^{1} \left(\frac{1}{\sqrt{1+\frac{1}{\beta^2}-x^2}} - \frac{1}{\alpha - \frac{1}{\beta} + \sqrt{1+\frac{1}{\beta^2}-x^2}} \right) dx \\
&\leq \frac{\alpha\beta-1}{\sqrt{1+\beta^2}} \int_{-1}^{1} \frac{1}{\sqrt{1+\frac{1}{\beta^2}-x^2}} dx.
\end{aligned}$$

The claim follows computing the integral. □

The previous proposition indicates that possibly $\lim_{\alpha\to\infty} M_{\alpha,\beta} = \infty$. To prove this, we establish a lower bound for $M_{\alpha,\beta}$ for large α. In what follows G denotes the function $G : \mathbb{R} \to (-c_0/2, c_0/2)$,

$$G(t) = \int_0^t \frac{1}{(1+\tau^2)^{\frac{5}{4}}} \, d\tau \text{ with } c_0 := \int_{\mathbb{R}} \frac{1}{(1+\tau^2)^{\frac{5}{4}}} \, d\tau = \mathcal{B}\big(1/2, 3/4\big) = 2.39628\ldots, \tag{6.2}$$

with $\mathcal{B}(\,.\,,\,.\,)$ the Beta-Function. The G-function played an important role in the study of the one-dimensional Willmore problem, i.e. of so called elastica, see [12, pp. 233–234] and [6, 7].

The following estimate from below holds true for any $\beta \neq 0$, irrespective of its sign.

Proposition 6.2 (A lower bound for the energy)**.** *Let $\beta \in \mathbb{R} \setminus \{0\}$. For $\alpha > 2|\beta|$ it holds that*

$$M_{\alpha,\beta} \geq \alpha \min\left\{G(-\beta)^2, (G(\alpha/2)+G(\beta))^2\right\} - 4\frac{\beta}{\sqrt{1+\beta^2}},$$

where the function G is defined in (6.2)*. In particular,* $\lim_{\alpha\to\infty} M_{\alpha,\beta} = \infty$.

Proof. For any $u \in N_{\alpha,\beta}$ we have

$$\mathcal{W}_h(u) \quad \geq \quad \int_{-1}^{1} \frac{u''(x)^2 u(x)}{(1+u'(x)^2)^{\frac{5}{2}}}\,dx - 4\frac{\beta}{\sqrt{1+\beta^2}}.$$

If $u(x) \geq \alpha/2$ for all $x \in [-1,1]$ then

$$\begin{aligned}
\mathcal{W}_h(u) \quad &\geq \quad \frac{\alpha}{2}\int_{-1}^{1} \frac{u''(x)^2}{(1+u'(x)^2)^{\frac{5}{2}}}\,dx - 4\frac{\beta}{\sqrt{1+\beta^2}} \\
&\geq \quad \frac{\alpha}{4}\left(\int_{-1}^{1} \frac{u''(x)}{(1+u'(x)^2)^{\frac{5}{4}}}\,dx\right)^2 - 4\frac{\beta}{\sqrt{1+\beta^2}} \\
&= \quad \alpha(G(-\beta))^2 - 4\frac{\beta}{\sqrt{1+\beta^2}}.
\end{aligned}$$

Otherwise, there exists $x_1 \in (0,1)$ such that $u(x) \geq \alpha/2$ in $[x_1,1]$ and $u'(x_1) \geq \alpha/2$. Proceeding similarly as before, Cauchy's inequality yields

$$\begin{aligned}
\mathcal{W}_h(u) \quad &\geq \quad 2\frac{\alpha}{2}\int_{x_1}^{1} \frac{u''(x)^2}{(1+u'(x)^2)^{\frac{5}{2}}}\,dx - 4\frac{\beta}{\sqrt{1+\beta^2}} \\
&\geq \quad \frac{\alpha}{1-x_1}\left(\int_{x_1}^{1} \frac{u''(x)}{(1+u'(x)^2)^{\frac{5}{4}}}\,dx\right)^2 - 4\frac{\beta}{\sqrt{1+\beta^2}} \\
&\geq \quad \alpha(G(\alpha/2)+G(\beta))^2 - 4\frac{\beta}{\sqrt{1+\beta^2}}.
\end{aligned}$$

One should observe that the function G is strictly increasing. In both cases we have that

$$\mathcal{W}_h(u) \geq \alpha \min\left\{G(\beta)^2, (G(\alpha/2)+G(\beta))^2\right\} - 4\frac{\beta}{\sqrt{1+\beta^2}}.$$

$\square$

According to Propositions 6.1 and 6.2, $M_{\alpha,\beta}$ grows linearly in $\alpha \to \infty$. We recall that for $\beta = 0$ the situation is different since $M_{\alpha,0} \to 0$, see [4, Lemma 3.2] and also Proposition 6.6 below.

6.1.2 On the sign of the hyperbolic curvature of minimisers

From Proposition 3.7 we infer the following convexity property for minimisers of the Willmore functional.

Lemma 6.3. *Let $u \in N_{\alpha,\beta}$ be a minimiser for $M_{\alpha,\beta}$. Then, $x \mapsto u'(x)$ is strictly decreasing on $[0,1]$.*

Proof. Since each minimiser satisfies $x + u(x)u'(x) < 0$ in $(0,1]$, the function u' is decreasing in a right neighbourhood of 0. We assume by contradiction that u' is not strictly decreasing on $(0,1]$. Then, there exist $0 < x_1 < x_2 \le 1$ such that $u'(x_1) = u'(x_2)$. We consider $u|_{[-x_1,x_1]}$ and rescale it to a function $w \in C^{1,1}([-x_2,x_2],(0,\infty))$. This function satisfies $w(x_2) = \frac{x_2}{x_1}u(x_1) > u(x_1) \ge u(x_2)$ and $w'(x_2) = u'(x_2)$. Moreover, by Remark 2.4 we conclude that

$$\int_{-x_2}^{x_2} \kappa_h[w]^2\, ds_h[w] = \int_{-x_1}^{x_1} \kappa_h[u]^2\, ds_h[u] < \int_{-x_2}^{x_2} \kappa_h[u]^2\, ds_h[u], \tag{6.3}$$

since $\kappa_h[u]$ is not identically zero in $[x_1,x_2]$. This follows since u solves the differential equation (2.5) and is not part of a geodesic circle. On the other hand, exploiting that u is a minimiser, we find

$$\begin{aligned}\int_{-x_2}^{x_2} \kappa_h[u]^2\, ds_h[u] &= \inf\Bigg\{ \int_{-x_2}^{x_2} \kappa_h[v]^2\, ds_h[v] \,:\, v \in C^{1,1}([-x_2,x_2],(0,\infty)),\ \text{symmetric},\\ &\qquad\qquad v(x_2) = u(x_2) \text{ and } v'(x_2) = u'(x_2)\Bigg\}\\ &\le \int_{-x_2}^{x_2} \kappa_h[w]^2\, ds_h[w],\end{aligned}$$

where in the last step we used that $w(x_2) > u(x_2)$ and Proposition 3.7. One should observe that the condition $0 > x + u(x)u'(x)$ is the rescaled version of $\alpha\beta > 1$ on the interval $[0,x]$. We have achieved a contradiction to (6.3). □

Theorem 6.4. *We assume that $\alpha\beta > 1$. Let $u \in N_{\alpha,\beta}$ be a minimiser for $M_{\alpha,\beta}$. Then, either $\kappa_h[u] < 0$ in $[0,1)$, or there exists $a \in (0,1)$ such that $\kappa_h[u] < 0$ in $[0,a)$ and $\kappa_h[u] > 0$ in $(a,1)$.*

Proof. We consider the auxiliary function $\varphi\colon [0,1] \to \mathbb{R}$ defined by $\varphi(x) := x + u(x)u'(x)$, where $(\varphi(x),0)$ is the centre and $r(x) := u(x)\sqrt{1+u'(x)^2}$, $x \in [0,1]$ the radius of the geodesic circle being tangential to the graph of u in $(x,u(x))$. From (3.2) we know that $\varphi(x) < 0$ in $(0,1]$, and $\varphi(0) = 0$. Hence, $\varphi(x)$ is decreasing for $x > 0$ sufficiently small. Since $\varphi'(x) = \left\{1+u'(x)^2\right\}^{\frac{3}{2}}\kappa_h[u](x)$, it follows that $\kappa_h[u] < 0$ in a right neighbourhood of 0. Viewing at (2.5) now as a second order equation for $\kappa_h[u]$ satisfying a strong maximum / minimum principle provided that maxima / minima are equal to zero yields that it suffices to show that $\kappa_h[u]$ has at most one sign change in $[0,1)$.

We assume by contradiction that there exist $0 < x_1 < x_0 < x_2 \le 1$ such that $\kappa_h[u] > 0$ in (x_1,x_0), $\kappa_h[u] < 0$ in (x_0,x_2) and $\varphi(x_1) = \varphi(x_2)$. We construct a new function with lower Willmore energy. This new function equals the original one on $[0,x_1]$. Then we take the arc of the circle with centre $(\varphi(x_1),0)$ and radius $r(x_1)$, starting at $(x_1,u(x_1))$ and ending where this arc intersects the straight line which connects $(\varphi(x_1),0) = (\varphi(x_2),0)$ and $(x_2,u(x_2))$. Finally, we attach the suitably rescaled original function $u|_{[x_2,1]}$. More precisely, with the scaling factor $\varrho = r(x_1)/r(x_2)$ the new function is

$$v(x) := \begin{cases} u(x) & \text{if } 0 \le x \le x_1, \\ \sqrt{r(x_1)^2 - (x-\varphi(x_1))^2} & \text{if } x_1 \le x \le x_2 + u'(x_2)u(x_2)(1-\varrho), \\ \varrho\, u\left(\frac{1}{\varrho}\big(x-(1-\varrho)\varphi(x_2)\big)\right) & \text{if } x_2 + u'(x_2)u(x_2)(1-\varrho) \le x \le \varrho + (1-\varrho)\varphi(x_2), \end{cases} \tag{6.4}$$

and extended by symmetry to $[-\ell(\varrho), \ell(\varrho)]$, setting $\ell(\varrho) := \varrho + (1-\varrho)\varphi(x_2)$. See Figure 14. The function v satisfies $v \in C^{1,1}([-\ell(\varrho), \ell(\varrho)], (0,\infty))$, $v(\ell(\varrho)) = \varrho\alpha$ and $v'(\ell(\varrho)) = -\beta$.

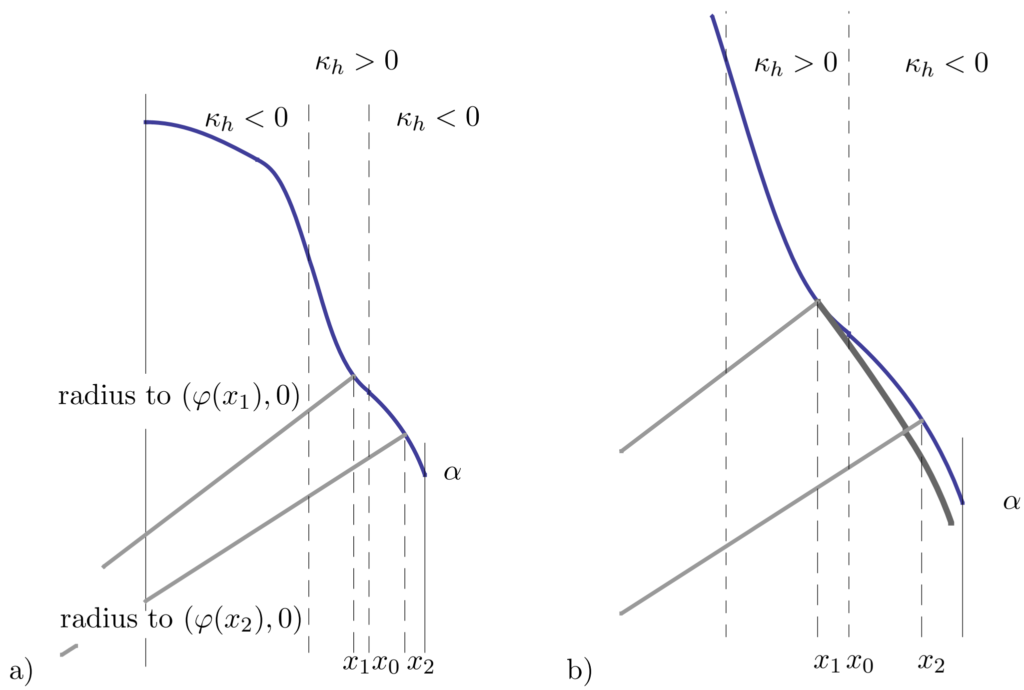


Figure 14: Proof of Theorem 6.4.

Note that $\varrho \le 1$. Indeed, one may write

$$r(x_2) = r(x_1) + \int_{x_1}^{x_2} \frac{u'(t)}{\sqrt{1+u'(t)^2}}\, \varphi'(t)\, dt. \tag{6.5}$$

By our assumption on φ and since $u'(x) \le 0$ in $[0,1]$, the integrand in (6.5) is negative in $[x_1, x_0]$ and positive in $[x_0, x_2]$. Moreover, since $p \mapsto \frac{p}{\sqrt{1+p^2}}$ is strictly increasing and, by Lemma 6.3, u' is strictly decreasing in $[0,1]$, also $\frac{u'}{\sqrt{1+u'^2}}$ is monotonically decreasing. Hence, splitting the integral in (6.5) and using that $\varphi(x_1) = \varphi(x_2)$ we get

$$r(x_2) > r(x_1) + \frac{u'(x_0)}{\sqrt{1+u'(x_0)^2}} \int_{x_1}^{x_0} \varphi'(t)\, dt + \frac{u'(x_0)}{\sqrt{1+u'(x_0)^2}} \int_{x_0}^{x_2} \varphi'(t)\, dt \;=\; r(x_1).$$

By scaling, the function $w(x) = \frac{1}{\ell(\varrho)}\, v\big(\ell(\varrho)x\big)$ defined in $[-1,1]$, satisfies

$$w'(1) = -\beta, \quad w(1) = \frac{\varrho\alpha}{\ell(\varrho)} \quad \text{and} \quad \mathcal{W}_h(w) < \mathcal{W}_h(u). \tag{6.6}$$

On the other hand, $\varrho < 1$, $\varphi(x_2) < 0$ give $\varrho > l(\varrho)$, and so $w(1) > \alpha = u(1)$. By monotonicity of the hyperbolic Willmore energy (see Proposition 3.12) we conclude that $\mathcal{W}_h(w) > \mathcal{W}_h(u)$. This contradicts (6.6). □

6.2 The case $\alpha\beta < 1$ and $\beta \geq 0$

6.2.1 Bounds on the energy

Proposition 6.5 (Upper bound for the energy)**.** *We have*

$$M_{\alpha,\beta} \leq \min\Big\{\frac{2(1-\alpha\beta)}{\sqrt{1+\beta^2}}\,\frac{1}{\alpha}, 8\tanh\left(\frac{\sqrt{1+\beta^2}}{\alpha} + \operatorname{arsinh}(\beta)\right) - 8\frac{\beta}{\sqrt{1+\beta^2}}\Big\}.$$

Proof. For $\beta > 0$, the first estimate follows with the same construction as in Proposition 6.1 considering the function $w \in N_{\alpha,\beta}$ given by (6.1); $w(x) = \alpha - \frac{1}{\beta} + \sqrt{1+\frac{1}{\beta^2} - x^2}$. Computing its Willmore energy we find

$$\begin{aligned}
\mathcal{W}_h(w) &= \frac{\alpha\beta - 1}{\sqrt{1+\beta^2}} \int_{-1}^{1} \left(\frac{1}{\sqrt{1+\frac{1}{\beta^2}-x^2}} - \frac{1}{\alpha - \frac{1}{\beta} + \sqrt{1+\frac{1}{\beta^2}-x^2}}\right) dx \\
&\leq \frac{1-\alpha\beta}{\sqrt{1+\beta^2}} \int_{-1}^{1} \frac{1}{\alpha - \frac{1}{\beta} + \sqrt{1+\frac{1}{\beta^2}-x^2}}\, dx \leq \frac{1-\alpha\beta}{\sqrt{1+\beta^2}}\,\frac{2}{\alpha}.
\end{aligned}$$

If $\beta = 0$, the function $w(x) \equiv \alpha$ directly gives $M_{\alpha,0} \leq \frac{2}{\alpha}$. Let f_α the function defined in (5.1). Notice that it is well defined since we assume that $\beta \geq 0$ and $\alpha\beta < 1$. From the calculations on p. 95 we see that

$$M_{\alpha,\beta} \leq \mathcal{W}_h(f_\alpha) \leq 8\tanh\left(\frac{\sqrt{1+\beta^2}}{\alpha}x_1\right) - 8\frac{\beta}{\sqrt{1+\beta^2}},$$

where $x_1 = 1 + \frac{\alpha}{\sqrt{1+\beta^2}}\operatorname{arsinh}(\beta)$. □

In the special case $\beta = 0$ we may now characterise the asymptotic behaviour of $M_{\alpha,0}$ for $\alpha \to \infty$. This is completely different from the case $\beta \neq 0$, cf. Proposition 6.2.

Proposition 6.6. *We assume that $\alpha > 0$ and $\beta = 0$. Then, one has*

$$\frac{2\alpha}{(\alpha+1)\sqrt{1+\alpha^2}} \leq M_{\alpha,0} \leq 8\tanh\left(\frac{1}{\alpha}\right).$$

Proof. Let $u_\alpha \in N_{\alpha,0}$ be a minimiser for $\mathcal{W}_h$ in $N_{\alpha,0}$ as constructed in Theorem 3.18 . It satisfies $u_\alpha(x) \leq \alpha + 1$ and $|u'_\alpha(x)| \leq 1/\alpha$, which yields

$$M_{\alpha,0} = \mathcal{W}_h(u_\alpha) \geq 2\int_0^1 \frac{1}{u_\alpha(x)\sqrt{1+u'_\alpha(x)^2}}\, dx \geq \frac{2\alpha}{(\alpha+1)\sqrt{1+\alpha^2}},$$

which is the estimate from below. The estimate from above was just proved in Proposition 6.5. □

6.2.2 On the sign of the hyperbolic curvature of minimisers

Theorem 6.7. *We assume that $\beta \geq 0$ and that $\alpha\beta < 1$. Let $u \in N_{\alpha,\beta}$ be a minimiser for $M_{\alpha,\beta}$. Then, $\kappa_h[u] > 0$ in $(-1, 1)$.*

Proof. The proof is along the lines of Theorem 6.4. We recall the main points and emphasise on what is different. We associate to u the auxiliary function $\varphi(x) := x + u(x)u'(x)$, $x \in [-1, 1]$. From (3.4) we know that $\varphi(0) = 0$ and $\varphi(x) > 0$ in $(0, 1]$. Since φ cannot be constant in an interval, $\varphi(x)$ increases in a right neighbourhood of 0 and hence $\kappa_h[u](x) > 0$ in a right neighbourhood of 0.

We now prove that $\varphi' \geq 0$ in $[0, 1]$. If $\varphi' < 0$ in some interval then there exist points $0 < x_0 < x' < 1$ such that $\varphi' \geq 0$ (i.e. $\kappa_h[u] \geq 0$) in $[0, x_0]$ and $\varphi' < 0$ (i.e. $\kappa_h[u] < 0$) in (x_0, x'). In particular, $u'' < 0$ in $[x_0, x']$. Let $x^* \in [0, x_0)$ be such that $u''(x) < 0$ in $(x^*, x']$. Then, there exist $x_1 \in [x^*, x_0)$ and $x_2 \in (x_0, x']$ such that $\varphi(x_1) = \varphi(x_2)$.

Then, with the same notation as in the proof of Theorem 6.4, we consider the function $v \in C^{1,1}([-\ell(\varrho), \ell(\varrho)], (0, \infty))$ defined as in (6.4). Then, $w(x) := \frac{1}{\ell(\varrho)} v(\ell(\varrho)x)$, $x \in [-1, 1]$, satisfies

$$w'(1) = -\beta, \quad w(1) = \frac{\varrho\alpha}{\ell(\varrho)} \quad \text{and} \quad \mathcal{W}_h(w) < \mathcal{W}_h(u). \tag{6.7}$$

Since $u'' < 0$ in $[x_1, x_2]$ and proceeding as in (6.5) one sees that $\varrho < 1$. Here, in contrast with the proof of Theorem 6.4, $\varphi > 0$ in $(0, 1)$ and so $\varrho < \ell(\varrho)$. Hence, $w(1) < u(1)$ and $\mathcal{W}_h(w) > \mathcal{W}_h(u)$ by the strict monotonicity of the energy (Proposition 3.19), which contradicts the inequality in (6.7). Then, φ being increasing in $[0, 1]$ implies that $\kappa_h[u] \geq 0$ in $[-1, 1]$. The strong minimum principle for (2.5) considered as a second order equation for $\kappa_h[u]$ and applied to a possible minimum 0 yields that $\kappa_h[u] > 0$ in $(-1, 1)$. □

6.3 The case $\beta < 0$ and $\alpha \geq \alpha_\beta$

6.3.1 Bounds on the energy

Proposition 6.8 (Upper bound of the energy)**.** *We have*

$$M_{\alpha,\beta} \leq (1 + \operatorname{arsinh}(-\beta)(\alpha - \alpha_\beta)) \frac{(-8\beta)}{\sqrt{1+\beta^2}}.$$

Proof. If $\alpha = \alpha_\beta$, the minimiser is $u_c(x) = \cosh(bx)/b$, $b = \operatorname{arsinh}(-\beta)$, which has vanishing mean curvature in $[-1, 1]$ and hyperbolic Willmore energy

$$\mathcal{W}_h(u_c) = -\frac{8\beta}{\sqrt{1+\beta^2}}.$$

If instead $\alpha > \alpha_\beta$, we consider the function $u := u_c + \delta_\alpha$ where $\delta_\alpha := \alpha - \alpha_\beta > 0$. Notice that $u \in N_{\alpha,\beta}$. Since $u_c \geq \frac{1}{b} > 0$ and $u_c'' > 0$ we have

$$\begin{aligned}
\mathcal{W}_h(u_c + \delta_\alpha) &= \int_{-1}^{1} \left(\frac{u_c''}{(1+u_c'^2)^{\frac{3}{2}}} + \frac{1}{(u_c+\delta_\alpha)\sqrt{1+u_c'^2}} \right)^2 (u_c + \delta_\alpha)\sqrt{1+u_c'^2}\, dx \\
&\leq \mathcal{W}_h(u_c) + \int_{-1}^{1} \left(\frac{u_c''}{(1+u_c'^2)^{\frac{3}{2}}} + \frac{1}{u_c\sqrt{1+u_c'^2}} \right)^2 \delta_\alpha \sqrt{1+u_c'^2}\, dx \\
&\leq \mathcal{W}_h(u_c) + b\delta_\alpha \int_{-1}^{1} \left(\frac{u_c''}{(1+u_c'^2)^{\frac{3}{2}}} + \frac{1}{u_c\sqrt{1+u_c'^2}} \right)^2 u_c \sqrt{1+u_c'^2}\, dx
\end{aligned}$$

which proves the proposition. □

The previous result together with Proposition 6.2 shows that also for $\beta < 0$, $M_{\alpha,\beta}$ grows linearly for $\alpha \to \infty$.

6.3.2 On the sign of the hyperbolic curvature of minimisers

Here we prefer a slightly less general formulation of the curvature statement and refer only to solutions as we have constructed. The reason is that we have to restrict the set of admissible functions in the case $-\beta < \alpha$.

Theorem 6.9. *We assume that $\beta < 0$ and that $\alpha \geq \alpha_\beta$. Let $u \in N_{\alpha,\beta}$ be an energy minimising solution of (1.4) as constructed in the proofs of Theorems 4.17 and 4.24. Then, either $\kappa_h[u] > 0$ in $[0,1)$, or there exists a point $a \in (0,1)$ such that $\kappa_h[u] > 0$ in $[0,a)$ and $\kappa_h[u] < 0$ in $(a,1)$.*

Proof. We have $u' > 0$ in $(0,1]$. We associate to u the function $\varphi(x) := x + u(x)u'(x)$, $x \in [-1,1]$, which satisfies $\varphi(0) = 0$ and $\varphi(x) > 0$ in $(0,1]$. Hence, $\varphi(x)$ increases in a right neighbourhood of 0 and so, $\kappa_h[u](x) > 0$ in a right neighbourhood of 0. In view of the strong maximum /minimum principle for (2.5) as a second order equation for $\kappa_h[u]$ applied to maximum /minimum equal to 0, we only need to exclude that there is a sign change from $\kappa_h[u] < 0$ to $\kappa_h[u] > 0$.

We assume by contradiction that there exist $0 < \tilde{x} < x_0 < x'$ such that $\kappa_h[u] < 0$ (i.e. $\varphi' < 0$) in $(\tilde{x}, x_0)$ and $\kappa_h[u] > 0$ (i.e. $\varphi' > 0$) in (x_0, x'). In particular, $u'' < 0$ in $[\tilde{x}, x_0]$ and so, also on a slightly larger interval $[\tilde{x}, x'') \supset [\tilde{x}, x_0]$. Then, we find $x_1 \in (\tilde{x}, x_0)$ and $x_2 \in (x_0, x'')$ with $\varphi(x_1) = \varphi(x_2)$.

We consider the function $v \in C^{1,1}([-\ell(\varrho), \ell(\varrho)], (0,\infty))$ as defined in (6.4). Using the same notation as in the proof of Theorem 6.4, one should notice that in this case $\varrho > 1$. Indeed, one starts from (6.5). By our assumption on φ and since $u'(x) > 0$ in $(0,1]$, the integrand in (6.5) is strictly negative in (x_1, x_0) and positive in (x_0, x_2). Moreover since u' is decreasing in (x_1, x_2), also $\frac{u'}{\sqrt{1+u'^2}}$ is monotonically decreasing. Hence, splitting the integral in (6.5) and using that $\varphi(x_1) = \varphi(x_2)$ we get

$$r(x_2) < r(x_1) + \frac{u'(x_0)}{\sqrt{1+u'(x_0)^2}} \int_{x_1}^{x_0} \varphi'(t)\,dt + \frac{u'(x_0)}{\sqrt{1+u'(x_0)^2}} \int_{x_0}^{x_2} \varphi'(t)\,dt \;=\; r(x_1).$$

Notice that even though $\varrho > 1$, $x_2 + u(x_2)u'(x_2)(1-\varrho) \geq x_1$.

By scaling, the function $w(x) = \frac{1}{\ell(\varrho)} v\big(\ell(\varrho)x\big)$ defined in $[-1,1]$ satisfies

$$w'(1) = -\beta, \quad w(1) = \frac{\varrho\alpha}{\ell(\varrho)} \quad \text{and} \quad \mathcal{W}_h(w) < \mathcal{W}_h(u). \tag{6.8}$$

On the other hand, since $\varphi > 0$ on $(0,1]$ we have $\varrho > l(\varrho)$, $w(1) > u(1)$ and hence $\mathcal{W}_h(w) \geq \mathcal{W}_h(u)$ by monotonicity of the hyperbolic Willmore energy (see Propositions 4.18 and 4.25), which contradicts the inequality in (6.8). □

6.4 The case $\beta < 0$ and $\alpha < \alpha_\beta$

6.4.1 Bounds on the energy

Proposition 6.10 (Upper bound of the energy)**.** *The following estimate holds*

$$M_{\alpha,\beta} \leq -\frac{8\beta}{\sqrt{1+\beta^2}} + 8\tanh\left(\frac{\operatorname{arsinh}(-\beta)}{\alpha}(\alpha_\beta - \alpha)\right).$$

Proof. For $\beta < 0$ and $\alpha < \alpha_\beta$ the function f_α defined in (5.1) is well defined. As usual we denote $b = \operatorname{arsinh}(-\beta)$. The claim follows then from

$$\begin{aligned} M_{\alpha,\beta} &\le \mathcal{W}_h(f_\alpha) = -\frac{8\beta}{\sqrt{1+\beta^2}} - 8\tanh\left(\frac{b\alpha_\beta}{\alpha}(x_0 - 1 + \frac{\alpha}{\alpha_\beta})\right) \\ &\le -\frac{8\beta}{\sqrt{1+\beta^2}} + 8\tanh\left(\frac{b\alpha_\beta}{\alpha}(1 - \frac{\alpha}{\alpha_\beta})\right). \end{aligned}$$

□

6.4.2 On the sign of the hyperbolic curvature of minimisers

Theorem 6.11. *Let $u \in N_{\alpha,\beta}$ be a minimiser for $M_{\alpha,\beta}$. Then, $\kappa_h[u] > 0$ in $(-1,1)$.*

Proof. We know that there exists $x_0 \in [0,1)$ such that $u'(x_0) = 0$, $u' > 0$ in $(x_0, 1]$ and $u' < 0$ in $(0, x_0)$. Then, $u|_{[-x_0,x_0]}$ is the rescaled minimiser of $M_{u(x_0)/x_0,0}$ and hence, by Theorem 6.7, $\kappa_h[u] > 0$ in $(-x_0, x_0)$.

It remains to study the sign of the curvature in $[x_0, 1]$. Again, we consider $\varphi(x) := x + u(x)u'(x)$, $x \in [x_0, 1]$. Since $u' > 0$ in $(x_0, 1]$, $\varphi(x_0) = x_0$ and $\varphi(x) > x_0$ in $(x_0, 1]$, $\varphi(x)$ increases in a right neighbourhood of x_0 and hence, $\kappa_h[u](x) > 0$ also in a right neighbourhood of x_0.

In view of the strong minimum principle of (2.5) considered as a second order equation for $\kappa_h[u]$ and applied to a possible minimum 0, is suffices to show that $\kappa_h[u] \ge 0$ everywhere. We assume by contradiction that there exist $x_0 < x' < x'' < 1$ such that $\kappa_h[u] > 0$ (i.e. $\varphi' > 0$) in $[0, x')$ and $\kappa_h[u] < 0$ (i.e. $\varphi' < 0$) in (x', x''). In particular, $u'' < 0$ in $[x', x'')$ and so, also on a slightly larger interval $(x^*, x'') \supset [x', x'')$. Finally, we may find $x_1 \in (x^*, x')$ and $x_2 \in (x', x'')$ with $\varphi(x_1) = \varphi(x_2)$.

Then, with the same notation as in the proof of Theorem 6.4, we consider the function $v \in C^{1,1}([-\ell(\varrho), \ell(\varrho)], (0,\infty))$ defined as in (6.4). Notice that in this case $\varrho < 1$. Indeed, by our assumption on φ and since $u'(x) > 0$ in $(x_0, 1]$, the integrand in (6.5) is strictly positive in $[x_1, x')$ and negative in $(x', x_2]$. Moreover since u' is strictly decreasing in $[x_1, x_2]$, also $\frac{u'}{\sqrt{1+u'^2}}$ is monotonically decreasing. Splitting the integral in (6.5) and using that $\varphi(x_1) = \varphi(x_2)$ we get

$$r(x_2) > r(x_1) + \frac{u'(x')}{\sqrt{1+u'(x')^2}} \int_{x_1}^{x'} \varphi'(t)\,dt + \frac{u'(x')}{\sqrt{1+u'(x')^2}} \int_{x'}^{x_2} \varphi'(t)\,dt \;=\; r(x_1).$$

Then, $w(x) := \frac{1}{\ell(\varrho)} v(\ell(\varrho)x)$, $x \in [-1,1]$, satisfies

$$w'(1) = -\beta, \quad w(1) = \frac{\varrho\alpha}{\ell(\varrho)} \quad \text{and} \quad \mathcal{W}_h(w) < \mathcal{W}_h(u). \tag{6.9}$$

Since $\varphi > 0$ on $(0,1]$ we have $\varrho < \ell(\varrho)$ and $w(1) < u(1)$. Therefore, $\mathcal{W}_h(w) > \mathcal{W}_h(u)$ by monotonicity of the energy (see Propositions 4.40 and 4.49), which contradicts the inequality in (6.9). □

7 Numerical studies and algorithms

We will try to approximate a solution $u(x)$ of the Willmore equation (1.4) by approximating the stationary limit $\widetilde{u}(x) = \lim_{t\to\infty} U(x,t)$ of the solution $U(x,t)$ of the Dirichlet problem of the

Willmore flow equation

$$\begin{cases} V = \triangle_\Gamma H + 2H^3 - 2HK \qquad \forall x \in (-1,1)\,, t > 0, \\ U(-1,t) = U(1,t) = \alpha, \qquad U_x(-1,t) = -U_x(1,t) = \beta \qquad \forall t > 0, \\ U(x,0) = u_0(x) \qquad \forall x \in [-1,1], \end{cases} \tag{7.10}$$

for a family $(\Gamma(t))_{t\in[0,\infty)}$ of axially symmetric surfaces parametrised by

$$\Gamma(t) := \{(x, U(x,t)\cos\varphi, U(x,t)\sin\varphi) :\ x \in [-1,1], \varphi \in [0,2\pi]\}\,.$$

Here H, K denote the quantities related to the surface $\Gamma(t)$ generated by the function $U(x,t)$ and V the normal velocity of $\Gamma(t)$ given by

$$V = \frac{U_t}{(1+U_x^2)^{1/2}}.$$

In order to derive the variational formulation of (7.10) we exploit the fact that the right hand side of (7.10) is linked with the derivative of the Willmore functional

$$\mathcal{W}(\Gamma) = \int_\Gamma H^2\, dA.$$

In fact, writing $\mathcal{W}(U)$ instead of $\mathcal{W}(\Gamma)$, we can show that

$$\mathcal{W}(U) = 2\pi\widetilde{\mathcal{W}}(U) \,+\, 2\pi\frac{\beta}{\sqrt{1+\beta^2}} \tag{7.11}$$

where

$$\widetilde{\mathcal{W}}(U) := \frac{1}{4}\int_{-1}^{+1}\left\{\frac{UU_{xx}^2}{(1+U_x^2)^{5/2}} \,+\, \frac{1}{U(1+U_x^2)^{1/2}}\right\} dx.$$

Thus, for the derivative in direction $\phi \in H_0^2(-1,1)$, we obtain

$$\begin{aligned} \langle\widetilde{\mathcal{W}}'(U),\phi\rangle \;&:=\; \tfrac{d}{d\varepsilon}\widetilde{\mathcal{W}}(U+\varepsilon\phi)\big|_{\varepsilon=0} \\ &=\; \frac{1}{4}\int_{-1}^{+1}\Big\{2\frac{UU_{xx}\phi_{xx}}{(1+U_x^2)^{5/2}} + \frac{U_{xx}^2\phi}{(1+U_x^2)^{5/2}} - 5\frac{UU_xU_{xx}^2\phi_x}{(1+U_x^2)^{7/2}} \\ &\qquad\qquad -\frac{\phi}{U^2(1+U_x^2)^{1/2}} - \frac{U_x\phi_x}{U(1+U_x^2)^{3/2}}\Big\}dx. \end{aligned} \tag{7.12}$$

Under the smoothness assumption $U \in H^4(-1,1)$ one can prove (see §2.3) that

$$\langle\widetilde{\mathcal{W}}'(U),\phi\rangle = -\int_{-1}^{+1} U\phi\Big(\triangle_\Gamma H + 2H^3 - 2HK\Big)dx \qquad \forall\phi \in H_0^2(-1,1). \tag{7.13}$$

Multiplying (7.10) with the test function $U\phi$ and integrating over $[-1,1]$ yields the following variational formulation :

For $t \geq 0$ find $U(\cdot,t) \in X$ such that $U(.,0) = u_0$ and

$$\int_{-1}^{+1}\frac{U(\cdot,t)U_t(\cdot,t)\phi}{(1+U_x(\cdot,t)^2)^{1/2}}dx \,+\, \langle\widetilde{\mathcal{W}}'(U(\cdot,t)),\phi\rangle = 0 \qquad \forall\phi \in H_0^2(-1,1),\ t > 0, \tag{7.14}$$

where $\langle \widetilde{\mathcal{W}}'(U(\cdot,t)),\phi\rangle$ is defined by (7.12) and

$$X := \{v \in H^2(-1,1) : \; v(-1) = v(1) = \alpha, \; v'(-1) = -v'(1) = \beta\}.$$

For the numerical solution of (7.14), we use the finite element method to get a finite dimensional nonlinear system of ODEs. To this end, we decompose the space interval $I = [-1,1]$ into elements $K_i = [x_{i-1}, x_i]$, $i = 1,\dots,N$, and define the finite element space $X_h \subset X$ as

$$X_h := \{v \in X : \; v\big|_{K_i} \in \mathbb{P}_3 \quad \forall\, i = 1,\dots,N\}, \tag{7.15}$$

where $\mathbb{P}_3$ denotes the space of polynomials with degree less or equal to 3. Note that $X_h \subset C^1(I,\mathbb{R})$, i.e. we use C^1-elements of third order. The degrees of freedom are the values of the function and of the first derivative at the nodes x_i where the values at the boundary points $x_0 = -1$ and $x_N = 1$ are prescribed by the values α and β due to $X_h \subset X$. Thus, the semi-discrete solution $U_h(\cdot,t) \in X_h$ of problem (7.14) can be represented as

$$U_h(x,t) = \sum_{j=1}^{2N+2} c_j(t)\varphi_j(x), \tag{7.16}$$

where the basis functions $\varphi_j \in C^1(I,\mathbb{R})$ are defined as follows. For each element K_i, it holds $\varphi_j\big|_{K_i} \in \mathbb{P}_3$ for all j. The first set of basis functions φ_{1+i}, $i = 0,\dots,N$, is responsible for the point values of the discrete function at the nodes x_i, i.e., it holds

$$\varphi_{1+i}(x_k) = \delta_{i,k}, \qquad \frac{\partial}{\partial x}\varphi_{1+i}(x_k) = 0 \qquad \forall\, k = 0,\dots,N, \quad i = 0,\dots N.$$

The second set φ_{N+2+i} is responsible for the values of the x-derivatives at the nodes x_i, i.e., it holds

$$\varphi_{N+2+i}(x_k) = 0, \qquad \frac{\partial}{\partial x}\varphi_{N+2+i}(x_k) = \delta_{i,k} \qquad \forall\, k = 0,\dots,N, \quad i = 0,\dots N.$$

These conditions for the definition of the basis functions φ_j imply the following meaning of the coefficients $c_j(t)$ in (7.16)

$$c_{1+i}(t) = U_h(x_i,t), \qquad c_{N+2+i}(t) = \frac{\partial}{\partial x}U_h(x_i,t) \qquad \forall\, i = 0,\dots,N,$$

where $c_1(t) = c_{N+1}(t) = \alpha$ and $c_{N+2}(t) = -c_{2N+2}(t) = \beta$ for all $t > 0$ due to the Dirichlet boundary conditions of $U_h(x,t)$. Note that the support of the basis functions φ_{1+i} and φ_{N+2+i} is local; it consists of the (at most two) elements that contain the node x_i. The initial condition is discretised as $U_h(x,0) = u_{0,h}(x) = \sum_{j=1}^{2N+2} c_{0,j}\varphi_j(x)$, where $u_{0,h} \in X_h$ is a suitable interpolant of u_0 in X_h, which can be defined, for instance, by the choice $c_{0,1+i} := u_0(x_i)$ and $c_{0,N+2+i} := \frac{\partial}{\partial x}u_0(x_i)$ for $i = 0,\dots,N$. Therefore, we have the initial conditions $c_j(0) = c_{0,j}$ for the unknown coefficient functions $c_j(t)$. For the discrete problem, we need the test space

$$X_{h,0} := \{v \in H^2_0(-1,1) : \; v\big|_{K_i} \in \mathbb{P}_3 \quad \forall\, i = 1,\dots,N\}.$$

Then, the semi-discrete variational problem reads :

$$\begin{aligned} &\text{For } t \ge 0 \text{ find } U_h(\cdot,t) \in X_h \text{ such that } U_h(.,0) = u_{0,h} \text{ and} \\ &\int_{-1}^{+1} \frac{U_h(\cdot,t)U_{ht}(\cdot,t)\phi_h}{(1+U_{hx}(\cdot,t)^2)^{1/2}}dx \; + \; \langle \widetilde{\mathcal{W}}'(U_h(\cdot,t)),\phi_h\rangle = 0 \qquad \forall \phi_h \in X_{h,0}, \; t > 0. \end{aligned} \tag{7.17}$$

Using the ansatz (7.16) for $U_h(\cdot,t)$ and taking the test functions $\phi_h = \varphi_i \in X_{h,0}$ for $i \in J_h := \{1,\dots,2N+2\}\setminus\{1,N+1,N+2,2N+2\}$, we see that (7.17) is equivalent to a nonlinear $(2N-2)$-dimensional system of ODEs for the coefficient functions $c_j(t)$, $j \in J_h$.

In the time discretisation, we calculate for a discrete time level t_n an approximation $U^n \in X_h$ of $U_h(\cdot,t_n)$. Starting with $t_0 = 0$ and $U^0 := u_{0,h}$, we assume that U^n is known. We choose a time step $k_n > 0$ and compute U^{n+1} at the time level $t_{n+1} := t_n + k_n$ from (7.17) by approximating the time derivative U_{ht} at $t = t_n$ by the first order backward difference formula

$$U_{ht}(t_n) \approx \frac{U^{n+1}-U^n}{k_n}.$$

In order to get a linear system of equations for U^{n+1} we replace in (7.17) several nonlinear terms of $U_h(\cdot,t)$ by the known function $U^n \in X_h$, i.e., we compute $U^{n+1} \in X_h$ from

$$\int_{-1}^{+1} \frac{U^n}{(1+(U_x^n)^2)^{1/2}}\Big(U^{n+1}-U^n\Big)\phi_h dx \;+\; k_n\langle \widetilde{\mathcal{W}}_n'(U^{n+1}),\phi_h\,\rangle = 0 \qquad \forall \phi_h \in S_h, \tag{7.18}$$

where $\widetilde{\mathcal{W}}_n'(U^{n+1})$ is the following linear approximation of $\widetilde{\mathcal{W}}\,'(U^{n+1})$:

$$\begin{aligned}\langle \widetilde{\mathcal{W}}_n'(U^{n+1}),\phi_h\,\rangle \;:=\; & \frac{1}{4}\int_{-1}^{+1}\Big\{2\frac{U^nU_{xx}^{n+1}\phi_{hxx}}{(1+(U_x^n)^2)^{5/2}} + \frac{(U_{xx}^n)^2\phi_h}{(1+(U_x^n)^2)^{5/2}} - 5\frac{U^n(U_{xx}^n)^2U_x^{n+1}\phi_{hx}}{(1+(U_x^n)^2)^{7/2}} \\ & -\frac{\phi_h}{(U^n)^2(1+(U_x^n)^2)^{1/2}} - \frac{U_x^{n+1}\phi_{hx}}{U^n(1+(U_x^n)^2)^{3/2}}\Big\}dx.\end{aligned}$$

Note that the places, where we have taken U^n and where U^{n+1}, have been chosen heuristically. Other choices are possible and will be studied in future.

Numerical experiments have shown that the choice of a constant time step $k_n = \triangle t$ for all $n = 0,1,\dots,$ does not lead to satisfying results. If the time step is too large the sequence $\{U^n\}$ can be divergent and if it is too small one needs a very large computing time to reach a stationary limit. Therefore, we have developed an adaptive time step control which is presented in Figure 15. In the step (b2) we discard the computed solution U^{n+1} if its energy has increased compared with U^n or if the relative change of the energy was too large. We divide the time step size by two and compute U^{n+1} again. In all other cases we accept the solution U^{n+1}. Moreover, we double the size for the next time step if the relative change of the energy was at least in two previous time steps too small and the doubled size is not larger than a prescribed value k_{max}.

In our numerical experiments, we have chosen the control parameters $\omega_{max} = 0.1$, $\omega_{min} = 0.01$, $k_{max} = 0.01$ (see Figure 15) and the initial time step size $k_0 = h^4$ where $h := \max_{1\le i\le N}|x_i - x_{i-1}|$ denotes the mesh-size. We accept U^{n+1} to be the stationary limit of our time marching algorithm if

$$k_n^{-1}|\mathcal{W}(U^{n+1})-\mathcal{W}(U^n)| < \varepsilon_{\mathcal{W}} \qquad \text{and} \qquad k_n^{-1}\|U^{n+1}-U^n\|_\infty < \varepsilon_U, \tag{7.19}$$

where the norm $\|\cdot\|_\infty$ is defined as

$$\|U_h\|_\infty := \max_{1\le j\le 2N+2}|c_j| \qquad \text{for} \qquad U_h = \sum_{j=1}^{2N+2} c_j\varphi_j \in X_h,$$

and $\varepsilon_{\mathcal{W}}$, ε_U are some prescribed tolerances which have been chosen as $\varepsilon_{\mathcal{W}} = \varepsilon_U = 10^{-4}$. We stop the time iteration if the criterion (7.19) is satisfied or if, in case (b2) of the adaptive time step control (Figure 15), for the halved time step size it holds $k_n/2 < \sqrt{eps}$, where eps is the relative floating-point accuracy, or if a maximum number n_{max} of iteration steps is reached (we have used $n_{max} = 360000$).

Computation of $(t_{n+1}, k_{n+1}, U^{n+1})$ *from* (t_n, k_n, U^n) *:*

(a) initialize: $\mathcal{W}_0 := \mathcal{W}(U^n)$ (formula (7.11)); $T^{accept} := 0\,;$ $N^{too\_small} := 0\,;$

(b) **while** $T^{accept} = 0$ **do**

  (1) compute: U^{n+1} by solving (7.18); $\mathcal{W} := \mathcal{W}(U^{n+1})\,;$

  (2) **if** $\mathcal{W} > \mathcal{W}_0$ or $|\mathcal{W} - \mathcal{W}_0| > \omega_{max}|\mathcal{W}_0|$ **then**
    $k_n := k_n/2\,;$

  (3) **else if** $|\mathcal{W} - \mathcal{W}_0| < \omega_{min}|\mathcal{W}_0|$ and $2k_n < k_{max}$ **then**
    $T^{accept} := 1\,;$
    if $N^{too\_small} \geq 2$ **then**
      $k_n := 2k_n\,;$ $N^{too\_small} := 0\,;$
    else
      $N^{too\_small} := N^{too\_small} + 1\,;$
    endif

  (4) **else**
    $T^{accept} := 1\,;$
  endif

enddo

(c) $k_{n+1} := k_n\,;$ $t_{n+1} := t_n + k_n\,;$

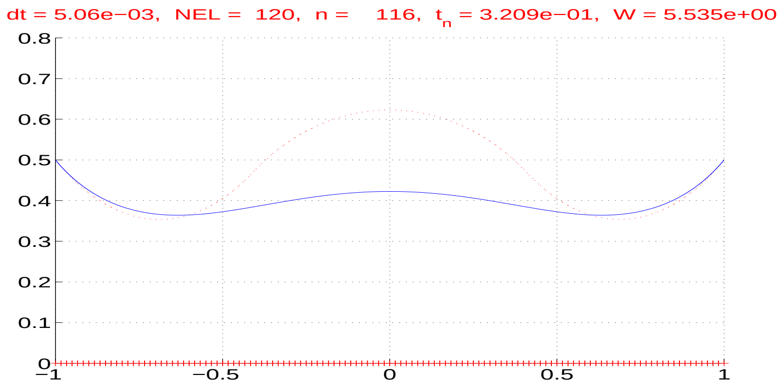
Figure 15: Time marching algorithm with control parameters ω_{max}, ω_{min} and k_{max}.

In the following, we describe our numerical results for three different settings of the boundary data α and β. In the first case, we combine the value $\alpha = 0.5$ with the three negative values $\beta \in \{-1, -5, -10\}$, see Figure 16. In the second case, we consider $\alpha = 0.5$ and the positive values $\beta \in \{1, 5, 10\}$, see Figure 17. Finally, in the third case, we study the situations where $\beta = 0$ and $\alpha \in \{0.5, 0.1, 0.01\}$, see Figure 18. The finite element mesh depends on the data α and β and is locally adapted near the boundary in the following way. The interval $I = [-1, 1]$ is decomposed into the three subintervals $\Omega_1 = [-1, -1 + \delta]$, $\Omega_2 = [-1 + \delta, 1 - \delta]$ and $\Omega_3 = [1 - \delta, 1]$ where

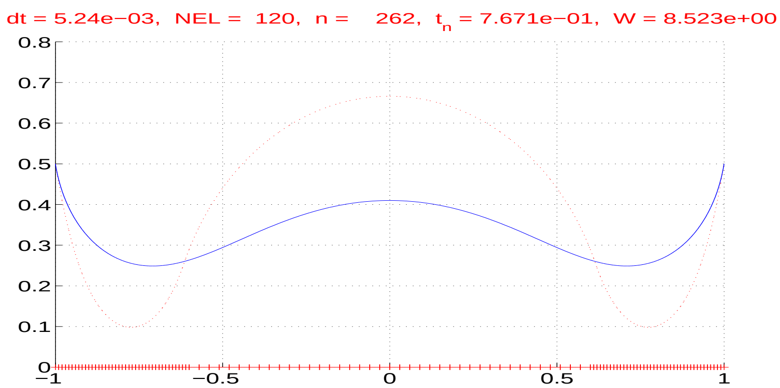
$$\delta := \min\{\frac{2}{3}, \omega_0 \min\{|\alpha|, \frac{1}{|\beta| + 10^{-6}}\}\}$$

with $\omega_0 = 2$ except for the case $(\alpha, \beta) = (0.01, 0)$ where $\omega_0 = 8$. Then the mesh is created by subdividing each subinterval Ω_k into $N_0 = 40$ equidistant elements. In each picture of Figures 16 - 18, the mesh is shown on the x-axis, the initial solution U^0 at $t_0 = 0$ is presented by the dotted line and the final solution U^n at the end t_n of the time iteration is given by the solid line. The parameters at the headline of the picture have the following meaning. `n` denotes the number of the last time step, `dt` the last time step size k_n, `NEL` the number of the finite elements and `W` the value of the Willmore functional $\mathcal{W}(U^n)$.

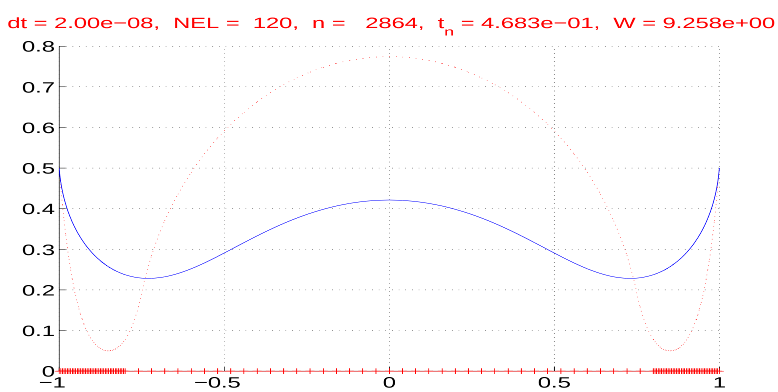
For nearly all cases, our numerical algorithm produced a discrete solution satisfying the approximate "stationarity" criterion (7.19) with the tolerances $\varepsilon_{\mathcal{W}} = \varepsilon_U = 10^{-4}$. The first exceptional case was $(\alpha, \beta) = (0.5, -10)$ where the algorithm at a time t_n could not find a next function U^{n+1} at a time $t_n + k_n$ with $k_n > \sqrt{eps}$ such that $\mathcal{W}(U^{n+1}) < \mathcal{W}(U^n)$. The other critical case was $(\alpha, \beta) = (0.01, 0)$ where for all n a new U^{n+1} with a smaller value of the Willmore functional



$\beta = -1$

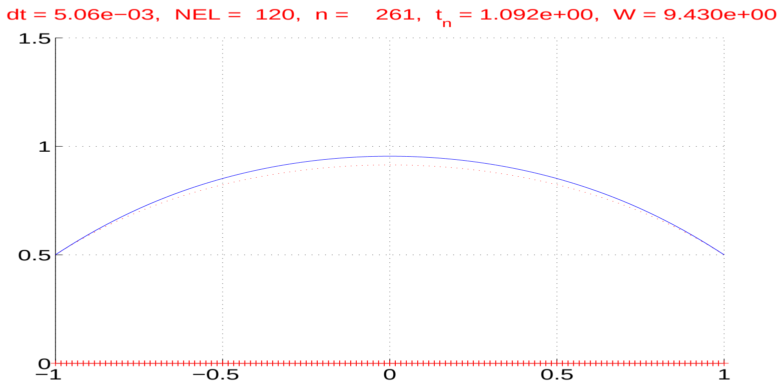


$\beta = -5$

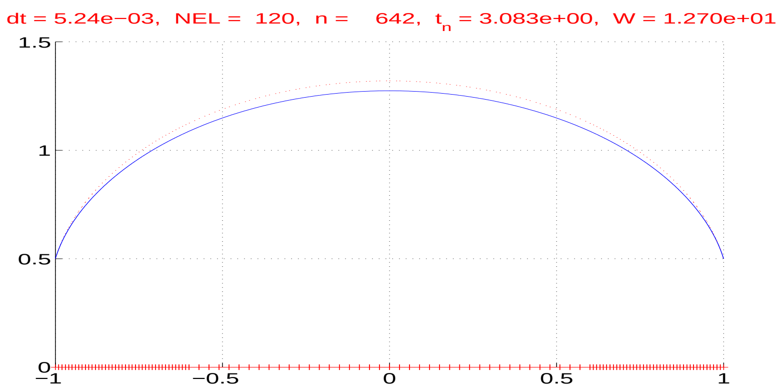


$\beta = -10: \quad k_n^{-1}\|U^{n+1} - U^n\|_\infty \approx 1.67e - 02, \quad$ stopped by $k_n/2 < \sqrt{eps}$

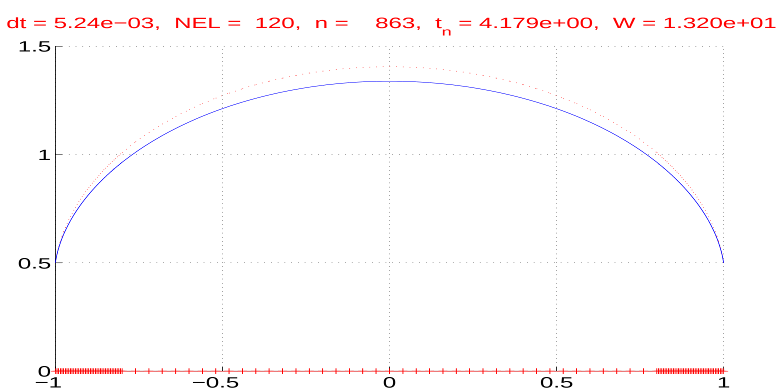
Figure 16: $\alpha = 0.5$ and $\beta < 0$



$\beta = 1$

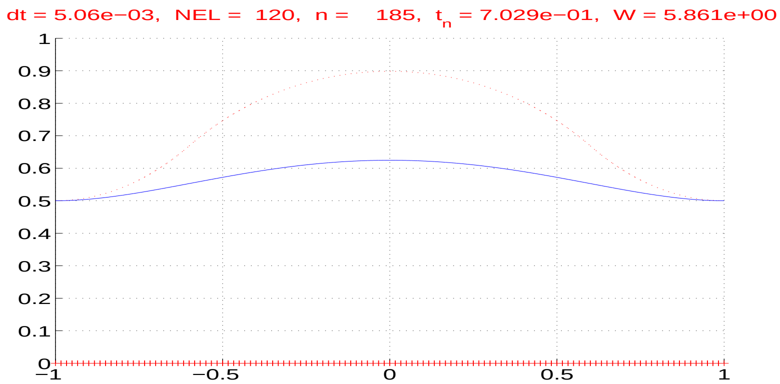


$\beta = 5$

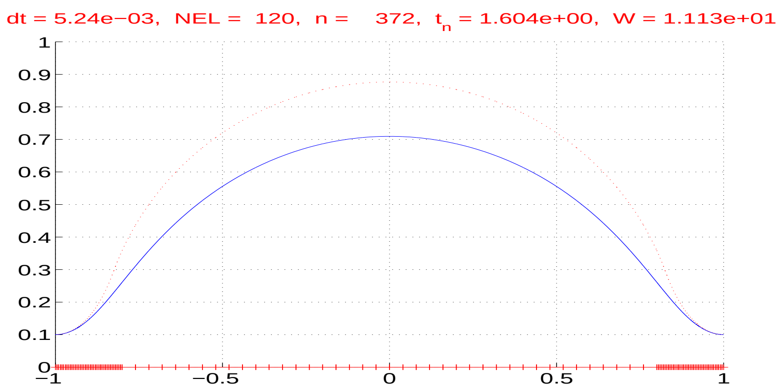


$\beta = 10$

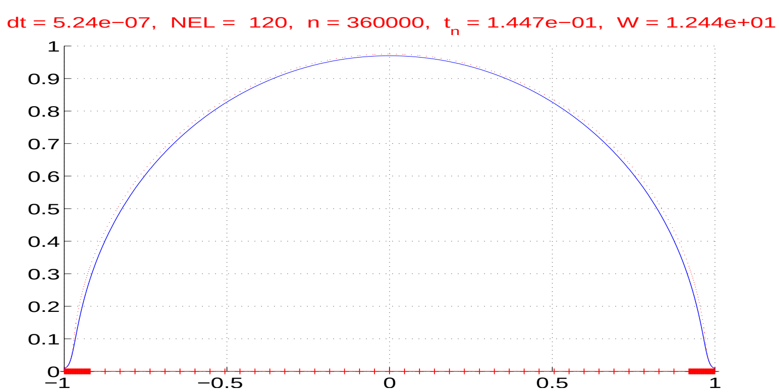
Figure 17: $\alpha = 0.5$ and $\beta > 0$



$\alpha = 0.5$



$\alpha = 0.1$



$\alpha = 0.01$: stopped by $n = n_{max}$, $\|U^{n+1} - U^n\|_\infty \approx 2.75e - 04$

Figure 18: $\beta = 0$

could be found but where the maximum number of $n_{max} = 360000$ time steps was reached without satisfying the criterion (7.19). On the other hand, the change of the graph of the discrete solution as well as the time step size over the last 99% of all time steps was very small. Here, further research is necessary to figure out the reason for this behaviour. Could it be that the first order time discretisation is not accurate enough or that the semi-implicit backward Euler exhibits some instabilities which lead to very small time steps? Another reason could be that the "exact" continuous Willmore flow is really creeping very slowly to the stationary limit. Let us finally note that, for such critical cases, a suitable choice of the initial function $U^0 = u_{0,h}$ is important for the convergence of the numerical solution to the stationary limit. Here a good analytical feeling is very helpful. We construct $u_{0,h} \in X_h$ as the interpolant of a suitable function $u_0 \in X$ as described above. In the case $\beta \leq 0$, we use $u_0 = f_\alpha$ with f_α defined in (5.1) which is a catenoid at the boundary fitted with an arc of a circle centered at the origin. For $\beta > 0$, we choose $u_0 = w$ with w defined in (6.1) which is an arc of a circle centered at $(0, \alpha - 1/\beta)$.

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Symmetric Willmore surfaces of revolution satisfying natural boundary conditions[1]

Matthias Bergner[2], Anna Dall'Acqua[3], Steffen Fröhlich[4]

Abstract

We consider the Willmore-type functional

$$\mathcal{W}_\gamma(\Gamma) := \int_\Gamma H^2\, dA - \gamma \int_\Gamma K\, dA,$$

where H and K denote mean and Gaussian curvature of a surface Γ, and $\gamma \in [0,1]$ is a real parameter. Using direct methods of the calculus of variations, we prove existence of surfaces of revolution generated by symmetric graphs which are solutions of the Euler-Lagrange equation corresponding to $\mathcal{W}_\gamma$ and which satisfy the following boundary conditions: the height at the boundary is prescribed, and the second boundary condition is the natural one when considering critical points where only the position at the boundary is fixed. In the particular case $\gamma = 0$ these boundary conditions are arbitrary positive height α and zero mean curvature.

Keywords. Natural boundary conditions, Willmore surfaces of revolution.
AMS classification. 49Q10; 53C42, 35J65, 34L30.

1 Introduction

For a smooth, immersed surface $\Gamma \subset \mathbb{R}^3$ and real parameters γ, μ, H_0, Nitsche in [14, 15] considered the functional

$$\mathcal{F}(\Gamma) = \int_\Gamma \Phi(H,K)\, dA \quad \text{with } \Phi(H,K) = \mu + (H - H_0)^2 - \gamma K, \tag{1.1}$$

where H is the mean curvature of the immersion, K its Gauss curvature, and dA its area element. In many applications, Γ is an idealised model for the interface occurring in real materials. The energy $\mathcal{F}(\Gamma)$ then reflects the surface tension and, therefore, elastic properties of this interface. Similar versions of this functional as model for elastic energies of thin plates were already studied by Poisson [17] in 1812, or Germain [7] in 1821. For a concise presentation we refer to Love's textbook [13]. In 1973, Helfrich [8] studied a functional quite similar to $\mathcal{F}$ from (1.1) as a model

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for biological bilayer membranes, see also [16] for a more recent survey on this subject. Therefore, $\mathcal{F}$ is sometimes referred to as *Helfrich functional.* Detailed historical information can also be found in Nitsche [14, 15].

From the mathematical point of view it is natural to assume a certain definiteness condition for the functional $\mathcal{F}$. More precisely, we require existence of a constant $C > -\infty$ such that $\mathcal{F}(\Gamma) \geq C$ holds true for all connected and orientable surfaces of regularity class C^2. As shown in [14], this condition imposes the following restrictions on the parameters

$$\mu \geq 0, \quad 0 \leq \gamma \leq 1, \quad \gamma H_0^2 \leq \mu(1-\gamma).$$

In the present work we study the special case $H_0 = \mu = 0$, where $\mathcal{F}$ takes the form

$$\mathcal{W}_\gamma(\Gamma) := \int_\Gamma H^2 \, dA - \gamma \int_\Gamma K \, dA, \quad 0 \leq \gamma \leq 1. \tag{1.2}$$

This functional models the elastic energy of thin shells. Willmore in [22] studied and popularised the functional $\mathcal{W}_0$, by now called *Willmore functional.*

Note that for $\gamma \in [0,1]$, the functional $\mathcal{W}_\gamma$ is non-negative. To see this, let $\kappa_1, \kappa_2 \in \mathbb{R}$ denote the principal curvatures of the surface. Then we compute

$$4(H^2 - \gamma K) = (\kappa_1+\kappa_2)^2 - 4\gamma\kappa_1\kappa_2 = (1-\gamma)(\kappa_1+\kappa_2)^2 + \gamma(\kappa_1-\kappa_2)^2 \geq 0 \quad \text{for } \gamma \in [0,1]$$

proving the non-negativity of $\mathcal{W}_\gamma$. Moreover, strict inequality $\mathcal{W}_\gamma(\Gamma) > 0$ holds for every non-planar surface Γ if $0 < \gamma < 1$.

We are mainly interested in minima or critical points of $\mathcal{W}_\gamma$. Such critical points $\Gamma \subset \mathbb{R}^3$ have to satisfy the *Willmore equation*

$$\Delta_\Gamma H + 2H(H^2 - K) = 0 \quad \text{on } \Gamma, \tag{1.3}$$

where Δ_Γ denotes the Laplace-Beltrami operator on Γ, see e.g. [22]. A solution of this non-linear fourth-order differential equation is called *Willmore surface.* Note that the Euler-Lagrange equation is independent of the value of γ since the integral over the Gauss curvature only contributes to the boundary terms on account of Gauss-Bonnet Theorem.

Existence and regularity results for closed Willmore surfaces of prescribed genus are extensively studied in the literature (see e.g., [1, 10, 11, 12, 20, 18]), while existence of Willmore surfaces *with prescribed boundaries* is by far less studied. In the presence of boundaries the partial differential equation (1.3) has to be accompanied by appropriate boundary conditions. Possible choices for them are presented in [14] and [15] along with corresponding existence results. Nitsche's results are based on perturbation arguments and require certain smallness conditions on the boundary data. On the other hand, Schätzle in [19] recently proved existence and regularity of branched Willmore immersions in $\mathbb{S}^n$ satisfying prescribed boundary conditions. By working in $\mathbb{S}^n$ some compactness problems could be overcome.

To present a complete analysis of at least special Willmore surfaces satisfying prescribed boundary conditions, we restrict ourselves to surfaces of revolution generated by rotating a symmetric graph in the $[x,y]$-plane about the x-axis. Existence and classical regularity of those axially symmetric Willmore surfaces with arbitrary symmetric Dirichlet boundary conditions were recently proved in [3, 4]. With the paper at hand we continue these studies. We solve the existence problem for Willmore surfaces of revolution with prescribed position at the boundary, and with a second boundary condition, which is the natural one when considering critical points of the Willmore functional in the class of surfaces of revolution generated by symmetric graphs where only the position at the boundary is fixed.

1.1 Main result

We consider surfaces of revolution $\Gamma \subset \mathbb{R}^3$ generated by rotating the graph of a smooth symmetric function $u\colon [-1,1] \to (0,\infty)$ about the x-axis. Within this class of surfaces we look for solutions of the Willmore equation (1.3) under the boundary conditions

$$u(\pm 1) = \alpha > 0 \quad \text{and} \quad H(\pm 1) = \frac{\gamma}{\alpha\sqrt{1+u'(\pm 1)^2}} \quad \text{for } \gamma \in [0,1].$$

Our main result is the following.

Theorem 1.1 (Existence and regularity)**.** *For each $\alpha > 0$ and for each $\gamma \in [0,1]$, there exists a positive and symmetric function $u \in C^\infty([-1,1],(0,\infty))$, i.e. $u(x) > 0$ and $u(x) = u(-x)$, such that the corresponding surface of revolution $\Gamma \subset \mathbb{R}^3$ solves*

$$\begin{cases} \triangle_\Gamma H + 2H(H^2 - K) = 0 \quad \text{on } \Gamma, \\[2ex] u(\pm 1) = \alpha \ \text{ and } \ H(\pm 1) = \dfrac{\gamma}{\alpha\sqrt{1+u'(\pm 1)^2}}. \end{cases} \tag{1.4}$$

This fourth-order system along with its natural boundary conditions can be found e.g. in [14], [15], or von der Mosel [21]. In Appendix A we recall how the second boundary condition in (1.4) arises as natural boundary condition for the functional $\mathcal{W}_\gamma$.

For special values of α and γ, explicit solutions of problem (1.4) are known. For example, if $\gamma = 1$ then the circular arc $u(x) = \sqrt{\alpha^2 + 1 - x^2}$ provides an explicit solution of (1.4) for arbitrary $\alpha > 0$. Next, let us define some real number α^* by

$$\alpha^* := \min_{y>0} \frac{\cosh(y)}{y} = \frac{\cosh(b^*)}{b^*} = \sinh b^* \approx 1.5088795\ldots \tag{1.5}$$

$$\text{with} \quad b^* \approx 1.1996786\ldots \quad \text{solving} \quad b^* \tanh(b^*) = 1. \tag{1.6}$$

In case of $\gamma = 0$ and $\alpha > \alpha^*$, there exist two catenoid solutions of (1.4) of the form $u(x) = \cosh(bx)/b$, $b > 0$ suitably chosen. These two solutions yield surfaces with vanishing mean curvature, i.e. minimal surfaces. Moreover, these explicit examples show that the solutions of problem (1.4) are, in general, not unique. Theorem 1.1 becomes particularly interesting for $\gamma = 0$ and $\alpha < \alpha^*$, as catenoid solutions do no longer exist under this assumption. For $\gamma = 0$ and $\alpha = 1$ there still exists an explicit solution given by $u(x) = 2 - \sqrt{2 - x^2}$, a piece of the well-known Clifford torus.

So for $\gamma = 0$ we have the following rough picture:
→ non-minimal solutions for $\alpha < \alpha^*$;
→ exactly one minimal surface solution for $\alpha = \alpha^*$;
→ two minimal surface solutions for $\alpha > \alpha^*$.

Existence of rotationally symmetric Willmore surfaces solution of (1.4) for $\gamma = 0$ and for all values of α was observed numerically by Fröhlich [6] in 2004, and by Kastian [9] as well as Grunau and Deckelnick [5]. Moreover, in [9] the presence of a third solution for $\alpha > \alpha^*$ was numerically observed, suggesting that α^* is a bifurcation point on the branch of minimal surface solutions. Recently, in [5] Deckelnick and Grunau proved that α^* is indeed a bifurcation point and so, at least locally, the existence also of a non-minimal solution for $\alpha > \alpha^*$ is settled. In the same paper, by a linearisation around the Clifford torus they prove existence of a solution to (1.4) for $\gamma = 0$ and α close to 1. Here we prove existence of solutions for the same boundary value problem for all $\alpha \in (0, \alpha^*)$.

Also the case $\gamma = 1$ is special. Up to some constant, $\mathcal{W}_1(u)$ equals the total elastic energy of u considered as a curve in the hyperbolic half-plane $\mathbb{R}^2_+ := \{(x, y) \in \mathbb{R}^2 : y > 0\}$ equipped with the metric $ds_h^2 := \frac{1}{y^2}(dx^2 + dy^2)$ (see e.g. [2], [3]). Thus, varying γ within $[0, 1]$, we interpolate between the "Euclidean" Willmore functional with $\gamma = 0$, and the "hyperbolic" Willmore functional for $\gamma = 1$.

The proof of Theorem 1.1 is based on the existence results from [4] for symmetric Willmore surfaces of revolution satisfying Dirichlet boundary conditions $u(\pm 1) = \alpha$ and $\mp u'(\pm 1) = \beta$ for $\alpha > 0$ and $\beta \in \mathbb{R}$ arbitrary. We construct a solution of (1.4) by minimising the Willmore energy for fixed α and variable β. Essential tools are the continuity and the monotonicity of the Willmore energy in β.

2 Notation. Dirichlet boundary value problem

2.1 Surfaces of revolution

We consider functions $u \in C^2([a, b], (0, \infty))$, $a < b$. Rotating the curve $(x, u(x)) \subset \mathbb{R}^2$ about the x-axis generates a *surface of revolution* $\Gamma \subset \mathbb{R}^3$ which can be parametrised by

$$\Gamma : f(x, \varphi) = \big(x, u(x)\cos\varphi, u(x)\sin\varphi\big) \in \mathbb{R}^3, \quad x \in [a, b], \ \varphi \in [0, 2\pi). \tag{2.1}$$

The term "surface" always refers to the mapping f as well as to the set Γ. The condition $u > 0$ implies that f is embedded in $\mathbb{R}^3$ and in particular immersed.

Let κ_1 and κ_2 denote the principal curvatures of $\Gamma \subset \mathbb{R}^3$, i.e. $\kappa_1 = -u''(x)(1 + u'(x)^2)^{-\frac{3}{2}}$ and $\kappa_2 = (u(x)\sqrt{1 + u'(x)^2})^{-1}$. Its *mean curvature* H and *Gaussian curvature* K are

$$\begin{aligned} H &= \frac{\kappa_1 + \kappa_2}{2} = -\frac{u''(x)}{2(1 + u'(x)^2)^{3/2}} + \frac{1}{2u(x)\sqrt{1 + u'(x)^2}}, \\ K &= \kappa_1\kappa_2 = -\frac{u''(x)}{u(x)(1 + u'(x)^2)^2}. \end{aligned}$$

For the total Gauss curvature we have

$$\int_\Gamma K\, dA = -2\pi \int_a^b \frac{u''(x)}{(1 + u'(x)^2)^{\frac{3}{2}}}\, dx = -2\pi \left. \frac{u'(x)}{\sqrt{1 + u'(x)^2}} \right|_a^b, \tag{2.2}$$

i.e. the Gauss-Bonnet theorem in our special situation. The integral is already determined by the boundary values $u'(a)$ and $u'(b)$. This fact will become essential for the Dirichlet problem discussed in Section 2.3. Furthermore, $\mathcal{W}_\gamma(\Gamma)$ takes the form

$$\begin{aligned} \mathcal{W}_\gamma(u) := \mathcal{W}_\gamma(\Gamma) &= \frac{\pi}{2} \int_a^b \left(\frac{u''(x)}{(1 + u'(x)^2)^{3/2}} - \frac{1}{u(x)\sqrt{1 + u'(x)^2}} \right)^2 u(x)\sqrt{1 + u'(x)^2}\, dx \\ &\quad + 2\pi\gamma \left. \frac{u'(x)}{\sqrt{1 + u'(x)^2}} \right|_a^b. \end{aligned} \tag{2.3}$$

An important property of the energy $\mathcal{W}_\gamma$ is the following

Lemma 2.1. *(Invariance of $\mathcal{W}_\gamma$ under rescaling)*
Given some function $u \in H^2([-1, 1], (0, +\infty))$ and $r > 0$, let $u_r \in H^2([-1/r, 1/r], (0, +\infty))$, $u_r(x) := u(rx)/r$ denote the rescaling of u by $1/r$. Then the mapping $r \mapsto \mathcal{W}_\gamma(u_r)$ is constant for $r \in (0, +\infty)$.

Proof. We note $u_r'(x) = u'(rx)$ and $u_r''(x) = ru''(rx)$, in particular $u_r'(\pm 1/r) = u'(\pm 1)$. Then we obtain

$$\begin{aligned} \mathcal{W}_\gamma(u_r) &= \frac{\pi}{2} \int_{-1/r}^{1/r} \left(\frac{ru''(rx)}{(1+u'(rx)^2)^{3/2}} - \frac{r}{u(rx)\sqrt{1+u'(rx)^2}} \right)^2 \frac{1}{r} u(rx) \sqrt{1+u'(rx)^2}\, dx \\ &\quad + 2\pi\gamma \left. \frac{u'(rx)}{\sqrt{1+u'(rx)^2}} \right|_{-1/r}^{1/r} = \mathcal{W}_\gamma(u) \end{aligned}$$

using formula (2.3) twice (first for $\mathcal{W}_\gamma(u_r)$ and then for $\mathcal{W}_\gamma(u)$) and the change of variables $\tilde{x} = rx$ in the integral. □

2.2 Notation

For $\alpha > \alpha^*$, α^* defined in (1.5), the following two numbers

$$b_1(\alpha) := \inf \left\{ b > 0 \ : \ \frac{\cosh b}{b} \le \alpha \right\} \quad \text{and} \quad b_2(\alpha) := \sup \left\{ b > 0 \ : \ \frac{\cosh b}{b} \le \alpha \right\} \tag{2.4}$$

are well-defined and satisfy the inequality $0 < b_1(\alpha) < b^* < b_2(\alpha) < +\infty$ with b^* from (1.6). Together with (1.5) we deduce

$$\sinh(b_1(\alpha)) < \sinh(b^*) = \alpha^* < \sinh(b_2(\alpha)). \tag{2.5}$$

Definition 2.2. *For $\alpha > 0$ and $\beta \in \mathbb{R}$ we introduce the space of functions*

$$\overline{N}_{\alpha,\beta} := \left\{ u \in H^2([-1,1]) \ : \ u(x) > 0 \ , \ u(x) = u(-x) \ , \ u(\pm 1) = \alpha \ \textit{and} \ u'(-1) = \beta \right\}$$

along with

$$\overline{T}_{\gamma,(\alpha,\beta)} := \inf \left\{ \mathcal{W}_\gamma(u) \ : \ u \in \overline{N}_{\alpha,\beta} \right\} \ \textit{for} \ \gamma \in [0,1] \ .$$

Due to technical reasons we shall not work within $\overline{N}_{\alpha,\beta}$, but within the smaller space

$$N_{\alpha,\beta} := \left\{ u \in \overline{N}_{\alpha,\beta} \ : \textit{if} \ \alpha > \alpha^* \ \textit{and} \ -\alpha < \beta \quad \textit{then} \quad u'(x) < \alpha \ \textit{in} \ [0,1] \right\} \tag{2.6}$$

with

$$T_{\gamma,(\alpha,\beta)} := \inf \left\{ \mathcal{W}_\gamma(u) \ : \ u \in N_{\alpha,\beta} \right\} \ \textit{for} \ \gamma \in [0,1] \ . \tag{2.7}$$

One easily sees that the space $N_{\alpha,\beta}$ is never empty and hence $T_{\gamma,(\alpha,\beta)}$ is well-defined. In Corollary 2.6 in the next section we show that the minimal energy $T_{\gamma,(\alpha,\beta)}$ is actually attained for all $\alpha > 0$, $\beta \in \mathbb{R}$ and $\gamma \in [0,1]$.

2.3 The Dirichlet boundary value problem

In this section we recall the existence result for the Dirichlet boundary value problem (2.8) below from [4]. First, this result holds true for $\gamma = 0$ and $\gamma = 1$. At the same time a solution to this problem is a critical point for $\mathcal{W}_\gamma$ independently of γ because, on account of (2.2), the total Gauss curvature is a constant depending only on β. Furthermore, we state monotonicity properties of the minimal energy $T_{\gamma,(\alpha,\beta)}$ in α.

Theorem 2.3. ([4, Th.1.1]) *For each $\alpha > 0$ and for each $\beta \in \mathbb{R}$, there exists a positive and symmetric function $u \in C^\infty([-1,1],(0,\infty))$ such that the corresponding surface of revolution $\Gamma \subset \mathbb{R}^3$ solves*

$$\begin{cases} \triangle_\Gamma H + 2H(H^2 - K) = 0 \quad \text{on } \Gamma, \\ u(\pm 1) = \alpha, \qquad u'(-1) = -u'(1) = \beta \end{cases} \tag{2.8}$$

Moreover, u has the following properties:

1) $\mathcal{W}_1(u) = T_{1,(\alpha,\beta)}$,

2) *if $\beta \geq 0$, then $u' > 0$ in $(-1,0)$,*

3) *if $\beta < 0$, then u has at most three critical points in $[-1,1]$.*

Property *1)*, which is not mentioned in [4, Th.1.1], holds due to the construction of u as minimiser of the functional $\mathcal{W}_1$ in the class $N_{\alpha,\beta}$. The monotonicity behaviour of $T_{1,(\alpha,\beta)}$ in α for fixed β was also studied in [4]. Those values of α and β, for which a catenoid or an arc of a circle solve (2.8), mark points where the monotonicity of this optimal energy w.r.t. α changes qualitatively. In particular, for $\beta > 0$ and $\alpha = \beta^{-1}$, a solution to (2.8) is an arc of the circle with center at the origin and going through $(1,\alpha)$, while for $\beta < 0$ and $\alpha = \alpha_\beta$ with

$$\alpha_\beta := \frac{\sqrt{1+\beta^2}}{\operatorname{arsinh}(-\beta)} \geq \alpha^* \tag{2.9}$$

the catenoid $u(x) = \cosh(bx)/b$, $b = \operatorname{arsinh}(-\beta)$ is a minimal surface solution to (2.8). Because of

$$T_{\gamma,(\alpha,\beta)} = T_{1,(\alpha,\beta)} + 4\pi(1-\gamma)\,\frac{\beta}{\sqrt{1+\beta^2}},$$

the minimal energies $T_{\gamma,(\alpha,\beta)}$ and $T_{1,(\alpha,\beta)}$ show the same monotonicity behaviour w.r.t. α as long as we keep γ and β fixed. Thus, the monotonicity results from [4] and [3] on $T_{1,(\alpha,\beta)}$ are carried over to the case $\gamma \in [0,1]$. We recall the results here and will give the proofs in Appendix C.

Proposition 2.4. *Let $\gamma \in [0,1]$ be fixed.*

(i) *For $\beta > 0$ and $\frac{1}{\beta} \leq \alpha' < \alpha$ it holds $T_{\gamma,(\alpha',\beta)} < T_{\gamma,(\alpha,\beta)}$.*

(ii) *For $\beta > 0$ and $0 < \alpha' < \alpha \leq \frac{1}{\beta}$ it holds $T_{\gamma,(\alpha',\beta)} > T_{\gamma,(\alpha,\beta)}$.*

(iii) *For $\beta = 0$ and $0 < \alpha' < \alpha$ it holds $T_{\gamma,(\alpha',\beta)} > T_{\gamma,(\alpha,\beta)}$.*

(iv) *For $\beta < 0$ and $0 < \alpha' < \alpha \leq \alpha_\beta$ it holds $T_{\gamma,(\alpha',\beta)} > T_{\gamma,(\alpha,\beta)}$.*

(v) *For $\beta < 0$ and $\alpha_\beta \leq \alpha' < \alpha$ it holds $T_{\gamma,(\alpha',\beta)} < T_{\gamma,(\alpha,\beta)}$.*

In order to prove Theorem 1.1 we require various important a priori estimates for solutions to (2.8) established in [4]. We recall them here and give the proofs in Appendix B. The real numbers b_1, b_2 are defined in (2.4) and α^* is defined in (1.5).

Proposition 2.5. *Let $\alpha > 0$, $\beta \in \mathbb{R}$ and $u \in C^\infty([-1,1],(0,\infty))$ be the function from Theorem 2.3 such that the corresponding surface of revolution $\Gamma \subset \mathbb{R}^3$ solves (2.8). Then u has the following qualitative properties:*

1. *If $\alpha \le \alpha^*$ then*

$$|u'(x)| \le \max\left\{|\beta|, \alpha^*, \frac{\sqrt{1+\beta^2}}{\alpha}\right\},$$

$$\sqrt{(\alpha+\max\{1,|\beta|\})^2 - x^2} \ge u(x) \ge \min\left\{\frac{1}{2}\frac{\alpha}{\sqrt{1+\beta^2}}, \frac{1}{2}\frac{\max\{|\beta|,\alpha^*\}}{e^{C_2}-1}\right\}$$

with $C_2 = 8(1+\max\{|\beta|,\alpha^*\}^2)$.

2. *If $\alpha > \alpha^*$ then*

$$|u'(x)| \le \max\left\{\sinh(b_2(\alpha)), |\beta|, \frac{\sqrt{1+\beta^2}}{\alpha}\right\},$$

$$\sqrt{(\alpha+\max\{1,|\beta|\})^2 - x^2} \ge u(x) \ge \min\left\{\frac{1}{2}\frac{\alpha}{\sqrt{1+\beta^2}}, \frac{\sinh(b_2(\alpha))}{e^{C_1}-1}, \frac{1}{2}\frac{\max\{|\beta|,\alpha^*\}}{e^{C_2}-1}, \frac{1}{b_2(\alpha)}\right\}$$

with $C_2 = 8(1+\max\{|\beta|,\alpha^*\}^2)$ *and* $C_1 = 2\cosh(2b_2(\alpha))(1+\operatorname{arsinh}(|\beta|)(\alpha-\alpha^*))$.

(2.i) If $-\sinh(b_1(\alpha)) \ge \beta > -\alpha$, we have

$$0 \le u'(x) \le -\beta < \alpha \quad \text{in } [0,1].$$

(2.ii) If $\beta > -\sinh(b_1(\alpha))$, we have

$$-\frac{1}{\alpha^*} \le u'(x) \le \sinh(b_1(\alpha)) \text{ in } [0,1] \text{ and } \sqrt{\alpha^2+1-x^2} \ge u(x) \ge \frac{1}{b_1(\alpha)}\cosh(b_1(\alpha)x).$$

Corollary 2.6. *Given any $\gamma \in [0,1]$, $\alpha > 0$ and $\beta \in \mathbb{R}$, there exists some function $u \in C^\infty([-1,1]) \cap N_{\alpha,\beta}$ such that the corresponding surface of revolution solves* (2.8) *and moreover $\mathcal{W}_\gamma(u) = T_{\gamma,(\alpha,\beta)}$ holds.*

Corollary 2.6 is an immediate consequence of Theorem 2.3 and Proposition 2.5 *(2.i)* and *(2.ii)* (the proposition gives that $u \in N_{\alpha,\beta}$ since for $\alpha > \alpha^*$, $\sinh(b_1(\alpha)) < \alpha$ by (2.5)).

3 Continuity and monotonicity of the energy in β

Throughout the following sections we consider fixed real numbers $\alpha > 0$ and $\gamma \in [0,1]$. In this section we analyse the behaviour of the optimal energy $T_{\gamma,(\alpha,\beta)}$ w.r.t. β. The results we obtain are the main ingredients for the proof of Theorem 1.1.

3.1 Continuity in β

Lemma 3.1. *Let $\gamma \in [0,1]$ be fixed. If $\alpha \le \alpha^*$, then $\beta \mapsto T_{\gamma,(\alpha,\beta)}$ is upper semi-continuous for $\beta \in \mathbb{R}$. If $\alpha > \alpha^*$, then $\beta \mapsto T_{\gamma,(\alpha,\beta)}$ is upper semi-continuous for $\beta \in \mathbb{R}\backslash\{-\alpha\}$.*

Proof. Given $u \in N_{\alpha,\beta}$ and $\varepsilon \in \mathbb{R}$ consider the symmetric function $u_\varepsilon(x) := u(x) + \frac{\varepsilon}{2}(1-x^2)$ with the properties $u_\varepsilon(\pm 1) = \alpha$, $u_\varepsilon'(-1) = \beta + \epsilon$. Then $u_\varepsilon \in \overline{N}_{\alpha,\beta+\varepsilon}$ will hold for $|\varepsilon| < \varepsilon_0$, $\varepsilon_0 > 0$ sufficiently small (to have $u_\varepsilon(x) > 0$ in $[-1,1]$). If either $\alpha \le \alpha^*$ or $-\beta > \alpha$ this implies $u_\varepsilon \in N_{\alpha,\beta+\varepsilon}$ for $|\epsilon|$ sufficiently small (see Definition 2.2). If, on the other hand, $\alpha > \alpha^*$ and $\beta > -\alpha$ then $u \in N_{\alpha,\beta}$ implies $u'(x) < \alpha$ in $[0,1]$ by Definition 2.2. This implies $u_\varepsilon'(x) < \alpha$ in $[0,1]$ for

$|\varepsilon| \leq \varepsilon_1$ and thus $u_\varepsilon \in N_{\alpha,\beta+\epsilon}$, if $0 < \varepsilon_1 \leq \varepsilon_0$ is chosen sufficiently small. The continuity of the mapping $\varepsilon \mapsto \mathcal{W}_\gamma(u_\varepsilon)$ gives

$$T_{\gamma,(\alpha,\beta)} = \inf_{u \in N_{\alpha,\beta}} \big[\lim_{\varepsilon\to 0} \mathcal{W}_\gamma(u_\varepsilon)\big] \geq \inf_{u \in N_{\alpha,\beta}} \big[\limsup_{\varepsilon\to 0} T_{\gamma,(\alpha,\beta+\varepsilon)}\big] = \limsup_{\varepsilon\to 0} T_{\gamma,(\alpha,\beta+\varepsilon)},$$

which just means that $\beta \mapsto T_{\gamma,(\alpha,\beta)}$ is upper semi-continuous. □

The proof of lower semi-continuity of $\beta \mapsto T_{\gamma,(\alpha,\beta)}$ is more involved and requires the a priori estimates from Proposition 2.5.

Lemma 3.2. *Let $\gamma \in [0,1]$ be fixed. If $\alpha \leq \alpha^*$, then $\beta \mapsto T_{\gamma,(\alpha,\beta)}$ is lower semi-continuous for $\beta \in \mathbb{R}$. If $\alpha > \alpha^*$, then $\beta \mapsto T_{\gamma,(\alpha,\beta)}$ is lower semi-continuous for $\beta \in \mathbb{R}\backslash\{-\alpha\}$.*

Proof. Because of

$$T_{\gamma',(\alpha,\beta)} = T_{\gamma,(\alpha,\beta)} + 4\pi(\gamma-\gamma')\frac{\beta}{\sqrt{1+\beta^2}}$$

it suffices to prove the result for one particular γ, we take $\gamma_0 := \frac{1}{2}$. Let $(\beta_k)_{k\in\mathbb{N}} \subset \mathbb{R}$ be some sequence converging to some $\beta \in \mathbb{R}$. Moreover, let u_k be the function from Corollary 2.6 satisfying

$$u_k \in N_{\alpha,\beta_k} \quad \text{and} \quad \mathcal{W}_{\gamma_0}(u_k) = T_{\gamma_0,(\alpha,\beta_k)}.$$

Since $(\beta_k)_{k\in\mathbb{N}}$ is uniformly bounded, Proposition 2.5 yields positive constants c_i, $i = 1, 2, 3$, depending only on α such that

$$0 < c_1 \leq u_k(x) \leq c_2 \quad \text{and} \quad |u_k'(x)| \leq c_3 \quad \text{in } [-1,1] \tag{3.10}$$

holds true for all $k \in \mathbb{N}$. If moreover $\alpha > \alpha^*$ and $-\alpha < \beta$, then Proposition 2.5 yields additionally

$$u_k'(x) \leq \max\big\{-\beta_k, \sinh(b_1(\alpha))\big\} \quad \text{in } [0,1]. \tag{3.11}$$

From the upper semi-continuity of Lemma 3.1 we deduce that $T_{\gamma_0,(\alpha,\beta_k)} = \mathcal{W}_{\gamma_0}(u_k) \leq c_4$ holds with some constant c_4. This is true since upper semi-continuous functions achieve a maximum on compact sets. These estimates imply

$$\begin{aligned} c_4 \geq \mathcal{W}_{\gamma_0}(u_k) &= \frac{\pi}{2}\int_{-1}^{1}\left(\frac{u_k''(x)^2 u_k(x)}{(1+u_k'(x)^2)^{\frac{5}{2}}} + \frac{1}{u_k(x)\sqrt{1+u_k'(x)^2}}\right) dx \\ &\geq \frac{\pi}{2}\frac{c_1}{(1+c_3^2)^{\frac{5}{2}}}\int_{-1}^{1} u_k''(x)^2\, dx. \end{aligned} \tag{3.12}$$

Note that due to the choice $\gamma_0 = \frac{1}{2}$ the boundary terms cancel each other. From (3.12) we obtain uniform boundness of the sequence in $H^2([-1,1])$, and, after passing to a subsequence, Rellich's embedding theorem ensures the existence of $u \in H^2([-1,1])$ such that

$$u_k \rightharpoonup u \text{ in } H^2([-1,1]) \text{ and } u_k \to u \text{ in } C^1([-1,1]).$$

The convergence in $C^1([-1,1])$ ensures that also u satisfies the bounds in (3.10), in particular $u(x) > 0$ in $[-1,1]$. If either $\alpha \leq \alpha^*$ or $-\alpha > \beta$ then $u \in \overline{N}_{\alpha,\beta} = N_{\alpha,\beta}$ holds. If, on the other hand, $\alpha > \alpha^*$ and $-\alpha < \beta$ holds then estimate (3.11) and inequality (2.5) yield

$$u'(x) \leq \max\big\{-\beta, \sinh(b_1(\alpha))\big\} < \alpha \quad \text{in } [0,1]$$

and thus $u \in N_{\alpha,\beta}$ also in this case. The strong convergence in $C^1([-1,1])$ and the weak convergence in $H^2([-1,1])$ yield

$$\begin{aligned}\mathcal{W}_{\gamma_0}(u_k) &= \frac{\pi}{2}\int_{-1}^{1}\left(\frac{u_k''(x)^2u(x)}{(1+u'(x)^2)^{\frac{5}{2}}}+\frac{1}{u(x)\sqrt{1+u'(x)^2}}\right)dx+o(1)\\ &\geq \frac{\pi}{2}\int_{-1}^{1}\left(\frac{u''(x)^2u(x)}{(1+u'(x)^2)^{\frac{5}{2}}}+\frac{1}{u(x)\sqrt{1+u'(x)^2}}\right)dx+o(1)=\mathcal{W}_{\gamma_0}(u)+o(1).\end{aligned}$$

Together with $u \in N_{\alpha,\beta}$ this shows

$$T_{\gamma_0,(\alpha,\beta)} \leq \mathcal{W}_{\gamma_0}(u) \leq \liminf_{k\to\infty} \mathcal{W}_{\gamma_0}(u_k) = \liminf_{k\to\infty} T_{\gamma_0,(\alpha,\beta_k)}$$

proving the claimed lower semi-continuity. □

The combination of the above two results now yields

Corollary 3.3. *Let $\gamma \in [0,1]$, $\alpha > 0$ be fixed. Then $\beta \mapsto T_{\gamma,(\alpha,\beta)}$ is continuous in $\mathbb{R}$ if $\alpha \leq \alpha^*$ while for $\alpha > \alpha^*$ it is continuous in $\mathbb{R}\backslash\{-\alpha\}$.*

3.2 Monotonicity results for large and small β

In this section we show that $\beta \mapsto T_{\gamma,(\alpha,\beta)}$ is an increasing function for sufficiently large positive values of β and a decreasing function for sufficiently small negative values of β. This allows us to restrict to 'bounded' values of β when looking for the absolute minimiser.

Lemma 3.4. *If $\gamma \in [0,1]$ and $\beta > \beta' \geq \alpha^{-1}$, then $T_{\gamma,(\alpha,\beta)} > T_{\gamma,(\alpha,\beta')}$.*

Proof. By Corollary 2.6 there exists some $u \in N_{\alpha,\beta}$ such that $\mathcal{W}_\gamma(u) = T_{\gamma,(\alpha,\beta)}$. Because of $u'(-1) = \beta > \beta'$ and $u'(0) = 0$ the following number

$$x^* := \inf\{x \in [-1,0] \,:\, u'(x) \leq \beta'\}$$

is well-defined and satisfies $x^* \in (-1,0)$, $u'(x^*) = \beta'$ and $u'(x) \geq \beta' > 0$ for all $x \in [-1,x^*]$. Hence, the function u is increasing on $[-1,x^*]$ and we deduce $u(x^*) \geq u(-1) = \alpha > \alpha|x^*|$. Now let $w \in C^\infty([-1,1])$ be the function obtained by rescaling $u|_{[x^*,-x^*]}$ to the interval $[-1,1]$, i.e. $w(x) := u(rx)/r$, $r = |x^*|$. By construction, $w'(-1) = \beta'$ and $w(\pm 1) > \alpha$. By the rescaling invariance of the energy (Lemma 2.1) and Proposition 2.4*(i)* (note $w(\pm1) > \alpha \geq \beta'^{-1}$) we finally get

$$T_{\gamma,(\alpha,\beta)} = \mathcal{W}_\gamma(u) \geq \mathcal{W}_\gamma(u|_{[x^*,-x^*]}) = \mathcal{W}_\gamma(w) \geq T_{\gamma,(w(\pm1),\beta')} > T_{\gamma,(\alpha,\beta')}.$$

Here we have used $\mathcal{W}_\gamma(u) \geq \mathcal{W}_\gamma(w)$ which follows from $\gamma \in [0,1]$. □

Remark 3.5. *Actually, this result can be generalised to the case $-\infty < \gamma \leq 1$. Using Corollary 2.6,* (2.3) *and Lemma 3.4 we find*

$$T_{\gamma,(\alpha,\beta)} = T_{1,(\alpha,\beta)} + 4\pi(1-\gamma)\frac{\beta}{\sqrt{1+\beta^2}} > T_{1,(\alpha,\beta')} + 4\pi(1-\gamma)\frac{\beta'}{\sqrt{1+\beta'^2}} = T_{\gamma,(\alpha,\beta')},$$

since $1-\gamma \geq 0$ and $\beta > \beta' \geq \alpha^{-1} > 0$.

In the following, we set

$$\beta_2(\alpha) := \begin{cases} 0 & \text{if } \alpha < \alpha^*, \\ -\sinh(b_2) & \text{if } \alpha \geq \alpha^*, \end{cases} \quad \text{with } b_2 = b_2(\alpha) \text{ defined in (2.4).} \tag{3.13}$$

A simple computation shows that, for $\beta < 0$, $\alpha > \alpha_\beta$ implies $\beta > \beta_2(\alpha)$, where α_β is defined by (2.9).

Lemma 3.6. *Let $\gamma \in [0,1]$ be fixed. If $\beta' < \beta \leq \min\{-\alpha, \beta_2(\alpha)\}$, then $T_{\gamma,(\alpha,\beta)} < T_{\gamma,(\alpha,\beta')}$.*

Proof. By Corollary 2.6 there exists some $u \in N_{\alpha,\beta'}$ such that $\mathcal{W}_\gamma(u) = T_{\gamma,(\alpha,\beta')}$. Because of $\beta' < -\alpha$ there exists $\overline{x} \in (-1,0)$ the smallest element such that $u(\overline{x}) = -\alpha\overline{x}$. Since $u'(-1) = \beta' < \beta \leq -\alpha$, $u'(\overline{x}) \geq -\alpha$, and u' is continuous, there exists $x^* \in (-1,\overline{x})$ such that $u'(x^*) = \beta$ and $u(x^*) < \alpha|x^*|$. We consider the function $w \in C^\infty([-1,1])$ obtained by rescaling $u|_{[x^*,-x^*]}$ to the interval $[-1,1]$. By construction there hold $w'(-1) = \beta$ and $w(\pm 1) < \alpha$. If $\alpha > \alpha^*$ the assumption $\beta \leq \beta_2(\alpha)$ gives $\alpha \leq \alpha_\beta$ with α_β defined in (2.9). In case of $\alpha \leq \alpha^*$ then clearly $\alpha \leq \alpha_\beta$ is also true. In both cases, Lemma 2.1 and Proposition 2.4*(iv)* (noting that $w(\pm 1) < \alpha \leq \alpha_\beta$) yield

$$T_{\gamma,(\alpha,\beta')} = \mathcal{W}_\gamma(u) \geq \mathcal{W}_\gamma(w) \geq T_{\gamma,(w(\pm 1),\beta)} > T_{\gamma,(\alpha,\beta)}.$$

Here we have used $\mathcal{W}_\gamma(u) \geq \mathcal{W}_\gamma(w)$ due to $\gamma \in [0,1]$. □

Remark 3.7. *This result still holds for all $\gamma \geq 0$ because*

$$T_{\gamma,(\alpha,\beta')} = T_{0,(\alpha,\beta')} - 4\pi\gamma\frac{\beta'}{\sqrt{1+\beta'^2}} > T_{0,(\alpha,\beta)} - 4\pi\gamma\frac{\beta}{\sqrt{1+\beta^2}} = T_{\gamma,(\alpha,\beta)},$$

which holds for $\gamma \geq 0$ and $\beta' < \beta \leq \min\{-\alpha, \beta_2(\alpha)\}$.

3.3 The case $\gamma = 0$

For this case we give a complete description of the monotonicity behaviour of $\beta \mapsto T_{0,(\alpha,\beta)}$ for all values of β. For $\alpha \leq \alpha^*$ this mapping is decreasing on $(-\infty, -\alpha]$ while it is increasing on $[-\alpha, \infty)$. For $\alpha > \alpha^*$ the behaviour is more complicated due to the presence of the two catenoid solutions whose energy $\mathcal{W}_0$ is zero.

Similarly to $\beta_2(\alpha)$, let us introduce

$$\beta_1(\alpha) := \begin{cases} -\alpha^* & \text{if } \alpha < \alpha^*, \\ -\sinh(b_1) & \text{if } \alpha \geq \alpha^*, \end{cases} \quad \text{with } b_1 = b_1(\alpha) \text{ defined in (2.4).} \tag{3.14}$$

Lemma 3.8. *If $\alpha^{-1} \geq \beta > \beta' \geq \max\{-\alpha, \beta_1(\alpha)\}$, then $T_{0,(\alpha,\beta)} > T_{0,(\alpha,\beta')}$.*

Proof. Given $\beta > \beta'$ we first define $b := -\operatorname{arsinh}(\beta)$, $b' := -\operatorname{arsinh}(\beta')$ and note $b < b'$. By Corollary 2.6 there exists some $u \in N_{\alpha,\beta}$ such that $\mathcal{W}_0(u) = T_{0,(\alpha,\beta)}$. Let $f(x)$ be the catenary with initial data $f(-1) = \alpha$, $f'(-1) = \beta$, i.e. the function

$$f(x) = \frac{\alpha}{\cosh b}\cosh\left(\frac{\cosh b}{\alpha}(x+1) - b\right). \tag{3.15}$$

At the point

$$x^* := -1 + \frac{\alpha}{\cosh b}(b - b') \tag{3.16}$$

we have $f'(x^*) = \beta'$. Note that $x^* < -1$ since $b < b'$. Let $v \in C^{1,1}([x^*, -x^*])$ be the symmetric function equal to f on $[x^*, -1]$ and equal to u in $(-1, 0]$. Furthermore, let $w \in C^{1,1}([-1,1])$ be

v rescaled to $[-1, 1]$. By construction it holds $w'(-1) = \beta'$. In order to apply the monotonicity property of the energy in α we need to show $w(\pm 1) < \alpha$. Since $\beta > \beta' \geq -\alpha$ we have $\sinh(x) < \alpha$ for all $x \in (b, b')$, and hence

$$\frac{\cosh(b') - \cosh(b)}{b' - b} < \alpha \quad \text{or equivalently} \quad \frac{\cosh(b')}{\cosh(b) - \alpha(b - b')} < 1.$$

From this inequality we see

$$w(\pm 1) = \frac{v(x^*)}{|x^*|} = \frac{\alpha \cosh(b')}{\cosh(b)} \frac{1}{1 - \frac{\alpha}{\cosh(b)}(b - b')} = \alpha \frac{\cosh(b')}{\cosh(b) - \alpha(b - b')} < \alpha. \tag{3.17}$$

Since the piece of catenoid has zero energy for $\gamma = 0$, and the energy $\mathcal{W}_\gamma$ is invariant under rescaling (Lemma 2.1), we obtain

$$T_{0,(\alpha,\beta)} = \mathcal{W}_0(u) = \mathcal{W}_0(w) \geq T_{0,(w(\pm 1), w'(-1))} = T_{0,(w(-1),\beta')}.$$

Now, if $\beta' \geq 0$, then, using $w(\pm 1) < \alpha < \beta'^{-1}$, Proposition 2.4*(ii)* yields $T_{0,(w(\pm 1),\beta')} > T_{0,(\alpha,\beta')}$. On the other hand, if $\beta' < 0$ we claim $\alpha \leq \alpha_{\beta'}$. This is clear if $\alpha \leq \alpha^*$, while if $\alpha > \alpha^*$ it is assured by the assumption $\beta' \geq -\sinh(b_1)$ which follows from the definition of $\beta_1(\alpha)$. Proposition 2.4*(iv)* now yields again $T_{0,(w(\pm 1),\beta')} > T_{0,(\alpha,\beta')}$. In both cases we obtain $T_{0,(\alpha,\beta)} > T_{0,(\alpha,\beta')}$. □

Combining our Lemmata 3.4, 3.6 and 3.8 with Corollary 3.3 for $\alpha \leq \alpha^*$ we obtain:

Corollary 3.9. *If $0 < \alpha \leq \alpha^*$, then $T_{0,(\alpha,\beta)}$ is increasing in β for $\beta \in [-\alpha, \infty)$ and decreasing for $\beta \in (-\infty, -\alpha]$. The mapping $\beta \mapsto T_{0,(\alpha,\beta)}$ achieves its global minimum at $\beta = -\alpha$.*

We still have to discuss the case $\alpha > \alpha^*$ and $\beta \in [\beta_2(\alpha), \beta_1(\alpha)]$. Here, the monotonicity behaviour becomes more involved due to the presence of the two catenoids corresponding to the two values $\beta_1(\alpha)$ and $\beta_2(\alpha)$ for the boundary datum β.

Lemma 3.10. *If $\alpha > \alpha^*$ and $-\alpha \geq \beta > \beta' \geq \beta_2(\alpha)$, then $T_{0,(\alpha,\beta)} > T_{0,(\alpha,\beta')}$.*

Proof. Note that the assumption $-\alpha > \beta' \geq \beta_2(\alpha)$ yields $\alpha \geq \alpha_{\beta'}$. The claim is proven quite similarly as Lemma 3.8. By Corollary 2.6 there exists some $u \in N_{\alpha,\beta}$ such that $\mathcal{W}_0(u) = T_{0,(\alpha,\beta)}$. Let $f(x)$ be the function from (3.15). At x^* defined as in (3.16), we have $f'(x^*) = \beta'$. Now consider the symmetric function $v \in C^{1,1}([x^*, -x^*])$ which is equal to f in $[x^*, -1]$ and to u in $(-1, 0]$. Furthermore, let $w \in C^{1,1}([-1, 1])$ be its rescaling to $[-1, 1]$. By construction, $w'(-1) = \beta'$ and $w(\pm 1) > \alpha$. Indeed, since $-\alpha \geq \beta > \beta'$ we have $\sinh(x) > \alpha$ for all $x \in (b, b')$ and also

$$\frac{\cosh(b') - \cosh(b)}{b' - b} > \alpha \quad \text{or equivalently} \quad \frac{\cosh(b')}{\cosh(b) - \alpha(b - b')} > 1.$$

This inequality implies $w(\pm 1) > \alpha$ which is proven just like (3.17). We then obtain the inequality

$$T_{0,(\alpha,\beta)} = \mathcal{W}_0(u) = \mathcal{W}_0(w) \geq T_{0,(w(\pm 1),\beta')} > T_{0,(\alpha,\beta')},$$

using Proposition 2.4*(v)* together with $w(\pm 1) > \alpha > \alpha_{\beta'}$. □

For $\alpha > \alpha^*$ and $\beta \in (-\alpha, \beta_1(\alpha)]$ the elements $u \in N_{\alpha,\beta}$ have the additional restriction $u'(x) < \alpha$ in $[0, 1]$ (compare Definition 2.2). This property shall be used now in order to prove monotonicity in $\beta \in (-\alpha, \beta_1(\alpha)]$.

Lemma 3.11. *If $\alpha > \alpha^*$ and $\beta_1(\alpha) \geq \beta > \beta' > -\alpha$, then $T_{0,(\alpha,\beta)} < T_{0,(\alpha,\beta')}$.*

Proof. Note that the assumption $-\alpha < \beta \le \beta_1(\alpha)$ yields $\alpha \ge \alpha_\beta$. By Corollary 2.6 there exists some $u \in N_{\alpha,\beta'}$ such that $\mathcal{W}_0(u) = T_{0,(\alpha,\beta')}$. Moreover, $\beta' \le u'(x) \le 0$ in $[-1,0]$ by Proposition 2.5. From this estimate together with $\beta' > -\alpha$ it follows that $u(x) > \alpha|x|$ for $x \in (-1,1)$. Since $u'(-1) = \beta' < \beta < 0$, $u'(0) = 0$ and u' is continuous, there exists $x^* \in (-1,0)$ such that $u'(x^*) = \beta$ and $u(x^*) > \alpha|x^*|$. Now let $w \in C^\infty([-1,1])$ be the rescaling of $u|_{[x^*,-x^*]}$ to the interval $[-1,1]$. By construction, $w'(-1) = \beta$ and $w(\pm 1) > \alpha$. Proposition 2.4*(v)* yields

$$T_{0,(\alpha,\beta')} = \mathcal{W}_0(u) \ge \mathcal{W}_0(w) \ge T_{0,(w(\pm1),\beta)} > T_{0,(\alpha,\beta)}.$$

□

Combining the previous results we have:

Corollary 3.12. *For fixed $\alpha > \alpha^*$, the function $\beta \mapsto T_{0,(\alpha,\beta)}$ is decreasing on the intervals $(-\infty, \beta_2(\alpha)]$ and $(-\alpha, \beta_1(\alpha)]$ while it is increasing on the intervals $[\beta_2(\alpha), -\alpha]$ and $[\beta_1(\alpha), +\infty)$.*

3.4 The case $\gamma \in [0,1]$

A combination of Lemmata 3.4 and 3.6 yields:

Corollary 3.13. *For $\gamma \in [0,1]$ and $\alpha \le \alpha^*$ the mapping $\beta \mapsto T_{\gamma,(\alpha,\beta)}$ is decreasing for $-\infty < \beta \le -\alpha$ and increasing for $\alpha^{-1} \le \beta < +\infty$.*

This result does not give us any information about the monotonicity if $-\alpha < \beta < \alpha^{-1}$. We may expect that there exists a unique $\tilde\beta = \tilde\beta(\alpha,\gamma) \in [-\alpha, \alpha^{-1}]$ such that $\beta \mapsto T_{\gamma,(\alpha,\beta)}$ is decreasing on $(-\infty, \tilde\beta]$ and increasing on $[\tilde\beta, +\infty)$. In fact, this claim is true for $\gamma = 0$ with $\tilde\beta = -\alpha$, due to Corollary 3.9. It is also true for $\gamma = 1$ where we can take $\tilde\beta = \alpha^{-1}$.

Corollary 3.14. *For $\gamma \in [0,1]$ and $\alpha > \alpha^*$ the mapping $\beta \mapsto T_{\gamma,(\alpha,\beta)}$ is decreasing on $(-\infty, \beta_2(\alpha)]$ and $(-\alpha, \beta_1(\alpha)]$, and increasing on $[\alpha^{-1}, \infty)$.*

Proof. For $\beta \ge \alpha^{-1}$ and $\beta \le \beta_2(\alpha)$ the claim follows from Lemmata 3.4 and 3.6. For $\beta \in (-\alpha, \beta_1(\alpha)]$, we note

$$T_{\gamma,(\alpha,\beta)} = T_{0,(\alpha,\beta)} - 4\pi\gamma \frac{\beta}{\sqrt{1+\beta^2}}.$$

Since $T_{0,(\alpha,\beta)}$ is decreasing by Corollary 3.12 on $(-\alpha, \beta_1(\alpha)]$ and $x \mapsto -x/\sqrt{1+x^2}$ is also decreasing for $x < 0$, for $\beta_1(\alpha) \ge \beta > \beta' > -\alpha$ we obtain

$$T_{\gamma,(\alpha,\beta')} = T_{0,(\alpha,\beta')} - 4\pi\gamma \frac{\beta'}{\sqrt{1+\beta'^2}} > T_{0,(\alpha,\beta)} - 4\pi\gamma \frac{\beta}{\sqrt{1+\beta^2}} = T_{\gamma,(\alpha,\beta)}.$$

The claim follows. □

Similarly to Corollary 3.14, this result does not yield information on the monotonicity if $\beta_1(\alpha) < \beta < \alpha^{-1}$. One may conjecture that there exists some $\tilde\beta = \tilde\beta(\alpha,\gamma) \in [\beta_1(\alpha), \alpha^{-1}]$ such that $\beta \mapsto T_{\gamma,(\alpha,\beta)}$ is decreasing on $(-\alpha, \tilde\beta]$ and increasing on $[\tilde\beta, +\infty)$.

Remark 3.15. *Similarly to the case $\gamma = 0$ treated in in Section 3.3, we can completely discuss the monotonicity behaviour of $\beta \mapsto T_{1,(\alpha,\beta)}$ for $\gamma = 1$. It is decreasing on $(-\infty, -\alpha]$ and on $(-\alpha, \alpha^{-1}]$ and increasing on $[\alpha^{-1}, +\infty)$. The global minimum $\beta = \alpha^{-1}$ corresponds to the circular arc $u(x) = \sqrt{\alpha^2 + 1 - x^2}$, $u \in N_{\alpha,\alpha^{-1}}$ which has zero energy $\mathcal{W}_1(u) = 0$.*

The proof is quite similar to the case $\gamma = 0$. Instead of adding a piece of a catenoid, as done in the proof of Lemmata 3.8 and 3.10, we now add a circular arc. While for $\gamma = 0$ adding a piece of catenoid does not change the energy $\mathcal{W}_0$, in the case of $\gamma = 1$ adding a circular arc does not change the energy $\mathcal{W}_1$. We point out that the procedure of adding 'pieces' with zero energy cannot be used for $0 < \gamma < 1$ since for this range of γ the energy $\mathcal{W}_\gamma$ is always larger than zero.

4 Proof of Theorem 1.1

We first study the case $\alpha \leq \alpha^*$. Setting $\beta^- := \min\{-\alpha, \beta_2(\alpha)\}$, $\beta^+ := \alpha^{-1}$, Corollary 3.13 implies

$$T_{\gamma,\alpha} := \inf_{\beta \in \mathbb{R}} T_{\gamma,(\alpha,\beta)} = \inf_{\beta^- \leq \beta \leq \beta^+} T_{\gamma,(\alpha,\beta)}.$$

The continuity of the energy in β, proven in Corollary 3.3, yields some $\beta^* \in [\beta^-, \beta^+]$ such that $T_{\gamma,\alpha} = T_{\gamma,(\alpha,\beta^*)}$. By Corollary 2.6 there exists some $u \in N_{\alpha,\beta^*} \cap C^\infty([-1,1])$ such that $\mathcal{W}_\gamma(u) = T_{\gamma,(\alpha,\beta^*)}$. Since u minimises the energy $\mathcal{W}_\gamma$ within the class $\cup_{\beta\in\mathbb{R}} N_{\alpha,\beta}$, it solves the boundary value problem (1.4).

Let us now study the case $\alpha > \alpha^*$. Here we set $\beta^- := \beta_1(\alpha) > -\alpha$, $\beta^+ := \alpha^{-1}$. Corollary 3.14 yields

$$T_{\gamma,\alpha} := \inf_{-\alpha < \beta < +\infty} T_{\gamma,(\alpha,\beta)} = \inf_{\beta^- \leq \beta \leq \beta^+} T_{\gamma,(\alpha,\beta)}.$$

Again, Corollary 3.3 gives some $\beta^* \in [\beta^-, \beta^+]$ such that $T_{\gamma,\alpha} = T_{\gamma,(\alpha,\beta^*)}$. Corollary 2.6 yields some $u \in N_{\alpha,\beta^*} \cap C^\infty([-1,1])$ such that $\mathcal{W}_\gamma(u) = T_{\gamma,(\alpha,\beta^*)}$. This function u minimises the energy $\mathcal{W}_\gamma$ within the class $\cup_{-\alpha<\beta<+\infty} N_{\alpha,\beta}$ and hence is solution of the boundary value problem (1.4). Here it is crucial that $\beta^* > -\alpha$.

Remark 4.1. *In the particular case $\alpha \leq \alpha^*$ and $\gamma = 0$ the monotonicity property of the energy in β (Corollary 3.9) yields that the constructed solution of (1.4) satisfies $u'(-1) = -\alpha$. One can verify this for the values of α for which an explicit solution to (1.4) is known. For $\alpha = 1$ this solution is a piece of the Clifford torus, i.e. the surface of revolution corresponding to $f(x) := 2 - \sqrt{2 - x^2}$. One sees that $f(-1) = 1$ and $f'(-1) = -1$. Another explicit solution is the catenoid $x \mapsto g(x) := \cosh(b^* x)/b^*$ with b^* defined in (1.6). This function has boundary value $g(-1) = \alpha^*$ with α^* defined in (1.5) and $g'(-1) = -\sinh(b^*) = -\alpha^*$ by definition of b^* and α^*.*

A Natural boundary conditions

The following lemma yields the first variation of the functional $\mathcal{W}_\gamma$.

Lemma A.1. *Let $u \in C^4([-1,1],(0,\infty))$. Then for all $\varphi \in H^2([-1,1]) \cap H^1_0([-1,1])$, we have*

$$\frac{d}{dt}\int_\Gamma H(u+t\varphi)^2\, dA[u+t\varphi]\Big|_{t=0} = -2\pi\left[H(x)\frac{u(x)\varphi'(x)}{1+u'(x)^2}\right]_{-1}^{1}$$

$$-2\pi\int_{-1}^{1} u(x)\varphi(x)\left(\Delta_\Gamma H(x) + 2H(H^2-K)\right)dx,$$

and

$$\frac{d}{dt}\int_\Gamma K[u+t\varphi]\, dA[u+t\varphi]\Big|_{t=0} = -2\pi\left[\frac{\varphi'(x)}{(1+u'(x)^2)^{3/2}}\right]_{-1}^{1},$$

Γ being the surface of revolution generated by $u + t\varphi$.

The first statement was proved in [5, Lemma 6]. The second identity follows directly if we write the Gauss curvature K in coordinates. Thus, the first variation of the composed functional $\mathcal{W}_\gamma(u)$ can be written as

$$\frac{d}{dt}\mathcal{W}_\gamma(u+t\varphi)\Big|_{t=0} = -2\pi\left[\left(H(x) - \frac{\gamma}{u(x)\sqrt{1+u'(x)^2}}\right)\frac{u(x)\varphi'(x)}{1+u'(x)^2}\right]_{-1}^{1}$$

$$-2\pi\int_{-1}^{1} u\varphi\left(\Delta_\Gamma H + 2H^3 - 2HK\right)dx$$

for all $\varphi \in H^2([-1,1]) \cap H^1_0([-1,1])$. The corresponding boundary value problem is given by (1.4). In order to provide a geometric interpretation of this boundary value problem, we observe

Lemma 2.2. *Let $x \in (-1,1)$ be fixed, and consider the curve $\varphi \mapsto X(x,\varphi)$ on Γ. Then it holds*

$$\kappa_n(x) = \frac{1}{u(x)\sqrt{1+u'(x)^2}}$$

for its normal curvature w.r.t. the surface unit normal vector

$$\nu(x,\varphi) = \big(u'(x), -\cos\varphi, -\sin\varphi\big)\,\frac{1}{\sqrt{1+u'(x)^2}}\,.$$

Proof. Parametrising the curve by arclength $s \in [0, 2\pi u(x)]$ gives

$$\begin{aligned}
X(s) &= \left(x, u(x)\cos\frac{s}{u(x)}, u(x)\sin\frac{s}{u(x)}\right),\\
X'(s) &= \left(0, -\sin\frac{s}{u(x)}, \cos\frac{s}{u(x)}\right),\\
X''(s) &= \left(0, -\frac{1}{u(x)}\cos\frac{s}{u(x)}, -\frac{1}{u(x)}\sin\frac{s}{u(x)}\right).
\end{aligned}$$

Thus, the normal curvature w.r.t. ν is given by

$$\kappa_n(x) = \langle X''(s), \nu\big(x, \frac{s}{u(x)}\big)\rangle = \frac{1}{\sqrt{1+u'(x)^2}}\frac{1}{u(x)}.$$

$\square$

On account of this lemma, the natural boundary data can be expressed in terms of the geometric quantity κ_n at the boundary of the surface: We can write (1.4) in the form

$$\begin{cases} \Delta_\Gamma H + 2H^3 - 2HK = 0 \quad \text{on } \Gamma,\\ u(\pm 1) = \alpha, \qquad H(\pm 1) = \gamma\kappa_n(\pm 1). \end{cases}$$

A detailed computation of natural boundary conditions even for Helfrich's functional can be found in the literature. We want to mention e.g. Nitsche [14], [15], and von der Mosel [21].

B Proof of Proposition 2.5

Here we collect the results from [4] needed to prove the a priori estimates for the function u of Theorem 2.3.

Proof of Proposition 2.5. We use the following facts. First, $\alpha \le \alpha^*$ implies $\alpha \le \alpha_\beta$ for all $\beta < 0$. For $\alpha \le \alpha^*$, the equality $\alpha = \alpha_\beta$ holds only when $\alpha = \alpha^*$ and $\beta = -\alpha^*$. For $\alpha > \alpha^*$ there exist $b_1 = b_1(\alpha)$ and $b_2 = b_2(\alpha)$ defined in (2.4) such that $b_1 < b^* < b_2$, with b^* defined in (1.6), and $\alpha = \cosh(b_1)/b_1 = \cosh(b_2)/b_2$. Finally, $\alpha > \alpha_\beta$ implies $\sinh(b_1) < -\beta < \sinh(b_2)$, while $\alpha < \alpha_\beta$ implies $-\beta < \sinh(b_1)$ or $-\beta > \sinh(b_2)$. Notice that $\sinh(b_1) < \alpha^* < \alpha < \sinh(b_2)$ for all $\alpha > \alpha^*$. These observations follow directly from the definition of α_β in (2.9) and the properties of the functions $y \mapsto \cosh(y)/y$ and $y \mapsto \sinh(y)$.

Proof of 1. This is the case $\alpha \le \alpha^*$. We start by estimating u'. If $\alpha\beta > 1$, u satisfies $u' \le 0$ in $[0,1]$ and $|u'(x)| \le \beta$ for all $x \in [-1,1]$ ([4, Th.3.11]). When $\alpha\beta = 1$, then we have the explicit solution $u(x) = \sqrt{1+\alpha^2-x^2}$ ([4, Lem.3.1]) and $|u'(x)| \le \alpha^{-1}$. If $\beta \ge 0$ and $\alpha\beta < 1$, u satisfies $x + u(x)u'(x) \ge 0$ and $u'(x) \le 0$ in $[0,1]$ ([4, Th.3.18]). It follows $|u'(x)| \le \alpha^{-1}$. In the case $\beta < 0$, following [4, Lem.4.27], u has at most three critical points in $[-1,1]$. Moreover, for $x \in [0,1]$ we have $u'(x) \le \max\{-\beta, \alpha^*\}$ ([4, Th. 4.48] if $\alpha < \alpha^*$, [4, Th.4.39] if $\alpha = \alpha^*$ and $\beta \ne -\alpha^*$ (using $\sinh(b_1) < \alpha^*$), and [4, Lem.4.1] if $\alpha = \alpha^*$ and $\beta = -\alpha^*$). If u has exactly one critical point in $[-1,1]$, then $u' \ge 0$ in $[0,1]$. Otherwise, there is $x_0 \in (0,1)$ so that $u'(x_0) = 0$, $u' > 0$ in $(x_0, 1]$, $u' < 0$ in $(0, x_0)$. With the same construction as in Lemma 3.16 in [4] we may assume that $x + u(x)u'(x) \ge 0$ in $[0,1]$. Since

$$u(x_0) \ge \frac{\alpha}{\operatorname{arsinh}(-\beta)(\alpha_\beta - \alpha)}\, x_0 \tag{2.18}$$

by Lemma 4.29 from [4], we get by definition of α_β (see (2.9))

$$u'(x) \ge -\frac{\operatorname{arsinh}(-\beta)(\alpha_\beta - \alpha)}{\alpha} \ge -\frac{\cosh(\operatorname{arsinh}(-\beta))}{\alpha} = -\frac{\sqrt{1+\beta^2}}{\alpha}.$$

We now estimate u from above. If $\alpha\beta > 1$, u satisfies $x + u(x)u'(x) \le 0$ in $[0,1]$ (see [4, Lem.3.9]), and integrating this inequality from 0 to $x \in (0,1]$ gives

$$u(x) \le \sqrt{u(0)^2 - x^2} \quad \text{with } u(0) \le \alpha + \beta$$

where the last inequality follows from $|u'(x)| \le \beta$ for $x \in [-1,1]$ ([4, Th.3.11]). When $\alpha\beta = 1$, then $u(x) = \sqrt{1+\alpha^2-x^2}$. If $\alpha\beta < 1$, the function u satisfies $x + u(x)u'(x) \ge 0$ in $[0,1]$ (for $\beta \ge 0$ [4, Lem.3.16], and the same inequality holds by the same reasoning for $\beta < 0$). Thus, integrating the inequality from x to 1 we find

$$u(x) \le \sqrt{1+\alpha^2-x^2} \le \sqrt{(1+\alpha)^2 - x^2} \quad \text{in } [-1,1].$$

It remains to prove the estimate of u from below. If $\beta \ge 0$, then $u' \le 0$ in $[0,1]$ ([4, Th.3.11] for $\alpha\beta > 1$, [4, Lem.3.1] when $\alpha\beta = 1$, and [4, Th.3.18] for $\alpha\beta < 1$ and $\beta \ge 0$). It directly follows $u(x) \ge u(1) = \alpha$. We consider now the case $\beta < 0$. If $\alpha = \alpha^* = \alpha_\beta$, then $\beta = -\alpha^*$ and $u(x) = \cosh(b^*x)/b^*$ with b^* defined in (1.6). In this case, $u(x) \ge 1/b^*$ and therefore $u(x) \ge \frac{1}{2}\alpha/\sqrt{1+\beta^2}$. In all the other cases, we have $\alpha < \alpha_\beta$. We recall Lemma 4.9 from [4]: Let $\nu := \max_{x\in[0,1]}\{u'(x)\}$ and $x_0 \ge 0$ so that $u'(x_0) = 0$ and $u' > 0$ in $(x_0, 1]$. Then,

$$\min_{x\in[0,1]} u(x) = u(x_0) \ge \nu \frac{1-x_0}{e^C - 1} \quad \text{with } C = \frac{1}{2}\nu\sqrt{1+\nu^2}\left(\mathcal{W}_1(u) + \frac{4\beta}{\sqrt{1+\beta^2}}\right). \tag{2.19}$$

We distinguish between $x_0 \le 1/2$ and $x_0 > 1/2$. In the first case, by the estimate on u' just proved ($u'(x) \le \max\{-\beta, \alpha^*\}$ in $[0,1]$), and taking the following energy estimate into account (see [4, Prop.6.10])

$$\mathcal{W}_1(u) \le \frac{-8\beta}{\sqrt{1+\beta^2}} + 8\tanh\left(\operatorname{arsinh}(-\beta)\frac{\alpha_\beta - \alpha}{\alpha}\right) \le 16, \tag{2.20}$$

inequality (2.19) gives us

$$\min_{x\in[0,1]} u(x) \ge \frac{1}{2}\frac{\max\{-\beta, \alpha^*\}}{e^{C_2} - 1} \text{ with } C_2 = 8(1 + \max\{-\beta, \alpha^*\}^2).$$

If $x_0 \ge 1/2$, it follows from Lemma 4.29 in [4] (see (2.18)) that

$$u(x) \ge u(x_0) \ge \frac{1}{2}\frac{\alpha}{\operatorname{arsinh}(-\beta)(\alpha_\beta - \alpha)} \ge \frac{1}{2}\frac{\alpha}{\cosh(\operatorname{arsinh}(-\beta))} = \frac{1}{2}\frac{\alpha}{\sqrt{1+\beta^2}}.$$

Proof of 2. This is the case $\alpha > \alpha^*$. We start by estimating the derivative. The case $\beta \geq 0$ can be treated as the case $\alpha \leq \alpha^*$. Indeed, the distinction between $\alpha \leq \alpha^*$ and $\alpha > \alpha^*$ is relevant only for $\beta < 0$. If $\beta < 0$, $\alpha \geq \alpha_\beta$ and $-\beta < \alpha$, then $0 \leq u'(x) \leq -\beta$ in $[0,1]$ by Theorem 4.24 in [4]. While if $\beta < 0$, $\alpha \geq \alpha_\beta$ and $-\beta \geq \alpha$, then $0 \leq u'(x) \leq \sinh(b_2)$, $x \in [0,1]$, ([4, Th.4.17]). It remains to consider the case $\alpha^* < \alpha < \alpha_\beta$. We proceed as in the case $\alpha \leq \alpha^*$ and $\beta < 0$. By [4, Lem.4.27] u has at most three critical points in $[-1,1]$. Moreover, for $x \in [0,1]$ we have $u'(x) \leq \max\{-\beta, \sinh(b_1)\} \leq \max\{-\beta, \sinh(b_2)\}$ ([4, Th.4.39]). If u has exactly one critical point in $[-1,1]$, then $u' \geq 0$ in $[0,1]$. Otherwise, let $x_0 \in (0,1)$ be so that $u'(x_0) = 0$. By Lemma 3.16 in [4] we may assume that $x + u(x)u'(x) \geq 0$ in $[0,1]$ and by Lemma 4.29 in [4] that $u(x_0)$ satisfies (2.18). Hence, we get by definition of α_β (see (2.9))

$$u'(x) \geq -\frac{x}{u(x)} \geq -\frac{x_0}{u(x_0)} \geq \frac{\operatorname{arsinh}(-\beta)(\alpha_\beta - \alpha)}{\alpha} = -\frac{\sqrt{1+\beta^2}}{\alpha}.$$

The estimate from above for u are proved with the same arguments used in the case $\alpha \leq \alpha^*$. The same is true for the estimate from below for u in the case $\beta \geq 0$. However, we need some new arguments for the estimate of u from below in the case $\beta < 0$. If $\alpha > \alpha_\beta$, we have $u' \geq 0$ in $[0,1]$ and $u'(x) \leq \sinh(b_2(\alpha))$ for $x \in [0,1]$ ([4, Th.4.17 and Th.4.24]). Here we use that $-\beta < \sinh(b_2(\alpha))$ if $-\beta < \alpha$. Then by (2.19) and the energy estimate ([4, Prop.6.8]):

$$\mathcal{W}_1(u) \leq \frac{-8\beta}{\sqrt{1+\beta^2}}(1 + \operatorname{arsinh}(-\beta)(\alpha - \alpha_\beta)) \leq 8(1 + \operatorname{arsinh}(-\beta)(\alpha - \alpha^*)),$$

we get

$$\min_{x\in[0,1]} u(x) \geq \frac{\sinh(b_2)}{e^{C_1} - 1} \text{ with } C_1 = 2\cosh(2b_2)(1 + \operatorname{arsinh}(-\beta)(\alpha - \alpha^*)).$$

If $\alpha = \alpha_\beta$, the solution is $u(x) = \cosh(b_1 x)/b_1$ or $u(x) = \cosh(b_2 x)/b_2$ with $b_1 < b_2$. Therefore $u(x) \geq 1/b_2$ for all $x \in [-1,1]$. When $\alpha < \alpha_\beta$, the idea is to use the estimate in (2.19). Let $x_0 \in [0,1)$ be such that $u'(x_0) = 0$ and $u' > 0$ in $(x_0, 1]$. If $x_0 \leq 1/2$ we proceed as for $\alpha > \alpha_\beta$. By the estimate on u' just established ($u' \leq \max\{-\beta, \sinh(b_1)\} \leq \max\{-\beta, \alpha^*\}$), and by the energy estimate in (2.20), inequality (2.19) gives us

$$\min_{x\in[0,1]} u(x) \geq \frac{1}{2}\frac{\max\{-\beta, \alpha^*\}}{e^{C_2} - 1} \text{ with } C_2 = 8(1 + \max\{-\beta, \alpha^*\}^2).$$

If $x_0 \geq 1/2$, the estimate $u(x) \geq \frac{1}{2}\alpha/\sqrt{1+\beta^2}$ follows directly from (2.18).

Proof of (2.i) The estimate is proven in Theorem 4.24 in [4].

Proof of (2.ii) In the special case $\beta > -\sinh(b_1(\alpha))$, Lemma 4.36 in [4] gives $u(x) \geq \cosh(b_1 x)/b_1$ and $u'(x) \leq \sinh(b_1)$ in $[0,1]$. If $u' \geq 0$ in $[0,1]$, then $u(x) \leq \alpha$. Otherwise by Lemma 4.27 in [4] there exists $x_0 \in (0,1)$ such that $u'(x_0) = 0$ and $u' < 0$ in $(0, x_0)$. We see that $u(x) \geq \cosh(b_1 x)/b_1$ implies $u(x_0) > \alpha^* x_0$. Since $x + u(x)u'(x) \geq 0$ in $[0,1]$ (proceeding as in [4, Lem. 3.16]), we find $u'(x) \geq -1/\alpha^*$ for $x \in [0,1]$, and also $u(x) \leq \sqrt{1 + \alpha^2 - x^2}$. □

C Monotonicity of the energy in α

Here we prove the monotonicity behaviour of the function $(0,\infty) \ni \alpha \mapsto T_{\gamma,(\alpha,\beta)}$ for $\gamma \in [0,1]$ and $\beta \in \mathbb{R}$ fixed.

Proof of Proposition 2.4. By the definition of $N_{\alpha,\beta}$ in (2.6), the one of $T_{\gamma,(\alpha,\beta)}$ given in (2.7) and formula (2.3) (see also (2.2)) we find

$$T_{\gamma,(\alpha,\beta)} = T_{1,(\alpha,\beta)} + 4\pi(1-\gamma)\frac{\beta}{\sqrt{1+\beta^2}}, \tag{2.21}$$

for all $\gamma \in [0,1]$, $\beta \in \mathbb{R}$ and $\alpha > 0$. Hence, the minimal energies $T_{\gamma,(\alpha,\beta)}$ and $T_{1,(\alpha,\beta)}$ have the same monotonicity behaviour with respect to α as long as we keep γ and β fixed. In [4] and [3] the monotonicity behaviuor in α of $T_{1,(\alpha,\beta)}$ has been studied. In the notation of those papers $\widetilde{M}_{\alpha,\beta}$ denotes $T_{1,(\alpha,\beta)}$ for $\alpha > \alpha^*$ and $-\sinh(b_1) \geq \beta \geq -\alpha$, while $M_{\alpha,\beta}$ denotes $T_{1,(\alpha,\beta)}$ for all the other values of α and β. With our notation, we may rewrite the monotonicity results in [4] and [3] as follows:

(i) For $\beta > 0$ and $\frac{1}{\beta} \leq \alpha' < \alpha$ it holds $T_{1,(\alpha',\beta)} < T_{1,(\alpha,\beta)}$ by [4, Prop.3.12].

(ii) For $\beta > 0$ and $0 < \alpha' < \alpha \leq \frac{1}{\beta}$ it holds $T_{1,(\alpha',\beta)} > T_{1,(\alpha,\beta)}$ by [4, Prop.3.19].

(iii) For $\beta = 0$ and $0 < \alpha' < \alpha$ it holds $T_{1,(\alpha',\beta)} > T_{1,(\alpha,\beta)}$ by [3, Th.2].

(iv) For $\beta < 0$ and $0 < \alpha' < \alpha \leq \alpha_\beta$ it holds $T_{1,(\alpha',\beta)} > T_{1,(\alpha,\beta)}$ by [4, Prop. 4.40 and 4.49].

(v) For $\beta < 0$ and $\alpha_\beta \leq \alpha' < \alpha$ it holds $T_{1,(\alpha',\beta)} < T_{1,(\alpha,\beta)}$ by [4, Prop.s 4.18 and 4.25].

The claim follows directly from the estimates above and (2.21). □

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Willmore surfaces of revolution bounding two prescribed circles[1]

Matthias Bergner[3], Anna Dall'Acqua[2], Steffen Fröhlich[4]

Abstract

We consider the family of smooth embedded rotationally symmetric annular type surfaces in $\mathbb{R}^3$ having two concentric circles contained in two parallel planes of $\mathbb{R}^3$ as boundary. Minimising the Willmore functional within this class of surfaces we prove the existence of smooth axi-symmetric Willmore surfaces having these circles as boundary. When the radii of the circles tend to zero we prove convergence of these solutions to the round sphere.

Keywords. Natural boundary conditions, Willmore surface, surface of revolution.
AMS classification. 49Q10; 53C42, 35J65, 34L30.

1 Introduction and main results

A smooth, immersed two-dimensional surface $\Gamma \subset \mathbb{R}^3$ is a Willmore surface if it is stationary with respect to compactly supported variations for the Willmore functional

$$\mathcal{W}(\Gamma) := \int_\Gamma H^2 \, dA \,. \tag{1}$$

Here H is the mean curvature of Γ. The Willmore functional is a special case of the more general Helfrich functional. These functionals are of geometric interest. They appear, in particular, in the theory of elasticity as models for the elastic energy of thin planes (see [7], [12] and [13]). The Euler-Lagrange equation (called Willmore equation) associated to (1) is

$$\triangle H + 2H(H^2 - K) = 0 \quad \text{on } \Gamma \tag{2}$$

where $\triangle$ denotes the Laplace-Beltrami operator on the surface Γ.

Many results concerning existence and regularity of closed Willmore surfaces are present in the literature, see for instance [1, 9, 14, 16]. We are interested in studying existence of Willmore surfaces with boundary and satisfying prescribed boundary conditions. Even though already in 1993 Nitsche in [12] attracted the attention to this problem not much is yet known. One of the main difficulties is that equation (2) is of fourth order and not uniformly elliptic. Moreover, the Willmore functional is not convex. Schätzle in [15] proved existence of Willmore immersions in

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$\mathbb{S}^n$ satisfying Dirichlet boundary conditions. Working on $\mathbb{S}^n$ some compactness problems could be overcome. Another approach to the problem is to study existence of solutions to (2) with boundary conditions under certain symmetry assumptions. This leads to the study of Willmore surfaces of revolution. Existence of Willmore surfaces of revolution generated by symmetric graphs satisfying arbitrary symmetric Dirichlet boundary conditions has been proven in [5] (see also [4]) by solving a minimisation problem. Scholtes in [17] studied the functional obtained by adding an additional area term to the Willmore functional. He could prove existence of minimisers in the class of surfaces of revolution generated by graphs satisfying prescribed (but not arbitrary) Dirichlet boundary data.

Another challenging boundary value problem is obtained by fixing only the boundary of the surfaces among which to vary. Since the problem is of fourth order, a second boundary condition 'arises' , the so-called 'natural' boundary condition. In the considered case the natural boundary condition is that the mean curvature has to be zero at the boundary (see [2, App.A] or [18]). This boundary value problem for surfaces of revolution generated by symmetric graphs has been studied in [2] and [6]. In this paper we extend the results from [2]. Here we consider surfaces of revolution generated by rotating a regular smooth curve along the x-axis. The boundary consists of two circles on planes parallel to the y,z-plane and centered at $(-1,0,0)$ and $(1,0,0)$ respectively. The radii are arbitrary, in particular the two circles do not necessarily have the same radius. Moreover, we do not restrict ourselves to graphs and neither to symmetric curves.

Before stating the main theorem we introduce for some parameter $\alpha_l > 0$ the number

$$\alpha_r^*(\alpha_l) := \inf_{\gamma\in\mathbb{R}} \frac{\alpha_l}{\cosh(\gamma)} \cosh\Big(\frac{2\cosh(\gamma)}{\alpha_l} + \gamma\Big) > 0\,. \tag{3}$$

Denoting by $S_r := \{re^{i\varphi} \,:\, \varphi \in \mathbb{R}\}$ the circle of radius r centered at the origin, our main result is the following:

Theorem 1.1. *Let $C_{\alpha_l} := \{-1\} \times S_{\alpha_l}$, $C_{\alpha_r} := \{1\} \times S_{\alpha_r}$ denote two concentric circles in parallel planes of $\mathbb{R}^3$ with radii $\alpha_l, \alpha_r > 0$. Then there exists some smooth, annular type Willmore surface $\Gamma \subset \mathbb{R}^3$ minimising the Willmore energy among all rotationally symmetric, annular type surfaces with boundary $C_{\alpha_l} \cup C_{\alpha_r}$. The surface Γ is embedded into $\mathbb{R}^3$ and admits the representation*

$$\Gamma = \{(x, u(x)\cos\varphi, u(x)\sin\varphi) \,:\, x \in [-1,1]\;,\; \varphi \in \mathbb{R}\} \tag{4}$$

with some function $u \in C^\infty([-1,1],(0,+\infty))$. The surface Γ is solution of the following boundary value problem

$$\begin{cases} \triangle H + 2H(H^2 - K) = 0 & \text{on } \Gamma, \\ \partial\Gamma = C_{\alpha_l} \cup C_{\alpha_r}, & H = 0 \text{ on } \partial\Gamma\,. \end{cases} \tag{5}$$

Finally, one of the following three alternatives holds:

a) If $\alpha_r > \alpha_r^*(\alpha_l)$, there exist precisely two such solutions Γ, both being catenoids with $H \equiv 0$.

b) If $\alpha_r = \alpha_r^*(\alpha_l)$, there exists precisely one such solution Γ, a catenoid with $H \equiv 0$.

c) If $\alpha_r < \alpha_r^*(\alpha_l)$, there exists at least one such solution Γ. Its mean curvature satisfies $H = 0$ on $C_{\alpha_l} \cup C_{\alpha_r}$ and $H \neq 0$ on $\Gamma\backslash(C_{\alpha_l} \cup C_{\alpha_r})$.

Naturally, alternative *c*) is the most interesting part of this result as the constructed Willmore surface is not a minimal surface. Alternative *c*) corresponds precisely to the case where no annular type minimal surface spanning the two concentric circles exists (see Proposition 2.1). Also note that the solution from part *c*) minimises under axi-symmetric variations but is only stationary under general (i.e. not necessarily axi-symmetric) variations. Presently, we do not know whether there exists some non-rotationally symmetric, annular type surface spanning $C_{\alpha_l} \cup C_{\alpha_r}$ with smaller Willmore energy than the one constructed in Theorem 1.1.

Our second result concerns the limit case when both α_l and α_r converge to zero, i.e. the bounding circles C_{α_l} and C_{α_r} collapse to the points $(-1,0,0)$ and $(1,0,0)$ respectively.

Theorem 1.2. *For α_l, $\alpha_r > 0$ let $\Gamma = \Gamma_{\alpha_l,\alpha_r}$ be the surface from Theorem 1.1 above and u_{α_l,α_r} be the positive function generating the surface $\Gamma_{\alpha_l,\alpha_r}$ as in (4). Then $\Gamma_{\alpha_l,\alpha_r}$ converges to the round sphere $\mathbb{S}^2 \subset \mathbb{R}^3$ as both $\alpha_l, \alpha_r \to 0$ in the sense that the functions u_{α_l,α_r} converge uniformly to the function $\sqrt{1-x^2}$ in $[-1,1]$.*

The asymptotic behavior of the minimisers in case of Willmore surfaces of revolution generated by symmetric graphs with prescribed Dirichlet boundary conditions is studied in [5]. In that paper it is proven that the functions generating the minimisers converge to the function $\sqrt{1-x^2}$ in $C^m([-1+\delta_0, 1-\delta_0])$ for any $\delta_0 > 0$. More precisely, in case of symmetric Dirichlet boundary conditions one has two parameters. One prescribes the same radius $\alpha > 0$ for both boundary circles. Another parameter $\beta \in \mathbb{R}$ describes the contact angle between the surface and the two planes containing the bounding circles. In the limit procedure in [5], β is kept fixed while α is converges to zero. A similar result is proven in [8] in case of symmetric natural boundary conditions.

1.1 Notation and structure of the paper

For $a, b \in \mathbb{R}$, $a < b$, let $c(t) = (x(t), y(t)) : [a,b] \to \mathbb{R} \times (0, +\infty)$ be some smooth regular curve and

$$\Gamma = \{(x(t), y(t)\cos\varphi, y(t)\sin\varphi) \;:\; t \in [a,b]\;,\; \varphi \in [0, 2\pi)\}$$

be the surface of revolution corresponding to c. The Willmore energy of Γ is given by

$$\mathcal{W}(c) = \frac{\pi}{2}\int_a^b \Big(\frac{x'y''-x''y'}{(x'^2+y'^2)^{3/2}} - \frac{x'}{y(x'^2+y'^2)^{1/2}}\Big)^2 y(x'^2+y'^2)^{1/2}\,dt\,.$$

If the curve c is in fact a graph over the x-axis, i.e. $c(t) = (t, u(t))$, then we obtain

$$\mathcal{W}(c) = \mathcal{W}(u) = \frac{\pi}{2}\int_a^b \Big(\frac{u''}{(1+u'^2)^{3/2}} - \frac{1}{u(1+u'^2)^{1/2}}\Big)^2 u(1+u'^2)^{1/2}\,dx\,. \tag{6}$$

Definition 1.3. *Let $\widetilde{T}_{\alpha_l,\alpha_r}$ denote the set of all regular curves $c \in W^{2,2}([-1,1], \mathbb{R} \times (0,+\infty))$ connecting the points $(-1,\alpha_l)$ and $(1,\alpha_r)$, i.e. $c(-1) = (-1,\alpha_l)$, $c(1) = (1,\alpha_r)$. Moreover, let T_{α_l,α_r} denote the set of all functions $u \in W^{2,2}([-1,1],(0,+\infty))$ with boundary conditions $u(-1) = \alpha_l$, $u(1) = \alpha_r$. Finally, we define*

$$\widetilde{M}_{\alpha_l,\alpha_r} = \inf_{c \in \widetilde{T}_{\alpha_l,\alpha_r}} \mathcal{W}(c) \quad \textit{and} \quad M_{\alpha_l,\alpha_r} = \inf_{u \in T_{\alpha_l,\alpha_r}} \mathcal{W}(u)\,.$$

In order to show that M_{α_l,α_r} is attained it is convenient to work in a smaller class than T_{α_l,α_r}.

Definition 1.4. *Given parameters $\alpha_l, \alpha_r > 0$, $L > 0$ we define the space*

$$T_{\alpha_l,\alpha_r,L} := \big\{u \in T_{\alpha_l,\alpha_r} \;:\; u(x) \geq L^{-1} \textit{ and } |u'(x)| \leq L \textit{ in } [-1,1]\big\}$$

as well as the numbers

$$M_{\alpha_l,\alpha_r,L} := \inf_{u \in T_{\alpha_l,\alpha_r,L}} \mathcal{W}(u)\;.$$

Remark 1.5. *The set $T_{\alpha_l,\alpha_r,L}$ is empty if $L > 0$ is too small. However, $T_{\alpha_l,\alpha_r,L}$ is non-empty and hence $M_{\alpha_l,\alpha_r,L}$ well-defined for sufficiently large L, see Lemma 3.1 below.*

The reason for working within the smaller class $T_{\alpha_l,\alpha_r,L}$ is that it is relatively simple to construct minimisers $u = u_L$ in this class. The main task consists in proving a priori estimates for these minimisers u_L independent of L.

The paper is organised as follows. In Section 2 we prove the equality $\widetilde{M}_{\alpha_l,\alpha_r} = M_{\alpha_l,\alpha_r}$. Hence it is sufficient to study the minimisation problem in the class of graphs. In Section 3 we show a priori estimates for minimisers in the smaller class $T_{\alpha_l,\alpha_r,L}$ and prove that these estimates are independent of L for L sufficiently large. This is the key point in the proof of Theorem 1.1 presented in Section 4. Finally in Section 5 we study the behavior of minimisers for $\alpha_l, \alpha_r \to 0$ and prove Theorem 1.2.

2 Reduction to the case of graphs and monotonicity property of the energy

Identifying some function $u \in T_{\alpha_l,\alpha_r}$ with its graph parametrisation $c(t) := (t, u(t)) \in \widetilde{T}_{\alpha_l,\alpha_r}$ we obtain the inclusion $T_{\alpha_l,\alpha_r} \subset \widetilde{T}_{\alpha_l,\alpha_r}$ and hence $\widetilde{M}_{\alpha_l,\alpha_r} \leq M_{\alpha_l,\alpha_r}$. The goal of this section is to prove the equality $\widetilde{M}_{\alpha_l,\alpha_r} = M_{\alpha_l,\alpha_r}$.

We start by determining for which data $\alpha_l, \alpha_r > 0$ a minimal surface actually is a solution of the boundary value problem (5). For this purpose we consider the catenaries through $(-1, \alpha_l)$, i.e. the one-parameter family

$$u_\gamma(x) := \frac{\alpha_l}{\cosh(\gamma)} \cosh\left(\frac{\cosh(\gamma)}{\alpha_l}(x+1) + \gamma\right), \quad x \in \mathbb{R} \tag{7}$$

with a parameter $\gamma \in \mathbb{R}$. We have $u_\gamma(-1) = \alpha_l$, $u'_\gamma(-1) = \sinh(\gamma)$ and vanishing Willmore energy $\mathcal{W}(u_\gamma) = 0$. The surface of revolution corresponding to u_γ is a minimal surface, called catenoid. A catenary belongs to T_{α_l,α_r} whenever there is a $\gamma \in \mathbb{R}$ such that $u_\gamma(1) = \alpha_r$. One can see that this is equivalent to $\alpha_r \geq \alpha_r^*(\alpha_l)$ with $\alpha_r^*(\alpha_l)$ defined in (3) in the introduction. We first prove the following result, which we already mentioned in the introduction.

Proposition 2.1. *For $\alpha_l, \alpha_r > 0$ let C_{α_l}, C_{α_r} denote the two circles from Theorem 1.1. Then one of the following three alternatives holds:*

a) If $\alpha_r > \alpha_r^*(\alpha_l)$, then there are precisely two annular type minimal surfaces spanning $C_{\alpha_l} \cup C_{\alpha_r}$, both being catenoids.

b) If $\alpha_r = \alpha_r^*(\alpha_l)$, there exists precisely one annular type minimal surface spanning $C_{\alpha_l} \cup C_{\alpha_r}$, a catenoid.

c) If $\alpha_r < \alpha_r^*(\alpha_l)$, no annular type minimal surface spanning $C_{\alpha_l} \cup C_{\alpha_r}$ exists.

Proof. Due to [11, Theorem 1.1] there exist at most two such minimal surfaces. In particular, all annular type minimal surfaces spanning $C_{\alpha_l} \cup C_{\alpha_r}$ must be surfaces of revolution, since otherwise one might produce infinitely many of them simply by rotation. However, catenoids (and planes) are the only minimal surfaces of revolution and the claim follows from definition of $\alpha_r^*(\alpha_l)$. □

A simple consequence is

Lemma 2.2. *Given $\alpha_l > 0$ let $\alpha_r^*(\alpha_l)$ be defined as in (3). A catenary belongs to the space T_{α_l,α_r} whenever $\alpha_r \geq \alpha_r^*(\alpha_l)$. In particular, $M_{\alpha_l,\alpha_r} = \widetilde{M}_{\alpha_l,\alpha_r} = 0$ is satisfied for any $\alpha_r \geq \alpha_r^*(\alpha_l)$.*

This lemma and a simple study of the function u_γ defined in (7) immediately yield part *a)* and *b)* of Theorem 1.1. Our next result describes a construction to replace a regular curve by a curve admitting a non-parametric representation with almost the same Willmore energy but lower boundary values.

Lemma 2.3. *Given $\alpha_l, \alpha_r > 0$, any curve $c \in \widetilde{T}_{\alpha_l,\alpha_r}$ and $\delta > 0$ there exist $\alpha_l' \in (0, \alpha_l)$, $\alpha_r' \in (0, \alpha_r)$ and some function $u \in T_{\alpha_l',\alpha_r'}$ with $\mathcal{W}(u) \le \mathcal{W}(c) + \delta$.*

Proof. For $\varepsilon > 0$ we define the curve $c_\varepsilon(t) = (x_\varepsilon(t), y_\varepsilon(t))$ by

$$y_\varepsilon(t) := \frac{1}{\varrho} y(t) \quad , \quad x_\varepsilon(t) := -1 + \frac{1}{\varrho}\int_{-1}^{t} \big(|x'(\tau)| + \varepsilon\big) d\tau \quad \text{for } t \in [-1, 1]$$

with the rescaling factor

$$\varrho = \varrho(\varepsilon) := \frac{1}{2}\int_{-1}^{1} \big(|x'(\tau)| + \varepsilon\big) d\tau \ge 1 + \varepsilon > 1 \, .$$

Note that c_ε is a regular curve, $c_\varepsilon \in W^{2,2}([-1, 1], \mathbb{R} \times (0, +\infty))$, $x_\varepsilon(-1) = -1$ and $x_\varepsilon(1) = 1$ are satisfied. Due to the conformal invariance of the Willmore functional, in particular the invariance with respect to translations and reflections, one finds $\mathcal{W}(c) = \mathcal{W}(c_0)$. Together with the continuity of $\varepsilon \mapsto \mathcal{W}(c_\varepsilon)$ one deduces the convergence $\mathcal{W}(c_\varepsilon) \to \mathcal{W}(c)$ as $\varepsilon \to 0$. Because of $x_\varepsilon'(t) \ge \frac{\varepsilon}{\varrho} > 0$ in $[-1, 1]$ the curve c_ε has a non-parametric representation $u_\varepsilon := y_\varepsilon \circ x_\varepsilon^{-1} \in W^{2,2}([-1, 1], (0, +\infty))$. The claim follows noting that $u_\varepsilon(-1) = \frac{y(-1)}{\varrho} < y(-1) = \alpha_l$, $u_\varepsilon(1) = \frac{y(1)}{\varrho} < y(1) = \alpha_r$ (since $\varrho > 1$) as well as $\mathcal{W}(u_\varepsilon) = \mathcal{W}(c_\varepsilon) \to \mathcal{W}(c)$ for $\varepsilon \to 0$. □

Lemma 2.4. *Given $\alpha_l, \alpha_r > 0$, any $u \in T_{\alpha_l,\alpha_r}$ and $\alpha_r' \ge \alpha_r$ there exists some $v \in T_{\alpha_l,\alpha_r'}$ with $\mathcal{W}(v) \le \mathcal{W}(u)$.*

Proof. We need to study only the case $\alpha_r' < \alpha_r^*(\alpha_l)$ since otherwise there exists some catenary $v \in T_{\alpha_l,\alpha_r'}$ with $\mathcal{W}(v) = 0$. For some parameter $\tau \in [-1, 1]$ consider the function

$$v_\tau(x) := \begin{cases} u(x) & \text{for } x \in [-1, \tau] \\ w(x) & \text{for } x \in (\tau, 1] \end{cases}$$

where $w(x)$ denotes the catenary with initial data $w(\tau) = u(\tau)$, $w'(\tau) = u'(\tau)$. Note that v_τ depends continuously on τ and satisfies $v_\tau(-1) = u(-1) = \alpha_l$. The function v_{-1} coincides with some catenary and thus $v_{-1}(1) \ge \alpha_r^*(\alpha_l) > \alpha_r' \ge \alpha_r$ must hold. The function v_1 coincides with $u \in T_{\alpha_l,\alpha_r}$ and hence $v_1(1) = u(1) = \alpha_r$. The intermediate value theorem yields some $\tau = \tau(\alpha_r') \in [-1, 1]$ such that $v_\tau(1) = \alpha_r'$, i.e. $v_\tau \in T_{\alpha_l,\alpha_r'}$. From the estimate

$$\mathcal{W}(u) \ge \mathcal{W}(u|_{[-1,\tau]}) = \mathcal{W}(v_\tau)$$

the claim follows with $v = v_\tau$. □

Lemmas 2.3 and 2.4 yield $\widetilde{M}_{\alpha_l,\alpha_r} = M_{\alpha_l,\alpha_r}$ (see Definition 1.3) and the monotonicity of the energy.

Corollary 2.5 ($\widetilde{M}_{\alpha_l,\alpha_r} = M_{\alpha_l,\alpha_r}$). *The equality $\widetilde{M}_{\alpha_l,\alpha_r} = M_{\alpha_l,\alpha_r}$ holds for any $\alpha_l, \alpha_r > 0$, i.e. any minimiser within the small class T_{α_l,α_r} is also a minimiser in the larger class $\widetilde{T}_{\alpha_l,\alpha_r}$.*

Proof. Because of $T_{\alpha_l,\alpha_r} \subset \widetilde{T}_{\alpha_l,\alpha_r}$ we only need to prove $\widetilde{M}_{\alpha_l,\alpha_r} \geq M_{\alpha_l,\alpha_r}$. Given any $c \in \widetilde{T}_{\alpha_l,\alpha_r}$ and $\delta > 0$ Lemma 2.3 yields some $\alpha_l' \in (0, \alpha_l)$, $\alpha_r' \in (0, \alpha_r)$ and $u \in T_{\alpha_l',\alpha_r'}$ such that $\mathcal{W}(u) \leq \mathcal{W}(c) + \delta$. Applying Lemma 2.4 twice one obtains some $v \in T_{\alpha_l,\alpha_r}$ with $\mathcal{W}(v) \leq \mathcal{W}(u)$. We conclude $\mathcal{W}(v) \leq \mathcal{W}(c) + \delta$ and hence $M_{\alpha_l,\alpha_r} \leq \mathcal{W}(c) + \delta$ for any $c \in \widetilde{T}_{\alpha_l,\alpha_r}$ and $\delta > 0$. This yields $M_{\alpha_l,\alpha_r} \leq \widetilde{M}_{\alpha_l,\alpha_r}$. □

Corollary 2.6 (Monotonicity of the energy)**.** *Let M_{α_l,α_r} be defined as in Definition 1.3 for $\alpha_l, \alpha_r > 0$. Then M_{α_l,α_r} is monotonically decreasing in α_l for each fixed α_r, and monotonically decreasing in α_r for each fixed α_l.*

By Corollary 2.5 the above result is also valid for $\widetilde{M}_{\alpha_l,\alpha_r}$.

3 A priori estimates for the constrained minimisers

In this section we prove a priori estimates for the minimisers in $T_{\alpha_l,\alpha_r,L}$ (see Definition 1.4).

We start with establishing an upper bound on the energy $M_{\alpha_l,\alpha_r,L}$ from Definition 1.4, assuming L to be sufficiently large.

Lemma 3.1. *For $\alpha_l, \alpha_r > 0$ there exists a constant L_0 depending only on α_l, α_r such that the energy satisfies $M_{\alpha_l,\alpha_r,L} < 4\pi$ whenever $L \geq L_0$.*

Proof. Consider the circular arc

$$v(x) := \sqrt{\frac{\alpha_r^2 + \alpha_l^2}{2} + 1 - x^2 + \frac{\alpha_r^2 - \alpha_l^2}{2} x} \quad \text{for } x \in [-1, 1] \tag{8}$$

which belongs to T_{α_l,α_r} and hence also to $T_{\alpha_l,\alpha_r,L}$, provided $L \geq L_0$ with

$$L_0 = L_0(\alpha_l, \alpha_r) := \max_{x \in [-1,1]} \left(v(x)^{-1} + |v'(x)| \right).$$

The surface of revolution corresponding to v is a piece of a sphere and hence $\mathcal{W}(v) < 4\pi$, as the Willmore energy of a sphere is 4π. We conclude $M_{\alpha_l,\alpha_r,L} < 4\pi$ whenever $L \geq L_0$. □

3.1 Estimates on the hyperbolic curvature of the minimisers

As already observed by Bryant and Griffiths [3] and Langer and Singer [10], there is an interesting relation between the Willmore energy of surfaces of revolution and the elastic energy of curves in the hyperbolic half-plane. Indeed, for $u \in T_{\alpha_l,\alpha_r}$ and $a, b \in [-1, 1]$, $a < b$, one has

$$\mathcal{W}(u|_{[a,b]}) = \frac{\pi}{2} \int_a^b \kappa_h^2(x) \frac{\sqrt{1 + u'^2}}{u} \, dx - 2\pi \Big[\frac{u'}{\sqrt{1 + u'^2}} \Big]_a^b \tag{9}$$

where

$$\kappa_h(x) := \frac{u u''}{(1 + u'^2)^{3/2}} + \frac{1}{(1 + u'^2)^{1/2}} = \frac{u u'' + 1 + u'^2}{(1 + u'^2)^{3/2}} \tag{10}$$

denotes the curvature of the planar curve $x \mapsto (x, u(x))$ with respect to the hyperbolic half-plane metric. Curves with $\kappa_h(x) \equiv 0$ are precisely the geodesics of the hyperbolic half-plane. These are semi-circles whose center lie on the x-axis or semi-lines parallel to the y-axis. These curves play an essential role in studying Willmore surfaces of revolution (see [4], [5] and [2]).

Using circles as barriers from below and catenaries as barriers from above we prove pointwise bounds on the hyperbolic curvature of any minimiser in $T_{\alpha_l,\alpha_r,L}$.

Lemma 3.2. *For $\alpha_l, \alpha_r > 0$ let L_0 be the constant from Lemma 3.1. Then the hyperbolic curvature of any minimiser $u \in T_{\alpha_l,\alpha_r,L}$, $L \geq L_0$, satisfies $0 \leq \kappa_h(x) \leq 2$, $x \in [-1,1]$. Moreover, the inequality $u(x) \leq v(x)$ holds in $[-1,1]$, v denoting the circular arc from (8).*

Proof.

1) We first prove the lower bound $\kappa_h(x) \geq 0$. For parameters $z \in \mathbb{R}$, $\varrho > 0$ define the function

$$s_{\varrho,z}(x) := \sqrt{\max\left\{\varrho^2 - (x-z)^2, 0\right\}} \quad , \ x \in \mathbb{R}.$$

Note that $s_{\varrho,z}$ restricted to $[z-\varrho, z+\varrho]$ is simply a semi-circle centered at $(z,0)$ of radius ϱ. For $z \in \mathbb{R}$ we next define

$$\begin{aligned} r(z) &:= \sup\{\varrho > 0 \ : \ s_{\varrho,z}(x) \leq u(x) \text{ for all } x \in [-1,1]\} \quad \text{and} \\ g(z) &:= \{x \in [-1,1] \ : \ u(x) = s_{r(z),z}(x)\} \,. \end{aligned}$$

Then $g(z)$ is a nonempty, closed subset of $[-1,1]$ for any $z \in \mathbb{R}$. We prove that $g(z)$ is actually a closed interval. Setting $x_1 := \inf g(z)$, $x_2 := \sup g(z)$ and $I := [x_1, x_2]$ we have $g(z) \subset I$. We are done if $x_1 = x_2$ or $g(z) = I$. Otherwise, let v be the function equal to u on $[-1,1]\backslash I$ and equal to $s_{r(z),z}$ on I. We first observe that $v \in T_{\alpha_l,\alpha_r,L}$. Indeed since $u = v$ on ∂I and $v|_I$ is a piece of a semicircle, $v(x) \geq \inf u(x) \geq L^{-1}$ holds on $[-1,1]$. Moreover, $v \in W^{2,2}([-1,1],(0,+\infty))$ and $|v'(x)| \leq L$ since, by construction, $u'(x_1) \geq v'(x_1)$ with equality if $x_1 \in (-1,1)$ and $u'(x_2) \leq v'(x_2)$ with equality if $x_2 \in (-1,1)$. Now, we compare the Willmore energies of u and v. Since $v|_I$ is a piece of a semicircle, its hyperbolic curvature vanishes there. Using formula (9) we estimate

$$\mathcal{W}(v) - \mathcal{W}(u) = \mathcal{W}\big(v|_I\big) - \mathcal{W}\big(u|_I\big) \leq 2\pi\Big[\frac{u'}{\sqrt{1+u'^2}}\Big]_{x_1}^{x_2} - 2\pi\Big[\frac{v'}{\sqrt{1+v'^2}}\Big]_{x_1}^{x_2} \leq 0\,,$$

using once again that $u'(x_2) \leq v'(x_2)$ and $u'(x_1) \geq v'(x_1)$ which follows from $u \geq v$ in I and $u = v$ on $\partial I = \{x_1, x_2\}$. This shows $\mathcal{W}(v) \leq \mathcal{W}(u)$. Furthermore, $u|_I \equiv v|_I$ must hold since otherwise we would obtain the strict inequality $\mathcal{W}(v) < \mathcal{W}(u)$, contradicting the assumption of u being a minimiser in $T_{\alpha_l,\alpha_r,L}$. This proves $I = g(z)$ for all $z \in \mathbb{R}$.

Now we can find some constant $M > 0$ such that $g(z) = \{-1\}$ for all $z \leq -M$ and $g(z) = \{1\}$ for all $z \geq M$. By continuity of the radius $r(z)$ in z and of the function u in x, the graph of the multi-mapping g is closed. It follows that, writing $g(z) = [x_1(z), x_2(z)]$ for $z \in [-M, M]$, the function x_1 is lower semi-continuous ($x_1 : \mathbb{R} \to \mathbb{R}$), while x_2 is upper semi-continuous. Then, given any $x_* \in [-1,1]$, an intermediate value argument (i.e. a bisection argument) yields some $z_* \in \mathbb{R}$ such that $x_* \in g(z_*)$. This means $s_{r(z_*),z_*}(x) \leq u(x)$ in $[-1,1]$ and $s_{r(z_*),z_*}(x_*) = u(x_*)$, i.e. the graph of u lies above the circle $s_{r(z_*),z_*}$ while it touches the circle at the point $(x_*, u(x_*))$. The circle $s_{r(z_*),z_*}$ has vanishing hyperbolic curvature everywhere and hence $\kappa_h(x_*) \geq 0$.

2) To prove that $u(x) \leq v(x)$ in $[-1,1]$, let us write v given in (8) as $v(x) = \sqrt{r^2 - (x-x_0)^2}$ for $r > 0$ and $x_0 \in \mathbb{R}$ choosen appropriately. We recall that $v(-1) = \alpha_l$ and $v(1) = \alpha_r$. The inequality $\kappa_h(x) \geq 0$ proven in part 1) together with (10) imply $0 \leq 2(1 + u'^2 + uu'') = \big[(x-x_0)^2 + u^2(x)\big]''$. Thus the mapping $x \mapsto \varphi(x) := (x-x_0)^2 + u^2(x)$ is convex. Noting $\varphi(-1) = \varphi(1) = r^2$, we deduce $\varphi(x) \leq r^2$ in $[-1,1]$ or equivalently $u(x) \leq \sqrt{r^2 - (x-x_0)^2} = v(x)$ in $[-1,1]$.

3) We now derive the upper bound $\kappa_h(x) \le 2$. The idea is similar to part 1). Instead of using semicircles from below, we approach the graph of u from above by suitable catenaries. Choose some function $v \in T_{\alpha_l,\alpha_r}$ such that $u(x) < v(x)$ holds for $x \in (-1,1)$, for example $v(x) := u(x) + 1 - x^2$. For parameters $\gamma \in \mathbb{R}$, $z \in [-1,1]$ let

$$c(x) = c_{\gamma,z}(x) := \frac{v(z)}{\cosh(\gamma)} \cosh\left(\frac{\cosh(\gamma)}{v(z)}(x-z) + \gamma\right) \quad \text{for } x \in \mathbb{R}$$

denote the catenary with initial data $c(z) = v(z)$, $c'(z) = \sinh(\gamma)$. For $z \in \mathbb{R}$ we also define

$$\begin{aligned} \gamma(z) &:= \sup\left\{\gamma \in \mathbb{R} \,:\, u(x) \le c_{\gamma',z}(x) \text{ for all } x \in [-1,z] \text{ and } \gamma' \le \gamma\right\} \quad \text{and} \\ g(z) &:= \left\{x \in [-1,z] \,:\, u(x) = c_{\gamma(z),z}(x)\right\}. \end{aligned}$$

As in part 1), we prove that $g(z)$ is some closed interval by setting $x_1 := \inf g(z)$, $x_2 := \sup g(z)$ and $I := [x_1, x_2]$. If $x_1 < x_2$, then let $w \in T_{\alpha_l,\alpha_r,L}$ denote the function equal to u on $[-1,1]\backslash I$ and equal to $c_{\gamma(z),z}$ on I. Here we note $x_2 < z$, $u'(x_2) = w'(x_2)$ and $u'(x_1) \le w'(x_1)$. Then the equation

$$\mathcal{W}(w) = \mathcal{W}(w|_{[-1,1]\backslash I}) = \mathcal{W}(u|_{[-1,1]\backslash I}) = \mathcal{W}(u) - \mathcal{W}(u|_I)$$

together with $\mathcal{W}(u) \le \mathcal{W}(w)$ imply $\mathcal{W}(u|_I) = 0$. However, this is only possible if $u|_I \equiv v|_I$ proving $I = g(z)$. We have $1 \in g(1)$ and $g(-1) = \{-1\}$. The continuity of the function $\gamma(z)$ in z and the continuity of the function u in x give that the graph of the multi-mapping g is closed. An intermediate value argument (as in part 1)) yields for any $x_* \in (-1,1)$ some $z_* \in (x_*, 1)$ with the properties $u(x) \le c_{\gamma(z_*),z_*}(x)$ in $[-1, z_*]$ and $u(x_*) = c_{\gamma(z_*),z_*}(x_*)$. The graph of u lies locally below the catenary $c_{\gamma(z_*),z_*}$ while it touches the catenary at the point $(x_*, u(x_*))$. The hyperbolic curvature of the catenary $c_{\gamma(z_*),z_*}$ is bounded from above by 2 and we obtain $\kappa_h(x_*) \le 2$.

□

Thanks to the pointwise estimates on the hyperbolic curvature of the minimiser we find that it is sufficient to get estimates on the minimiser from below and of the derivative at the boundary in order to get pointwise estimates of the first and second order derivative of the function in the interior of the interval.

Corollary 3.3. *For $\alpha_r, \alpha_l > 0$ let L_0 be the constant from Lemma 3.1. Let $u \in T_{\alpha_l,\alpha_r,L}$, $L \ge L_0$, be a minimiser for the Willmore energy in this class. Let $K > 0$ and $\varepsilon > 0$ be such that $u'(-1) \ge -K$, $u'(1) \le K$ as well as $u(x) \ge \varepsilon > 0$ in $[-1,1]$. Then u satisfies the estimates*

$$|u'(x)| \le C \text{ in } [-1,1] \quad \text{and} \quad |u''(x)| \le 2(1+C^2)^{3/2}\varepsilon^{-1} \quad \text{a.e. in } [-1,1]$$

with the constant $C = C(K,\varepsilon) = (2+\max\{\alpha_l,\alpha_r\}K)\varepsilon^{-1}$. In particular, $u \in W^{2,\infty}([-1,1],(0,+\infty))$ is true.

Proof. The inequality $\kappa_h(x) \ge 0$ from Lemma 3.2 together with (10) imply $1 + u'^2 + uu'' = (x + uu')' \ge 0$. Therefore the mapping $x \mapsto x + u(x)u'(x)$ is increasing. In particular

$$-1 + \alpha_l u'(-1) \le x + u(x)u'(x) \le 1 + \alpha_r u'(1) \text{ for all } x \in [-1,1], \tag{11}$$

and that gives

$$|u'(x)| \le (2 + \max\{\alpha_l, \alpha_r\}K)\varepsilon^{-1} = C \text{ for all } x \in [-1,1].$$

The inequality $0 \le \kappa_h(x) \le 2$ from Lemma 3.2 together with (10) also yield

$$-1 \le \frac{uu''}{(1+u'^2)^{3/2}} \le 2 \quad \text{a.e. in } [-1,1]$$

and we conclude

$$|u''(x)| \le 2(1+C^2)^{3/2}\varepsilon^{-1} \text{ a.e. in } [-1,1] \text{ and } u \in W^{2,\infty}([-1,1],(0,+\infty)) \ .$$

□

In order to prove Theorem 1.1 it remains to show the a priori estimates $u'(-1) \ge -K$, $u'(1) \le K$ and $u(x) \ge \varepsilon$ with constants K, ε only depending on α_l and α_r but not on L. These estimates are proved in the following section.

3.2 The remaining a priori estimates

We start by proving some estimates on the Willmore energy from below. This yields (see Corollary 3.7 below) a bound on the length of the interval where a function with Willmore energy bounded by 4π is allowed to become small.

Lemma 3.4. *Consider $a, b \in [-1,1]$, $a < b$. The Willmore energy of $u \in W^{2,2}([a,b],(0,+\infty))$ satisfies the two lower bounds*

$$\mathcal{W}(u) \ge -2\pi\Big[\frac{u'}{\sqrt{1+u'^2}}\Big]_a^b \quad \text{and} \quad \mathcal{W}(u) \ge \frac{\pi}{2}\int_a^b \frac{1}{u\sqrt{1+u'^2}}dx - \pi\Big[\frac{u'}{\sqrt{1+u'^2}}\Big]_a^b .$$

Proof. Starting from (6) and using the inequality $(p-q)^2 \ge -4pq$ one gets

$$\mathcal{W}(u) \ge -2\pi\int_a^b \frac{u''}{(1+u'^2)^{3/2}}dx = -2\pi\Big[\frac{u'}{\sqrt{1+u'^2}}\Big]_a^b .$$

Similarly, we get another estimate from below on the energy starting again from formula (6) and using the inequality $(p-q)^2 \ge q^2 - 2pq$:

$$\mathcal{W}(u) \ge \frac{\pi}{2}\int_a^b \frac{1}{u\sqrt{1+u'^2}}dx - \pi\int_a^b \frac{u''}{(1+u'^2)^{3/2}}dx = \frac{\pi}{2}\int_a^b \frac{1}{u\sqrt{1+u'^2}}dx - \pi\Big[\frac{u'}{\sqrt{1+u'^2}}\Big]_a^b .$$

□

Lemma 3.5. *Let $u \in W^{2,2}([0,1],(0,+\infty))$ satisfy $0 < u(x) \le \frac{1}{20}$. Then $\mathcal{W}(u) > \pi$.*

Proof. Set $I := [\frac{1}{4}, \frac{3}{4}]$ and $\varepsilon := \frac{1}{20}$. One of the following three cases will apply.

a) If $|u'(x)| \le 1$ for all $x \in I$, Lemma 3.4 then yields

$$\mathcal{W}(u) \ge \frac{\pi}{2}\int_I \frac{1}{u\sqrt{1+u'^2}} - \pi\Big[\frac{u'}{\sqrt{1+u'^2}}\Big]_{1/4}^{3/4} \ge \frac{\pi}{4\varepsilon\sqrt{2}} - \frac{2\pi}{\sqrt{2}} = \frac{3\pi}{\sqrt{2}} > \pi \ .$$

b) If $u'(x_1) > 1$ for some $x_1 \in I$, then the mean value theorem yields some $x_2 \in (3/4, 1)$ such $u'(x_2) \le 4\varepsilon$ (since $0 < u(x) \le \varepsilon$ in $[0,1]$). Together with Lemma 3.4 we deduce

$$\mathcal{W}(u) \ge \mathcal{W}(u|_{[x_1,x_2]}) \ge 2\pi\Big[\frac{-u'}{\sqrt{1+u'^2}}\Big]_{x_1}^{x_2} \ge 2\pi\Big[\frac{1}{\sqrt{2}} - \frac{4\varepsilon}{\sqrt{1+16\varepsilon^2}}\Big] > \pi \ .$$

c) The remaining case $u'(x_1) < -1$ for some $x_1 \in I$ can be treated as case b).

□

Remark 3.6. *The smallness condition $0 < u(x) \leq \frac{1}{20}$ is surely not optimal. However, note that the constant function $u(x) \equiv \frac{1}{2}$ has Willmore energy $\mathcal{W}(u) = \pi$. Lemma 3.5 will be false if one only requires $0 < u(x) \leq \frac{1}{2}$ instead.*

Corollary 3.7. *Let $u \in W^{2,2}([a,b],(0,+\infty))$, $a, b \in [-1,1]$ with $a < b$, satisfy $\mathcal{W}(u) < 4\pi$ and $0 < u(x) \leq \varepsilon$ in $[a,b]$ for some $\varepsilon > 0$. Then $b - a < 80\varepsilon$ must hold.*

Proof. The claim is proved by contradiction. Let us assume that $\frac{b-a}{80} \geq \varepsilon$. Then the functions

$$u_k(x) := \frac{4}{b-a}\, u\Big(a + \frac{b-a}{4}(x+k)\Big) \quad \text{for } x \in [0,1]\ ,\ k = 0, \ldots, 3\ ,$$

satisfy $0 < u_k(x) \leq \frac{1}{20}$ in $[0,1]$. Lemma 3.5 yields $\mathcal{W}(u_k) \geq \pi$ and together with the invariance of the Willmore energy under translations and rescaling one obtains

$$\mathcal{W}(u) = \sum_{k=0}^{3} \mathcal{W}(u_k) \geq \sum_{k=0}^{3} \pi = 4\pi$$

contradicting the assumption $\mathcal{W}(u) < 4\pi$. □

Comparing the minimisers with catenaries from above, we now obtain an estimate on the derivative at the boundary of the interval and then an estimate from below independent of L. The following lemma gives a bound on the slope of the catenaries that lie completely above the minimiser. The idea is that if the slopes of these catenaries become very large, the catenaries get arbitrarily close to the x-axis and so does the graph of u, lying completely below all these catenaries. Applying Corollary 3.7, we show that this costs too much Willmore energy.

Lemma 3.8. *For $a \in [0,1]$ and $\lambda > 0$ let $u \in W^{2,2}([-1,a],(0,+\infty))$ satisfy $\mathcal{W}(u) < 4\pi$ and $u(a) \leq \lambda$. Assume furthermore that there exists $\gamma_* \in \mathbb{R}$ such that*

$$u(x) \leq c_\gamma(x) \quad \textit{for all}\, x \in [-1,a] \quad \textit{and} \quad \gamma \leq \gamma_*$$

where c_γ denotes the catenary with initial data $c_\gamma(a) = \lambda$ and $c'_\gamma(a) = \sinh(\gamma)$, i.e.

$$c_\gamma(x) := \frac{\lambda}{\cosh(\gamma)} \cosh\Big(\frac{\cosh(\gamma)}{\lambda}(x-a) + \gamma\Big)\ . \tag{12}$$

Then $\gamma_* \leq \max\{162, \lambda\}$ must hold.

Proof. Denote $\bar\gamma := \max\{160, \lambda - 2\}$. We may assume $\gamma_* > \bar\gamma$ since otherwise we are done. For arbitrary $\gamma \in [\bar\gamma, \gamma_*]$ we define $x_\gamma := a - \frac{\lambda\gamma}{\cosh(\gamma)} \in (-1, a)$ with the property

$$u(x_\gamma) \leq c_\gamma(x_\gamma) = \frac{\lambda}{\cosh(\gamma)}\ .$$

For all $x \in [a - \lambda\bar\gamma/\cosh(\bar\gamma), a - \lambda\gamma_*/\cosh(\gamma_*)]$ there exists $\gamma \in [\bar\gamma, \gamma_*]$ such that $x = x_\gamma$. We conclude

$$u(x) \leq \frac{\lambda}{\cosh(\bar\gamma)} \leq \frac{\lambda\bar\gamma}{160\cosh(\bar\gamma)} \quad \text{for all } x \in \Big[a - \frac{\lambda\bar\gamma}{\cosh(\bar\gamma)}, a - \frac{\lambda\gamma_*}{\cosh(\gamma_*)}\Big]\ .$$

Then Corollary 3.7 yields

$$\frac{\lambda\bar{\gamma}}{\cosh(\bar{\gamma})} - \frac{\lambda\gamma_*}{\cosh(\gamma_*)} < \frac{\lambda\bar{\gamma}}{2\cosh(\bar{\gamma})} .$$

We conclude

$$\frac{\bar{\gamma}}{2\cosh(\bar{\gamma})} < \frac{\gamma_*}{\cosh(\gamma_*)} \leq \frac{\gamma_* - 2}{2\cosh(\gamma_* - 2)}$$

and hence $\gamma_* \leq \bar{\gamma} + 2$, proving the claim. $\square$

Theorem 3.9 (Boundary gradient estimate)**.** *Consider $\alpha_r, \alpha_l > 0$ and let L_0 be the constant from Lemma 3.1. Any minimiser u for the Willmore energy in the class $T_{\alpha_l,\alpha_r,L}$, $L \geq L_0$, satisfies the estimates*

$$u'(-1) \geq -\sinh\big(\max\{162, \alpha_l\}\big) \quad \textit{and} \quad u'(1) \leq \sinh\big(\max\{162, \alpha_r\}\big) .$$

Proof. We only prove the upper bound for $u'(1)$ as the proof of the lower bound for $u'(-1)$ is similar. For $\gamma \in \mathbb{R}$ let $c_\gamma(x)$ denote the catenary with initial data $c_\gamma(1) = \alpha_r$, $c'_\gamma(1) = \sinh(\gamma)$ (i.e. c_γ is the catenary given in (12) with $\lambda = \alpha_r$ and $a = 1$). We define the number

$$\gamma_* := \sup\big\{\gamma \in \mathbb{R} \,:\, u(x) \leq c_{\gamma'}(x) \text{ for all } x \in [-1,1] \text{ and } \gamma' \leq \gamma\big\} .$$

From $c_{\gamma_*}(1) = u(1)$ one easily deduces $u'(1) \geq c'_{\gamma_*}(1) = \sinh(\gamma_*)$. We proceed by proving the equality $u'(1) = c'_{\gamma_*}(1)$. It is convenient to distinguish two cases. If the function u satisfies $u(x) < c_{\gamma_*}(x)$ for all $x \in [-1,1)$, the definition of γ_* yields $u'(1) \leq c'_{\gamma_*}(1)$, proving the equality. If instead $u(x_*) = c_{\gamma_*}(x_*)$ for some $x_* \in [-1,1)$, we consider the function $v \in T_{\alpha_l,\alpha_r,L}$ that is equal to u on $[-1,x_*]$ and equal to c_{γ_*} on $[x_*,1]$. The inequality

$$\mathcal{W}(u) \leq \mathcal{W}(v) = \mathcal{W}(v|_{[-1,x_*]}) = \mathcal{W}(u|_{[-1,x_*]}) = \mathcal{W}(u) - \mathcal{W}(u|_{[x_*,1]})$$

implies $\mathcal{W}(u|_{[x_*,1]}) = 0$. However, this is only possible if $u|_{[x_*,1]} \equiv v|_{[x_*,1]}$ holds, proving $u'(1) = v'(1) = c'_{\gamma_*}(1) = \sinh(\gamma_*)$ also in the second case. Now Lemma 3.8 with $a = 1$ and $\lambda = u(1) = \alpha_r$ yields $\gamma_* \leq \max\{162, \alpha_r\}$ and hence $u'(1) = \sinh(\gamma_*) \leq \sinh\big(\max\{162, \alpha_r\}\big)$. $\square$

In the next result we construct at every point $x \in [-1,1]$ a catenary lying completely above the graph of u, while touching the graph at the point $(x, u(x))$. Using Lemma 3.8, we can control the slope of this catenary and hence also the distance of the catenary to the x-axis (see inequality (13) below). The catenaries are constructed with the same idea as in Lemma 3.2.

Theorem 3.10 (Estimate from below)**.** *For $\alpha_r, \alpha_l > 0$ let L_0 be a constant as in Lemma 3.1. Any minimiser u of the Willmore energy in $T_{\alpha_l,\alpha_r,L}$, with $L \geq L_0$ large enough, satisfies*

$$u(x) \geq \frac{\min\{\alpha_l, \alpha_r\}}{\cosh\left(\max\{162, \alpha_l + 2, \alpha_r + 2\}\right)} \quad \textit{for all } x \in [-1,1] .$$

Proof. We proceed as in the proof of Lemma 3.2 part 3). Let $v \in T_{\alpha_l,\alpha_r,L}$ denote the circular arc defined by (8). Consider $\tilde{v} \in T_{\alpha_l,\alpha_r,L}$ defined by $\tilde{v}(x) = v(x) + 1 - x^2$, $x \in [-1,1]$. We have $\min\{\alpha_l, \alpha_r\} \leq \tilde{v}(x) \leq \max\{\alpha_l, \alpha_r\} + 2$ in $[-1,1]$. It follows from Lemma 3.2 that $u(x) < \tilde{v}(x)$ holds in $(-1,1)$ and $u(\pm 1) = \tilde{v}(\pm 1)$. For parameters $\gamma \in \mathbb{R}$, $z \in [0,1]$ let

$$c(x) = c_{\gamma,z}(x) := \frac{\tilde{v}(z)}{\cosh(\gamma)} \cosh\left(\frac{\cosh(\gamma)}{\tilde{v}(z)}(x - z) + \gamma\right) \quad \text{for } x \in \mathbb{R}$$

denote the catenary with initial data $c(z) = \tilde{v}(z)$ and $c'(z) = \sinh(\gamma)$. Next we define

$$\gamma_*(z) := \sup\big\{\gamma \in \mathbb{R} \,:\, u(x) \leq c_{\gamma',z}(x) \text{ for all } x \in [-1,z] \text{ and } \gamma' \leq \gamma\big\} .$$

Lemma 3.8, applied to $u|_{[-1,z]}$ with $\lambda = \tilde{v}(z)$, yields the upper bound

$$\gamma_*(z) \le \max\{162, \tilde{v}(z)\} \le \max\big\{162, \max\{\alpha_l, \alpha_r\} + 2\big\} = \max\{162, \alpha_l + 2, \alpha_r + 2\}$$

and hence

$$c_{\gamma_*(z),z}(x) \ge \frac{\tilde{v}(z)}{\cosh(\gamma_*)} \ge \frac{\min\{\alpha_l, \alpha_r\}}{\cosh\left(\max\{162, \alpha_l + 2, \alpha_r + 2\}\right)} \quad \text{for all } x \in [-1, z] \text{ and } z \in [0,1]\ . \tag{13}$$

To finish the proof, we show that for any $x \in [0,1]$ we can find $z \in [0,1]$ such that $u(x) = c_{\gamma_*(z),z}(x)$. This together with (13) yields the claim. For $z \in [-1,1]$ we define the set valued function

$$g(z) := \big\{x \in [-1, z] \,:\, u(x) = c_{\gamma_*(z),z}(x)\big\}$$

and note that $g(z)$ is non-empty and closed. Moreover, proceeding as in the proof of Lemma 3.2 part 3) we find that $g(z)$ is a closed interval for any $z \in [-1,1]$ and since $1 \in g(1)$, $g(-1) = \{-1\}$, an intermediate value argument yields for any $x_* \in [-1,1]$ some $z_* \in [x_*, 1]$ such that $x_* \in g(z_*)$, i.e. $u(x_*) = c_{\gamma_*(z_*),z_*}(x_*)$, holds. Together with (13) we conclude

$$u(x) \ge \frac{\min\{\alpha_l, \alpha_r\}}{\cosh\left(\max\{162, \alpha_l + 2, \alpha_r + 2\}\right)} \quad \text{for all } x \in [0,1]\ .$$

Note that (13) is valid only for $z \in [0,1]$ so that the above reasoning only works for $x \in [0,1]$. However, by considering the reflection $\tilde{u}(x) := u(-x)$, which is a minimiser in the class $T_{\alpha_r,\alpha_l,L}$, one obtains the same estimate also for $x \in [-1,0]$. □

Combining Corollary 3.3, Theorems 3.9 and 3.10 we obtain the desired estimates.

Theorem 3.11. *Given $\alpha_l, \alpha_r > 0$ there exists some constant $C = C(\alpha_l, \alpha_r) > 0$ such that any minimiser u for the Willmore energy in the class $T_{\alpha_l,\alpha_r,L}$, $L \ge C$, satisfies the estimates*

$$u(x) \ge \frac{1}{C} \quad \textit{and} \quad |u'(x)| \le C \quad \textit{in } [-1,1]\ .$$

Remark 3.12. *It is important to note that the constant C of this result depends only on α_l and α_r but is independent of L.*

4 Construction of a minimiser

Proof of Theorem 1.1. Lemma 2.2 and a simple study of the function u_γ defined in (7) yield immediately part $a)$ and $b)$ of the claim. We divide the proof of part $c)$ into three steps.

1) Let L_0 be a constant from Lemma 3.1. For $L \ge L_0$ the set $T_{\alpha_l,\alpha_r,L}$ from Definition 1.4 is non-empty and $M_{\alpha_l,\alpha_r,L} < 4\pi$ holds. We now prove the existence of a minimiser for the Willmore energy in $T_{\alpha_l,\alpha_r,L}$, $L \ge L_0$. Fix some $u \in T_{\alpha_l,\alpha_r,L}$. Starting from (6) and using the inequality $(p-q)^2 \ge \frac{1}{2}p^2 - q^2$ we compute

$$\begin{aligned} \mathcal{W}(u) &\ge \frac{\pi}{2}\int_{-1}^{1}\Big(\frac{(u'')^2 u}{2(1+u'^2)^{5/2}} - \frac{1}{u(1+u'^2)^{1/2}}\Big)dx \\ &\ge \frac{\pi}{4L(1+L^2)^{5/2}}\int_{-1}^{1}(u'')^2 dx - \pi L\ . \end{aligned}$$

In particular, a bound on $\mathcal{W}(u)$ implies a bound on u'' in $L^2([-1,1])$ and hence a bound on u in the space $W^{2,2}([-1,1],(0,+\infty))$. Now let $\{u_k\}_{k\in\mathbb{N}}$ be a minimising sequence for the

Willmore energy in $T_{\alpha_l,\alpha_r,L}$, i.e. $\mathcal{W}(u_k) \to M_{\alpha_l,\alpha_r,L}$ for $k \to \infty$. By the argument above u_k is then uniformly bounded in $W^{2,2}([-1,1],(0,+\infty))$. A subsequence u_k converges weakly in $W^{2,2}([-1,1],(0,+\infty))$ and, by compact embedding, also strongly in $C^1([-1,1],(0,+\infty))$ to some limit function $u \in W^{2,2}([-1,1],(0,+\infty))$. From the strong convergence in C^1 we deduce $u(-1)=\alpha_l$, $u(1)=\alpha_r$, $u(x) \geq L^{-1}$, $|u'(x)| \leq L$ in $[-1,1]$ and hence $u \in T_{\alpha_l,\alpha_r,L}$. A lower semi-continuity argument yields

$$\mathcal{W}(u) \leq \liminf_{k\to\infty} \mathcal{W}(u_k) = M_{\alpha_l,\alpha_r,L}\ .$$

On the other hand, $u \in T_{\alpha_l,\alpha_r,L}$ implies $\mathcal{W}(u) \geq M_{\alpha_l,\alpha_r,L}$ and hence $\mathcal{W}(u) = M_{\alpha_l,\alpha_r,L}$. Thus, u is indeed a minimiser of the Willmore energy in the class $T_{\alpha_l,\alpha_r,L}$. Moreover, Corollary 3.3 yields $u \in W^{2,\infty}([-1,1],(0,+\infty)) = C^{1,1}([-1,1],(0,+\infty))$.

2) Let $C = C(\alpha_l,\alpha_r)$ denote the constant from Theorem 3.11 and $u = u_C$ be a minimiser for the Willmore energy in the class $T_{\alpha_l,\alpha_r,C}$. We prove that this u is a minimiser in the large class T_{α_l,α_r}. Given $v \in T_{\alpha_l,\alpha_r}$, choose some constant $L \geq C$ large enough such that $v \in T_{\alpha_l,\alpha_r,L}$. If $w \in T_{\alpha_l,\alpha_r,L}$ denotes a minimiser in the class $T_{\alpha_l,\alpha_r,L}$, then Theorem 3.11 shows in fact $w \in T_{\alpha_l,\alpha_r,C}$. Because of $L \geq C$, w is also a minimiser in the class $T_{\alpha_l,\alpha_r,C}$ and we obtain $\mathcal{W}(u) = \mathcal{W}(w) \leq \mathcal{W}(v)$. Since $v \in T_{\alpha_l,\alpha_r}$ is arbitrary, u must be a minimiser in the class T_{α_l,α_r}, proving the claim. Moreover, u also provides a minimiser in the even larger space $\widetilde{T}_{\alpha_l,\alpha_r}$ of immersed regular curves by Corollary 2.5.

3) With the same arguments as in [4, Thm.3.9 Step 2] one can prove $u \in C^\infty([-1,1])$. Let $\Gamma = \Gamma(u)$ denote the surface of revolution corresponding to u. The Euler-Lagrange equation satisfied by Γ is given by $\triangle H + 2H(H^2-K) = 0$ on Γ, where $\triangle$ denotes the Laplace-Beltrami operator on the surface Γ. Moreover, $H = 0$ on $C_{\alpha_l} \cup C_{\alpha_r}$ arises as the natural boundary condition for our variational problem (see [2, App.A] or [18]). In Lemma 3.2 we have proven that the solution Γ lies locally on one side of the catenoid, in particular $H \geq 0$ or $H \leq 0$ everywhere on Γ, the sign depending on the choice of the normal vector. From the strong maximum principle, applied to the second order elliptic equation $\triangle H + 2H(H^2-K) = 0$ we deduce either $H \equiv 0$ on Γ or $H \neq 0$ on $\Gamma \backslash (C_{\alpha_l} \cup C_{\alpha_r})$. The case $H \equiv 0$ corresponds to $\alpha_r \geq \alpha_r^*$ when the minimiser is a minimal surface of revolution, i.e. some catenoid.

□

Corollary 4.1. *For $\alpha_l, \alpha_r > 0$ let M_{α_l,α_r} be defined as in Definition 1.3 and $\alpha_r^*(\alpha_l)$ be defined as in (3). Then $\alpha_r \mapsto M_{\alpha_l,\alpha_r}$ is strictly monotonically decreasing in $(0,\alpha_r^*(\alpha_l))$.*

Proof. Let α_r, α_r' satisfy $0 < \alpha_r < \alpha_r' < \alpha_r^*(\alpha_l)$. Let $u \in T_{\alpha_l,\alpha_r}$ be a minimiser for the Willmore energy in T_{α_l,α_r}. Then u solves the corresponding Euler-Lagrange equation, that is u is solution of the fourth order ordinary differential equation given in [5, Lemma 2.2]. In particular, u does not coincide locally with a catenary. With the construction in Lemma 2.4 we find a $v \in T_{\alpha_l,\alpha_r'}$ such that $\mathcal{W}(v) \leq \mathcal{W}(u)$ and v coincides with a catenary on $[x_*,1]$ for some $x_* \in (-1,1)$. Hence $\mathcal{W}(v) < \mathcal{W}(u)$ and also $M_{\alpha_l,\alpha_r'} < M_{\alpha_l,\alpha_r}$. □

In [2] we studied the case of symmetric boundary conditions $\alpha = \alpha_l = \alpha_r$, minimising there only within the class symmetric graphs. We could prove that for $\alpha < \alpha^* = \inf_{\gamma\in\mathbb{R}} \frac{\cosh(\gamma)}{\gamma} \approx 1.5089$ the minimisers satisfy $u'(-1) = -u'(1) = -\alpha$. We cannot expect the same behavior in the more general case studied in this paper, but still we can show the following.

Lemma 4.2. *Given $\alpha_l, \alpha_r > 0$, let u be a minimiser for the Willmore energy in T_{α_l,α_r}. Then $u'(-1) < 0$ and $u'(1) > 0$ must hold.*

Proof. We prove only that $u'(1) > 0$ since the proof of $u'(-1) < 0$ is similar. We proceed by contradiction. If $u'(1) < 0$, let c be the catenary such that $c(1) = u(1) = \alpha_r$ and $c'(1) = u'(1)$ and $x_0 > 1$ be such that $c(x_0) = \alpha_r$. We take the function $\tilde{w} \in W^{2,2}([-1, x_0], (0, +\infty))$ that is equal to u on $[-1, 1]$ and equal to c on $(1, x_0]$. We denote by w the function defined on $[-1, 1]$ obtained from $\tilde{w}$ by appropriate translation and rescaling. By construction, $w(-1) < \alpha_l$ and $w(1) < \alpha_r$. Lemma 2.4 applied twice yields a function $v \in T_{\alpha_l,\alpha_r}$ such that

$$\mathcal{W}(v) \leq \mathcal{W}(w) = \mathcal{W}(\tilde{w}) = \mathcal{W}(u)\,.$$

Hence v is also a minimiser in T_{α_l,α_r}. By construction v coincides with a catenary on an interval of positive length and therefore v is equal to a catenary on the entire interval $[-1, 1]$, since both v and the catenary are solutions of the fourth order Euler-Lagrange equation with the same initial values. We obtain $\mathcal{W}(v) = 0$, a contradiction to the assumption $\alpha_r < \alpha_r^*(\alpha_l)$.

In the case $u'(1) = 0$ the construction is the same as above with the only difference that the point x_0 is chosen so that $\cosh((x_0 - 1)/\alpha_r) < (x_0 + 1)/2$. □

5 Convergence to a sphere for $\alpha_l, \alpha_r \to 0$

Here we study the behavior of the minimisers, which admits a representation as in (4), as both α_l and α_r converge to zero. In this situation the two circles defining the boundary of the surface $\Gamma_{\alpha_l,\alpha_r}$ collapse to points. We will show that $\Gamma_{\alpha_l,\alpha_r}$, the surface of revolution generated by the graph of the positive function u_{α_l,α_r}, converges to the round sphere $\mathbb{S}^2$ in the sense that the functions u_{α_l,α_r} converge uniformly to the function $\sqrt{1-x^2}$ in $[-1, 1]$ as $\alpha_l, \alpha_r \to 0$. In the case of symmetric boundary conditions $\alpha_l = \alpha_r$ this result was proved in [8].

We start by proving that the energy of Γ converges to the energy of a round sphere, i.e. to 4π.

Lemma 5.1. *For $a, b \in [-1, 1]$, $a < b$, let $u \in W^{2,2}([a, b], (0, +\infty))$ satisfy $\mathcal{W}(u) < 4\pi$ and $\max\{u(a), u(b)\} \leq \varepsilon^2$ for $\varepsilon < \min\{\frac{b-a}{2}, \frac{1}{80}e^{-12}\}$. Then the following estimates are satisfied*

$$\mathcal{W}(u) \geq 4\pi\big(1 - \delta(\varepsilon)\big) \quad \text{and} \quad \int\limits_{a+\varepsilon}^{b-\varepsilon} \kappa_h^2(x) \frac{\sqrt{1 + u'(x)^2}}{u(x)} dx \leq 8\,\delta(\varepsilon)$$

with κ_h the hyperbolic curvature of u as defined in (10) *and*

$$\delta(\varepsilon) := 1 - \sqrt{1 + \frac{12}{\log(80\varepsilon)}} > 0\,. \tag{14}$$

Proof. We first prove the following: Close to each boundary point there is a point with large derivative (in absolute value). Applying Corollary 3.7 to u restricted to the interval $[a, a + \varepsilon]$ we get that there exist some $x_* \in [a, a+\varepsilon]$ such that $u(x_*) \geq \frac{\varepsilon}{80}$. We set $L := \sup\{u'(x) : x \in [a, a+\varepsilon]\}$ and $I := \{x \in [a, a+\varepsilon] : u'(x) \geq 0\}$. Notice that, due to the assumption on ε, L is strictly positive. Moreover, I is not necessarily an interval but it is a closed set, by the continuity of u'. We choose some $x_1 \in [a, a + \varepsilon]$ with $u'(x_1) = L$. From Lemma 3.4 we first deduce

$$4\pi > \mathcal{W}(u) \geq \frac{\pi}{2} \int_a^b \frac{1}{u\sqrt{1 + u'^2}} dx - 2\pi$$

and continue by estimating

$$\begin{aligned} 12 \quad &\geq \quad \int_a^b \frac{1}{u\sqrt{1+u'^2}}dx \geq \int_I \frac{1}{u\sqrt{1+u'^2}}dx \geq \int_I \frac{u'}{uL\sqrt{1+L^2}}dx \geq \frac{1}{1+L^2}\int_a^{x_*} \frac{u'}{u}dx \\ &= \quad \frac{1}{1+L^2}\log\frac{u(x_*)}{u(a)} \geq \frac{1}{1+L^2}\log\frac{\varepsilon}{80\varepsilon^2} = \frac{-\log(80\varepsilon)}{1+L^2}\,. \end{aligned}$$

After suitably rearranging one obtains

$$\frac{u'(x_1)}{\sqrt{1+u'(x_1)^2}} = \frac{L}{\sqrt{1+L^2}} \geq \sqrt{1+\frac{12}{\log(80\varepsilon)}}\ .$$

where we use $0<\varepsilon<\frac{1}{80}e^{-12}$. In a similar way we can find some $x_2 \in [b-\varepsilon, b]$ such that

$$\frac{u'(x_2)}{\sqrt{1+u'(x_2)^2}} \leq -\sqrt{1+\frac{12}{\log(80\varepsilon)}}\ .$$

From Lemma 3.4 applied to $u|_{[x_1,x_2]}$ we obtain

$$\mathcal{W}(u) \geq \mathcal{W}(u|_{[x_1,x_2]}) \geq -2\pi\Big[\frac{u'}{\sqrt{1+u'^2}}\Big]_{x_1}^{x_2} \geq 4\pi\big(1-\delta(\varepsilon)\big)\ ,$$

with $\delta(\varepsilon)$ defined in (14). Moreover, using $x_1 \leq a+\varepsilon$, $x_2 \geq b-\varepsilon$ together with formula (9) for the Willmore energy one deduces

$$\frac{\pi}{2}\int\limits_{a+\varepsilon}^{b-\varepsilon} \kappa_h^2 \frac{\sqrt{1+u'^2}}{u}dx \leq \frac{\pi}{2}\int_{x_1}^{x_2} \kappa_h^2 \frac{\sqrt{1+u'^2}}{u}dx = \mathcal{W}(u|_{[x_1,x_2]}) + 2\pi\Big[\frac{u'}{\sqrt{1+u'^2}}\Big]_{x_1}^{x_2} < 4\pi\delta(\varepsilon)\ ,$$

proving the second estimate in the claim. □

An immediate consequence is the convergence of the energy to the one of the sphere.

Corollary 5.2. *The energy M_{α_l,α_r} from Definition 1.3 converges to 4π as $\alpha_l, \alpha_r \to 0$.*

Lemma 5.3. *Let $\varepsilon_0 > 0$ be such that $\delta(\varepsilon_0) = \frac{1}{2}$ with $\delta(\varepsilon)$ defined in (14). For $\alpha_l, \alpha_r > 0$ such that $\min\{\alpha_l, \alpha_r\} \leq \varepsilon^2$ with $\varepsilon < \min\{\varepsilon_0, \frac{1}{80}e^{-12}\}$ let u be a minimiser for the Willmore energy in T_{α_l,α_r}. Then u satisfies*

$$u(x) \geq \varepsilon^2 \quad \textit{and} \quad |u'(x)| \leq (2+\varepsilon^2\sinh(162))\varepsilon^{-2} \quad \textit{for all}\ x \in [-1+3\varepsilon, 1-3\varepsilon]\ .$$

Proof. We have $\mathcal{W}(u) = M_{\alpha_l,\alpha_r} < 4\pi$ by Lemma 3.1. We prove the first claim by contradiction. Let us assume that there exist $\varepsilon < \min\{\varepsilon_0, \frac{1}{80}e^{-12}\}$ and some $x_* \in [-1+3\varepsilon, 1-3\varepsilon]$ with $u(x_*) < \varepsilon^2$. Then Lemma 5.1, applied on the intervals $[-1, x_*]$ and $[x_*, 1]$, proves $\mathcal{W}(u|_{[-1,x_*]}) \geq 4\pi(1-\delta(\varepsilon)) > 2\pi$ as well as $\mathcal{W}(u|_{[x_*,1]}) > 2\pi$. This implies $\mathcal{W}(u) > 2\pi + 2\pi = 4\pi$, contradicting $\mathcal{W}(u) < 4\pi$ and proving the first claim. To prove the second inequality we first deduce from Theorem 3.9 that $u'(-1) \geq -\sinh(162)$ and $u'(1) \leq \sinh(162)$ must hold. These estimates and $u(x) \geq \varepsilon^2$ in $[-1+3\varepsilon, 1-3\varepsilon]$, just proved, combined with the estimate (11) in the proof of Corollary 3.3 give

$$|u'(x)| \leq (2+\max\{\alpha_l,\alpha_r\}\sinh(162))\varepsilon^{-2} \leq (2+\varepsilon^2\sinh(162))\varepsilon^{-2}\ .$$

□

We are now ready to prove Theorem 1.2.

Theorem 5.4. *Let $\{\alpha_{l,n}\}_{n\in\mathbb{N}}, \{\alpha_{r,n}\}_{n\in\mathbb{N}}$ be two strictly positive sequences converging to zero. For each $n \in \mathbb{N}$ let u_n be a minimiser for the Willmore energy in $T_{\alpha_{l,n},\alpha_{r,n}}$. Then u_n converges uniformly on $[-1,1]$ to the function $u_0(x) := \sqrt{1-x^2}$.*

Proof. Without loss of generality we may assume that $\alpha_{l,n}, \alpha_{r,n} \leq 1$ for all $n \in \mathbb{N}$. Defining the sequence $\varphi_n(x) := x^2 + u_n^2(x)$, it suffices to show that φ_n converge uniformly to $\varphi_0 \equiv 1$. From Lemma 3.2 it follows that $u_n(x) \leq \max\{\alpha_{l,n}, \alpha_{r,n}\} + 1$ for all n, and hence φ_n is uniformly bounded from above. If κ_n denotes the hyperbolic curvature of u_n, then we have the relation

$$\kappa_n = \frac{u_n u_n'' + 1 + u_n'^2}{(1+u_n'^2)^{3/2}} = \frac{\varphi_n''}{2(1+u_n'^2)^{3/2}} \,. \tag{15}$$

Lemma 3.2 implies $\kappa_n(x) \geq 0$ and hence $\varphi_n'' \geq 0$ in $[-1,1]$. From (11) together with Theorem 3.9 we conclude for all $n \in \mathbb{N}$

$$-1 - \alpha_{l,n}\sinh(162) \leq x + u_n(x)u_n'(x) = \frac{1}{2}\varphi_n'(x) \leq 1 + \alpha_{r,n}\sinh(162) \quad \text{for } x \in [-1,1]\,.$$

Hence $\varphi_n'(x)$ is uniformly bounded in $[-1,1]$ and, after passing to some subsequence, φ_n converges uniformly in $[-1,1]$ to some limit function $\varphi_0 \in C^{0,1}([-1,1],\mathbb{R})$. From $\varphi_n(-1) = 1 + \alpha_{l,n}^2$, $\varphi_n(1) = 1 + \alpha_{r,n}^2$ we deduce $\varphi_0(-1) = 1 = \varphi_0(1)$. We prove now that φ_0 is a linear function. Fixing $\delta > 0$, we first observe that Lemma 5.1 yields

$$0 = \lim_{n\to\infty} \int_{-1+\delta}^{1-\delta} \kappa_n^2 \frac{\sqrt{1+u_n'^2}}{u_n}\, dx\,,$$

while Lemma 5.3 shows

$$\inf_{\substack{x\in[-1+\delta,1-\delta]\\ n\in\mathbb{N}}} u_n(x) = m > 0 \quad , \qquad \sup_{\substack{x\in[-1+\delta,1-\delta]\\ n\in\mathbb{N}}} |u_n'(x)| = L < +\infty\,.$$

From (15), $u_n \leq 2$ for all $n \in \mathbb{N}$ together with the estimate above we reach

$$0 = \lim_{n\to\infty} \int_{-1+\delta}^{1-\delta} \kappa_n^2 \frac{\sqrt{1+u_n'^2}}{u_n}\, dx \geq \frac{1}{8(1+L^2)^{5/2}} \lim_{n\to\infty} \int_{-1+\delta}^{1-\delta} (\varphi_n'')^2\, dx\,.$$

The sequence φ_n'' converges to zero in $L^2(-1+\delta, 1-\delta)$ and we obtain $\varphi_0 \in W^{2,2}([-1+\delta,1-\delta],(0,\infty))$ with $\varphi_0'' \equiv 0$ in $(-1+\delta, 1-\delta)$ for any $\delta > 0$. Thus, φ_0 is a linear function and because of $\varphi_0(-1) = 1 = \varphi_0(1)$ we finally obtain $\varphi_0 \equiv 1$, as claimed. □

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Uniqueness for the Homogeneous Dirichlet Willmore boundary value problem[1]

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Abstract

We prove that a Willmore surface which has its boundary on a strict star-shaped two-dimensional domain and which intersects the plane of the domain with a zero angle, along the boundary, is necessarily a piece of the plane.

Keywords. Willmore surfaces, Dirichlet boundary conditions, Pohozaev identity, conformal Gauss map.
AMS classification. 35G25, 49Q10, 53A30, 53C42.

1 Introduction

A Willmore surface is a critical point for the Willmore functional, that for an immersed surface $\Phi : \Sigma \to \mathbb{R}^3$ is given by

$$W(\Phi(\Sigma)) = \int_\Sigma H^2\, dS\,,$$

with H the mean-curvature and dS the area form induced on $\Phi(\Sigma)$ by the canonical metric in $\mathbb{R}^3$. Here $H = \frac{1}{2}(\lambda_1 + \lambda_2)$ with λ_1, λ_2 the principal curvature of $\Phi(\Sigma)$. The Willmore functional models the elastic energy of thin cells or biological membranes. It has also applications in image processing. It is well known that for closed surfaces without boundary the Willmore functional is invariant under conformal transformations. The Euler-Lagrange equation (called Willmore equation) is

$$\Delta H + 2H(H^2 - K) = 0\,, \tag{1.1}$$

with Δ the Laplace-Beltrami operator on $\Phi(\Sigma)$ and K the Gauss curvature of $\Phi(\Sigma)$. For surfaces with boundary we consider only interior variations. Equation (1.1) is of fourth order and, since Δ depends on $\Phi(\Sigma)$, it is a quasilinear one. Moreover, the ellipticity is not uniform.

Existence of closed (without boundary) Willmore surfaces of prescribed genus has been proved in [18] and [1]. The regularity issue has been solved in [16] establishing that any Willmore surface is real analytic. In all these works the conformal invariance of the Willmore functional plays a key role.

In part of the literature, the functional

$$\tilde{W}(\Phi(\Sigma)) = \int_\Sigma (H^2 - K)\, dS\,, \tag{1.2}$$

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is referred to as the Willmore functional. This is well behaving under conformal transformations in $\mathbb{R}^3$. Indeed, it is trivially invariant under Euclidean transformations as well as under scaling. If I is an inversion with center a point $p \notin \Phi(\Sigma)$ then $\tilde{W}(I(\Phi(\Sigma))) = \tilde{W}(\Phi(\Sigma))$ (see Willmore, Ch.7.3 [21] or Weiner [20]). For surfaces without boundary the difference between $W(\Phi(\Sigma))$ and $\tilde{W}(\Phi(\Sigma))$ is the total Gauss curvature that is equal to the Euler Characteristic of the surface. Instead for surfaces with boundary, with the Gauss-Bonnet Theorem we get

$$\int_{\Sigma} K \, dS = 2\pi\chi(\Phi(\Sigma)) - \int_{\partial\Sigma} \kappa_g \, ds \,, \tag{1.3}$$

with $\chi(\Phi(\Sigma))$ the Euler charachteristik of $\Phi(\Sigma)$ and κ_g the geodesic curvature of the boundary.

We are interested in studying Willmore surfaces with boundary satisfying prescribed boundary conditions. The first to study boundary value problems for Willmore surfaces was Nitsche in [13]. He describes several choices of boundary value problems for the Willmore equation and established existence results for small data. Most of the works in the literature concerns Dirichlet boundary data. By this we mean that the boundary of the surface is fixed and also that the tangent space of the surface along the boundary is fixed. (See [3], [4] and [8] for results on natural boundary conditions.) Notice that due to (1.3) the difference between $W(\Phi(\Sigma))$ and $\tilde{W}(\Phi(\Sigma))$ (defined in (1.2)) is a fixed constant for surfaces satisfyng the same Dirichlet boundary conditions and of the same topological type.

The studies of Willmore surfaces with boundary in the literature follow two streams. On one side, there are existence results under special symmetries. In [6] and [7] existence of Willmore surfaces of revolution generated by graphs satisfying arbitrary symmetric Dirichlet boundary conditions has been proved. In this case, the boundary consists of two circles with the same radius and center on the axis with respect to which we rotate. The second boundary condition prescribes the derivative of the function at the boundary. One has existence of Willmore surfaces for all choices of the radius and for all values of the derivative at the boundary. This is in great contrast with the correspondent results for minimal surface, where there is a critical value of the radius under which there do not exists minimal surfaces having the two circles as boundary. More general approaches are in [17] and [14]. Schätzle in [17] proves existence of Willmore immersions in $\mathbb{S}^n$ satisfying Dirichlet boundary conditions. Under certain smallness assumptions on the energy, he can then project these surfaces into $\mathbb{R}^n$ to get embedded Willmore surfaces. Palmer in [14] proves (among other results) that a Willmore surface of disk type which has its boundary on a circle and which intersects the plane of the circle in a constant angle is a spherical cap or a flat disk.

In this work we extend the result of Palmer in [14] concerning the case of zero Dirichlet boundary data. Let $\Omega \subset \mathbb{R}^2$ be a smooth bounded domain which is strictly star-shaped with respect to $x_0 \in \Omega$. Given $u : \Omega \to \mathbb{R}$ a sufficiently smooth function with $u|_{\partial\Omega} = 0$ and $\nabla u|_{\partial\Omega} = 0$, we consider the surface Γ in $\mathbb{R}^3$ given by the graph of u. Is it true that Γ is a Willmore surface if and only if Γ is a subset of the plane $\{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_3 = 0\}$? Or in other words, Γ being a Willmore surface, does it imply and require u being constant and $u \equiv 0$? The answer is yes and this is the main result of this work.

Theorem 1.1. *Let $\Omega \subset \mathbb{R}^2$ be a smooth bounded strictly star-shaped domain. Let $u : \Omega \to \mathbb{R}$ be a smooth function with $u|_{\partial\Omega} = 0$ and $\nabla u|_{\partial\Omega} = 0$ and let $\Gamma \subset \mathbb{R}^3$ be the surface given by the graph of u.*

Then Γ is a Willmore surface if and only if $u \equiv 0$ in Ω.

Of course, due to the conformal invariance of the equation, it is not a restriction that we consider the plane $\{z = 0\} \subset \mathbb{R}^3$.

In general we do not expect uniqueness for the Willmore Dirichlet boundary value problems. Even in the presence of some extra symmetries. Indeed, in the case of surfaces of revolution generated by symmetric graphs with symmetric boundary data one can numerically find two different minimisers. So there is numerical evidence not only of two solutions of the Euler-Lagrange equation but also two different surfaces with the same Willmore energy. On the other hand, the author does not know what to expect in the case of graphs.

The proof of Theorem 1.1 consists of two steps. In the first we prove that, under the assumptions, Γ being a Willmore surface implies that the mean curvature and all second order derivative of u are zero at the boundary. This is done in the spirit of Pohozaev identity, i.e. multiplying the equation by test functions (the choice of which is due to the invariances of the equations) and then integrate. The second step is as in [14]. By a result of Bryant [2] we may associate to the Willmore surface a holomorphic function via the conformal Gauss map. By the first step of the proof this function is zero at the boundary and therefore identically zero. Then a classification theorem of Bryant yields the result. In the appendices we recall the definition of the conformal Gauss map and the results of Bryant.

1.1 Willmore graphs with Dirichlet boundary conditions

Let $\Omega \subset \mathbb{R}^2$ be a smooth bounded domain which is strictly star-shaped with respect to $x_0 \in \Omega$. We recall that a domain Ω is strictly starshaped with respect to x_0 ($x_0 \in \Omega$) when $(z - x_0) \cdot \nu > 0$ for every $z \in \partial\Omega$ with ν the exterior normal to $\partial\Omega$ in z. Without loss of generality, we assume from this point on that Ω is strictly star-shaped with respect to 0.

We consider $u \in C^4(\Omega; \mathbb{R})$ satisfying homegeneous Dirichlet boundary conditions, i.e. such that $u|_{\partial\Omega} = 0$ and $\nabla u|_{\partial\Omega} = 0$. The graph of u parametrises the surface Γ:

$$\Gamma \,:\, \Omega \ni (x, y) \mapsto (x, y, u(x, y))^t \in \Gamma \subset \mathbb{R}^3.$$

The first fundamental form and the normal are given as follows:

$$(g_{ij}) = \begin{pmatrix} 1 + u_x^2 & u_x u_y \\ u_x u_y & 1 + u_y^2 \end{pmatrix}, \; g = \det(g_{ij}) = 1 + |\nabla u|^2 = 1 + u_x^2 + u_y^2$$
$$\vec{n} = \frac{1}{\sqrt{g}}(-u_x, -u_y, 1)\,,$$

while the mean curvature and the Gauss curvature are

$$H = \frac{1}{2g^{3/2}}((1 + u_y^2)u_{xx} - 2u_x u_y u_{xy} + (1 + u_x^2)u_{yy})\,,$$
$$K = \frac{1}{g^2}(u_{xx}u_{yy} - u_{xy}^2)\,,$$

and finally the Laplace-Beltrami operator is given by

$$\begin{aligned} \Delta f &= \frac{1}{\sqrt{g}}\frac{\partial}{\partial x}\left(\frac{1}{\sqrt{g}}\big((1 + u_y^2)\frac{\partial}{\partial x}f - u_x u_y \frac{\partial}{\partial y}f\big)\right) \\ &\quad + \frac{1}{\sqrt{g}}\frac{\partial}{\partial y}\left(\frac{1}{\sqrt{g}}\big(- u_x u_y \frac{\partial}{\partial x}f + (1 + u_x^2)\frac{\partial}{\partial y}f\big)\right)\,. \end{aligned}$$

Hypothesis 1.2. *$\Omega \subset \mathbb{R}^2$ is a $C^{4,\alpha}$, $\alpha \in (0, 1)$, bounded domain which is strictly star-shaped with respect to $0 \in \mathbb{R}^2$. $u \in C^4(\overline{\Omega}; \mathbb{R})$ is such that $u|_{\partial\Omega} = 0$ and $\nabla u|_{\partial\Omega} = 0$. The surface Γ parametrised by the graph of u is a Willmore surface, that is a solution of* (1.1)

2 $H = 0$ on $\partial\Omega$

In this section we prove that all second order derivatives of u are zero at the boundary. Due to the boundary conditions, the smoothness of u and of the domain Ω, the second order tangential derivative and also the second order mixed derivative of u are zero. It remains to show that the second order normal derivative is zero.

The main result is the following.

Proposition 2.1. *Assume Hypothesis 1.2 and let ν denote the exterior normal to $\partial\Omega \subset \mathbb{R}^2$. Then, $u_{\nu\nu} = 0$ on $\partial\Omega$. In particular, H the mean curvature of Γ satisfies $H = 0$ on $\partial\Omega$.*

Corollary 2.2. *Assume Hypothesis 1.2. Then, $D^\alpha u = 0$ on $\partial\Omega$ for all $\alpha \in \mathbb{N}_0^3$ with $|\alpha| \leq 2$. In particular, H the mean curvature of Γ satisfies $H = 0$ on $\partial\Omega$.*

We prove Proposition 2.1 in the spirit of Pohozaev identity. Due to the conformal invariance of the Willmore functional, we expect to find invariant quantities. By testing the Willmore equation (1.1) with appropriate test functions we get two integral identities (Lemmas 2.3 and 2.4) from which Proposition 2.1 follows directly. At this point we use that the domain Ω is strictly star-shaped.

Lemma 2.3. *Assume Hypothesis 1.2. Then we have*

$$5\int_\Omega \frac{H^2}{\sqrt{g}}\,dz - 2\int_\Omega \frac{H}{g}(u_{xx}+u_{yy})\,dz + \int_\Omega H^2\sqrt{g}\,dz = 0\,.$$

Proof. Multiplying (1.1) by u and integrating over Ω we get

$$\int_\Omega u\Delta H\,dz + 2\int_\Omega H^3 u\,dz - 2\int_\Omega HKu\,dz = 0\,. \tag{2.1}$$

Using that $u = 0$ on $\partial\Omega$, we integrate by parts in the first integral obtaining

$$\begin{aligned}
&\int_\Omega u\Delta H\,dz \\
= \;& -\int_\Omega \frac{1}{g}[u_xH_x + u_yH_y]\,dz + \int_\Omega \frac{u}{\sqrt{g}}[u_x\partial_x H^2 + u_y\partial_y H^2]\,dz \\
& + \int_\Omega \frac{u}{g}[H_x(u_yu_{xy} - u_xu_{yy}) + H_y(u_xu_{xy} - u_yu_{xx})]\,dz\,.
\end{aligned}$$

Integrating by parts once more we find

$$\begin{aligned}
&\int_\Omega u\Delta H\,dz \\
= \;& +\int_\Omega \frac{H}{g}(u_{xx}+u_{yy})\,dz - 2\int_\Omega \frac{H}{g^2}(u_x^2u_{xx} + 2u_yu_xu_{xy} + u_y^2u_{yy})\,dz \\
& -\int_\Omega \frac{H^2}{\sqrt{g}}(u_x^2+u_y^2)\,dz - 2\int_\Omega H^3u\,dz \\
& +2\int_\Omega H^2\sqrt{g}\,dz - \int_\Omega \frac{H}{g}(u_{xx}+u_{yy})\,dz + 2\int_\Omega uHK\,dz \\
= \;& 5\int_\Omega \frac{H^2}{\sqrt{g}}\,dz - 2\int_\Omega \frac{H}{g}(u_{xx}+u_{yy})\,dz \\
& -2\int_\Omega H^3u\,dz + \int_\Omega H^2\sqrt{g}\,dz + 2\int_\Omega uHK\,dz\,.
\end{aligned}$$

The claim follows from the formula above and (2.1). $\square$

Lemma 2.4. *Assume Hypothesis 1.2. Then we have*

$$\int_\Omega (5\frac{H^2}{\sqrt{g}} + \sqrt{g}H^2 - 2\frac{H}{g}(u_{xx}+u_{yy}))\,dz - \int_{\partial\Omega} H^2(x\nu_x + y\nu_y)\,d\omega = 0\ ,$$

with $\nu = (\nu_x, \nu_y)$ the exterior normal to the boundary.

Proof. We multiply (1.1) by $z\cdot\nabla u = xu_x + yu_y$ and integrate over Ω. We obtain three terms as in (2.1). Integrating by parts the first term we get

$$\begin{aligned}
&\int_\Omega (xu_x + yu_y)\Delta H\,dz \\
= &\int_\Omega \frac{xu_x + yu_y}{\sqrt{g}}\left(\partial_x\left(\frac{1}{\sqrt{g}}((1+u_y^2)H_x - u_xu_yH_y)\right)\right)\,dz \\
&+\int_\Omega \frac{xu_x + yu_y}{\sqrt{g}}\left(\partial_y\left(\frac{1}{\sqrt{g}}(-u_xu_yH_x + (1+u_x^2)H_y)\right)\right)\,dz \\
= &-\int_\Omega \frac{H_xu_x + H_yu_y}{g}\,dz - \int_\Omega \sqrt{g}(x\partial_xH^2 + y\partial_yH^2)\,dz \\
&+\int_\Omega \frac{xu_x + yu_y}{\sqrt{g}}\left(u_x\partial_xH^2 + u_y\partial_yH^2\right)\,dz \\
&-\int_\Omega \frac{H_x}{g}(yu_{xy} - xu_{yy})\,dz - \int_\Omega \frac{H_y}{g}(xu_{xy} - yu_{xx})\,dz\ .
\end{aligned}$$

Integrating once more by parts we get also some boundary terms

$$\begin{aligned}
&\int_\Omega (xu_x + yu_y)\Delta H\,dz \\
= &\ 5\int_\Omega \frac{H^2}{\sqrt{g}}\,dz + \int_\Omega \sqrt{g}H^2\,dz - 2\int_\Omega \frac{H}{g}(u_{xx}+u_{yy})\,dz \\
&-2\int_\Omega H^3(xu_x + yu_y)\,dz + 2\int_\Omega HK(xu_x + yu_y)\,dz \\
&-\int_{\partial\Omega}(x\nu_x + y\nu_y)H^2\,d\sigma - \int_{\partial\Omega} H\nu_x(yu_{xy} - xu_{yy})\,d\sigma \\
&-\int_{\partial\Omega} H\nu_y(xu_{xy} - yu_{xx})\,d\sigma\ ,
\end{aligned} \tag{2.2}$$

with ν the exterior normal to $\partial\Omega$. Here we also use that $g \equiv 1$ on $\partial\Omega$. We concentrate on the boundary terms. At the boundary, $u_{xx} = \nu_x^2 u_{\nu\nu}$, $u_{xy} = \nu_x\nu_y u_{\nu\nu}$ and $u_{yy} = \nu_y^2 u_{\nu\nu}$. Therefore,

$$\begin{aligned}
&-\int_{\partial\Omega}(x\nu_x + y\nu_y)H^2\,d\sigma \\
&-\int_{\partial\Omega} H(\nu_x(yu_{xy} - xu_{yy}) + \nu_y(xu_{xy} - yu_{xx}))\,d\sigma \\
= &-\int_{\partial\Omega}(x\nu_x + y\nu_y)H^2\,d\sigma \\
&-\int_{\partial\Omega} Hu_{\nu\nu}(y\nu_x^2\nu_y - x\nu_x\nu_y^2 + x\nu_x\nu_y^2 - y\nu_x^2\nu_y)\,d\sigma \\
= &-\int_{\partial\Omega} H^2(x\nu_x + y\nu_y)\,d\sigma\ .
\end{aligned}$$

From the equation above and (2.2) we get

$$\begin{aligned} 0 &= \int_\Omega (xu_x + yu_y)(\Delta H + 2H(H^2 - K))\, dz \\ &= 5\int_\Omega \frac{H^2}{\sqrt{g}}\, dz + \int_\Omega \sqrt{g} H^2\, dz - 2\int_\Omega \frac{H}{g}(u_{xx} + u_{yy})\, dz \\ &\quad - \int_{\partial\Omega} H^2(x\nu_x + y\nu_y)\, d\sigma\ . \end{aligned}$$

□

Proof of Proposition 2.1. Combining the results of Lemmas 2.3 and 2.4 we get

$$\int_{\partial\Omega} H^2(x\nu_x + y\nu_y)\, d\sigma = 0\,.$$

This yields $H = 0$ on $\partial\Omega$ since $u \in C^4(\overline{\Omega})$ and Ω is strictly starshaped. We have also $u_{\nu\nu} = 0$ on $\partial\Omega$ since $H = u_{\nu\nu}/2$ at the boundary. □

Since the Willmore equation is a fourth order elliptic p.d.e. the Dirichlet boundary conditions together with the information that also all the second derivatives of u vanish at the boundary is not sufficient to conclude that $u \equiv 0$ in Ω. We would also need that the third derivatives of u are zero at the boundary. Instead of this, in the next section we prove that u is identically zero using that the graph of u is a smooth Willmore surface with a boundary component made of umbilics.

Remark 2.5. *By integrating directly equation* (1.1) *over* Ω*, we get a third integral equation*

$$\int_{\partial\Omega} \nabla H \cdot \nu\, d\sigma = 0\,. \tag{2.3}$$

Unfortunately, in general from this integral equality does not follow $\nabla H = 0$ *on* $\partial\Omega$*. If* Ω *is a ball and* u *is rotationally symmetric, we infer from* (2.3) *that* $\nabla H = 0$ *on* $\partial\Omega$*. Together with* $H = 0$ *on* $\partial\Omega$ *this would imply* $H \equiv 0$ *in* Ω *and hence* $u \equiv 0$ *in* Ω*.*

3 Proof of the main result

In the previous section we have proved that all second order derivatives of u vanishes at the boundary. In particular, that the boundary of the surface given by the graph of u is made of umbilic points. Theorem 1.1 follows from this observation together with some deep results of Bryant. We present in the appendix a brief survey of the concepts and results we need.

Proof of Theorem 1.1. Let Φ denote the parametrisation of Γ given by the graph of u, i.e.

$$\Phi : \Omega \to \mathbb{R}^3, \quad (x, y) \mapsto (x, y, u(x, y)).$$

By the Riemann mapping theorem there exists a conformal map ψ from the unit disk $B_1(0) \subset \mathbb{R}^2$ into Ω such that $\psi(B_1(0)) = \Omega$. Moreover, by the regularity assumption on $\partial\Omega$, $\psi : \overline{B_1(0)} \to \bar{\Omega}$ is of class $C^{4,\alpha}$, the same regularity as $\partial\Omega$ as in Hypothesis 1.2(See [15, Theorem 3.6]).

Further, by the theorem on existence of conformal (or isothermal) coordinates (see [12, Theorem 9.3.1]) there exists $\xi : \overline{B_1(0)} \to \overline{B_1(0)}$ an homeomorphismus of class $C^{4,\alpha}$ up to the boundary such that

$$f : B_1(0) \to \mathbb{R}^3, \quad f := \Phi \circ \psi \circ \xi\,,$$

is a conformal parametrisation for $\Phi(\Omega)$.

Let (u, v) denote the coordinates in $B_1(0)$ and $z = u + iv$ be the associated complex structure. Let n denote a unit normal vector field on $\Phi(\Omega) = f(B_1(0))$. Let φ denote the Hopf differential associated to f, i.e.

$$\varphi = \frac{1}{2}((f_{uu}, n) - (f_{vv}, n) - 2i(f_{uv}, n)) = 2(f_{zz}, n)\,,$$

with $\partial_z = \frac{1}{2}(\partial_u - i\partial_v)$ and $\partial_{\bar z} = \frac{1}{2}(\partial_u + i\partial_v)$.

We first show that $\varphi = 0$ on $\partial B_1(0)$. From Corollary 2.2 it follows that $D^\alpha \Phi = 0$ on $\partial\Omega$ for all $\alpha \in \mathbb{N}_0^3$ with $|\alpha| = 2$. Therefore, $D^\alpha f \cdot n = 0$ on $\partial B_1(0)$ for all $\alpha \in \mathbb{N}_0^3$ with $|\alpha| = 2$ and, consequently, $\varphi = 0$ on $\partial B_1(0)$. In Proposition 2.1 we had already that also the mean curvature satisfies $H = 0$ on $\Phi(\partial\Omega) = f(\partial B_1(0))$. To prove the theorem we proceed now as in [14, page 1587].

Differentiating the Hopf differential and the mean curvature along the boundary $\partial B_1(0)$ in the tangential direction one finds $0 = \partial_\theta \varphi$ and $0 = \partial_\theta H$. Since $\partial_\theta = i(z\partial_z - \bar z \partial_{\bar z})$ we get

$$z\varphi_z = \bar z \varphi_{\bar z} \text{ and } zH_z = \bar z H_{\bar z} \text{ on } \partial B_1(0). \tag{3.1}$$

Let now q be defined by

$$q = \begin{cases} \frac{1}{4}\varphi^2(H^2 + \Delta \log \varphi) & \text{if } \varphi \neq 0\,, \\ -\varphi_z H_z & \text{if } \varphi = 0\,, \end{cases}$$

with $\Delta = \frac{1}{4}e^\mu \partial_z\partial_{\bar z}$ and e^μ the conformal factor (i.e. $e^\mu = 2f_z \cdot f_{\bar z} = f_u \cdot f_u = f_v \cdot f_v$). Since f is a Willmore immersion, q is a holomorphic function by Lemma B.4 and Proposition B.5 in the appendix. Since $\varphi = 0$ on $\partial B_1(0)$ using (3.1) we have

$$-q = \varphi_z H_z = z\bar z \varphi_z H_z = (\bar z)^2 \varphi_{\bar z} H_z \text{ on } \partial B_1(0)\,.$$

By the Codazzi equation $\varphi_{\bar z} = e^\mu H_z$ (see (B3) in the appendix) and using (3.1) we get

$$-q = (\bar z)^2 e^\mu H_z H_z = (\bar z)^3 e^\mu z H_z H_z = (\bar z)^4 e^\mu H_{\bar z} H_z \text{ on } \partial B_1(0)\,.$$

Hence, $z^4 q$ is a holomorphic function that is real valued on $\partial B_1(0)$. By the maximum principle, $z^4 q = a \in \mathbb{R}$ in $B_1(0)$. Since q is holomorphic, we get that necessarily $a = 0$ and hence $q \equiv 0$ in $B_1(0)$. By the classification theorem of Bryant (see Theorem C.3 in the appendix), it follows that $\Phi(\Omega) = f(B_1(0))$ is a piece of a sphere or, after a Möbius transformation, a piece of a minimal surface.

Due to the boundary conditions, the surface cannot be a piece of a proper sphere. Then, there exists a conformal transformation h in $\mathbb{R}^3$ such that $(h \circ \Phi)(\Omega)$ is a minimal surface with a boundary component made of umbilic points. Here we use that the set of umbilic points is a conformal invariant, see [2, page 32] or [11, Lemma P6.7]. Then, the Hopf differential of $(h \circ \Phi)(\Omega)$ is holomorphic, zero at the boundary and therefore it is identically zero. Here we use that the Hopf differential of surfaces with constant mean curvature is holomorphic (see (B3)). The claim follows. □

A The conformal Gauss map

The conformal Gauss map associates to each point of a two-dimensional surface its central sphere which can be considered as a point in the unit sphere $\mathbb{S}_1^4$ in the five dimensional Minkowski space. This map is important in the study of Willmore surfaces since by this transformation, a Willmore surface corresponds (away from its umbilic points) to a minimal surface in $\mathbb{S}_1^4$. This observation goes back to Thomsen, [19]. In this section we describe the geometric constructions that lead to the definition of the conformal Gauss map. We follow the presentation in [9].

Let $f : \Sigma \to \mathbb{R}^3$ be a smooth immersion of a two-dimensional orientable surface Σ. Let $n : \Sigma \to \mathbb{S}^2$ be a normal vectorfield. We consider the central sphere of f at $f(s)$, $s \in \Sigma$. This is the 2-dimensional sphere in $\mathbb{R}^3$ going through $f(s) \in \mathbb{R}^3$ and with mean curvature equal to the mean curvature of f in $f(s)$. We denote the central sphere by $S_r(p)$ with $r = r(s) \in \mathbb{R} \cup \{\pm\infty\}$ the 'radius' and $p = p(s) \in \mathbb{R}^3$ the center. If $H(s)$ denotes the mean curvature of f in $f(s)$, then $r = 1/H(s)$ and $p = f(s) + rn(s)$.

Let Φ denote the inverse of the stereographic projection into $\mathbb{R}^3$ given by $\Phi : \mathbb{R}^3 \to \mathbb{S}^3 \setminus \{(0,0,0,1)^t\}$ with

$$\Phi((y^1, y^2, y^3)^t) = \frac{1}{1 + \|y\|^2}(2y^1, 2y^2, 2y^3, \|y\|^2 - 1)^t .$$

Since Φ is conformal, $\Phi(S_r(p)) \subset \mathbb{S}^3$ is a two-dimensional sphere. There exists a unique three-dimensional sphere that intersects $\mathbb{S}^3$ orthogonally along $\Phi(S_r(p))$. We denote its center by $Z(\Phi(S_r(p)))$. In this way we get a mapping

$$\begin{aligned} f_1 : \Sigma &\to \mathbb{R}^4 \cup \{\infty\} , \\ s &\mapsto Z(\Phi(S_r(p))) = (2p, \|p\|^2 - r^2 - 1)\frac{1}{\|p\|^2 - r^2 + 1} , \end{aligned} \tag{A1}$$

where, as before, $r = r(s) = 1/H(s)$ and $p = p(s) = f(s) + rn(s) \in \mathbb{R}^3$. Here $\| \cdot \|$ is the Euclidean norm in $\mathbb{R}^3$. (For this formula it is convenient to see Φ as the restriction to $\mathbb{R}^3$ of $G : \mathbb{R}^4 \to \mathbb{R}^4$ with G the inversion with respect to the 3-sphere of radius $\sqrt{2}$ and center $(0,0,0,1)^t$. If $\Phi(S_r(p))$ is an equatorial sphere in $\mathbb{S}^3$, then $f_1(s) = \infty$. This is the case if $\|p\|^2 + 1 = r^2$.)

Notice that in (A1) we write a vector in $\mathbb{R}^4$ via two components. The first is a vector in $\mathbb{R}^3$, while the second is a real number. Similarly, in the following we write elements in $\mathbb{R}^5$ via three components. The first is a vector in $\mathbb{R}^3$, while the other two components are real numbers. The formulas become nicer with this convention.

Now, to take care of the points sent to ∞, we look at $\mathbb{R}^4$ as the subset $\{[y, 1] : y \in \mathbb{R}^4\}$ of $\mathbb{RP}^4$. We get then the map

$$\begin{aligned} f_2 : \Sigma &\to \mathbb{RP}^4 , \\ s &\mapsto \big[p, \tfrac{1}{2}(\|p\|^2 - r^2 - 1), \tfrac{1}{2}(\|p\|^2 - r^2 + 1)\big] . \end{aligned}$$

As a final step we consider as a target $\mathbb{R}^5$ with the Lorentzian metric

$$g(X, Y) = \sum_{i=1}^{4} X^i Y^i - X^5 Y^5 , \quad X, Y \in \mathbb{R}^5, \tag{A2}$$

signature $(+, +, +, +, -)$, and the map

$$\begin{aligned} Y : \Sigma &\to (\mathbb{R}^5, g) , \\ s &\mapsto \frac{1}{r}\big(p, \tfrac{1}{2}(\|p\|^2 - r^2 - 1), \tfrac{1}{2}(\|p\|^2 - r^2 + 1)\big) . \end{aligned}$$

This is the conformal Gauss map associated to $f : \Sigma \to \mathbb{R}^3$. The normalisation factor $1/r$ is chosen in such a way that

$$Y(\Sigma) \subset \mathbb{S}^4_1 := \{Y \in (\mathbb{R}^5, g) : g(Y, Y) = 1\} ,$$

i.e. the image of Y is a subset of the unit sphere in $(\mathbb{R}^5, g)$. Since $r = r(s) = 1/H(s)$ and $p = p(s) = f(s) + rn(s)$ we have

$$\begin{aligned} Y(s) &= H(s)\left(f(s), \frac{1}{2}(\|f(s)\|^2 - 1), \frac{1}{2}(\|f(s)\|^2 + 1)\right) \\ &\quad + (n(s), (f(s), n(s)), (f(s), n(s)))\ , \end{aligned}$$

with $(\cdot,\cdot)$ the Euclidean scalar product in $\mathbb{R}^3$. It is convenient to write the conformal Gauss map as

$$\begin{aligned} s &\mapsto Y(s) = H(s)X(s) + T(s) \quad \text{with} \\ X(s) &= \left(f(s), \frac{1}{2}(\|f(s)\|^2 - 1), \frac{1}{2}(\|f(s)\|^2 + 1)\right) \\ \text{and } T(s) &= (n(s), (f(s), n(s)), (f(s), n(s)))\ . \end{aligned} \tag{A3}$$

Notice that $g(X(s), X(s)) = 0$ while $g(T(s), T(s)) = 1$.

We will see in the next section that the conformal Gauss map is (indeed) conformal with degeneracies at the umbilic points of Σ. Further, we study the properties of the conformal Gauss map associated to a Willmore surface.

Remark A.1. Notice that if $f : \Sigma \to \mathbb{R}^3$ is a sphere than the image of the associated conformal Gauss map is a fixed point in $\mathbb{S}^4_1$.

Remark A.2. The name conformal Gauss map has been used by Bryant. Thomsen in [19] used instead the concept of sphere congruence. A *sphere congruence* is a smooth mapping $S : \Sigma \to \{\text{spheres in } \mathbb{R}^3\}$ with Σ a two-dimensional manifold. This mapping induces a new mapping $Y : \Sigma \to \mathbb{S}^4_1$ which assigns to each sphere in $\mathbb{R}^3$ a point in $\mathbb{S}^4_1$ with the same construction as above. That is, to a sphere in $\mathbb{R}^3$ with center p and radius r we associate the vector

$$\frac{1}{r}(p, \frac{1}{2}(\|p\|^2 - r^2 - 1), \frac{1}{2}(\|p\|^2 - r^2 + 1)) \in \mathbb{R}^5\,. \tag{A4}$$

In the same way we may associate to points in $\mathbb{R}^3$ a vector in $\mathbb{R}^5$. Renormalizing (A4) by multiplying it by r and taking $r \to 0$ we see that

$$\mathbb{R}^3 \ni x \mapsto X = (x, \frac{1}{2}(\|x\|^2 - 1), \frac{1}{2}(\|x\|^2 + 1)) \in \mathbb{R}^5\,. \tag{A5}$$

Notice that the images of points in $\mathbb{R}^3$ are $X \in L$ with $L := \{X \in \mathbb{R}^5 \text{ such that } g(X, X) = 0 \text{ and } X^5 - X^4 = 1\}$. The mapping given in (A5) is an isometry from $\mathbb{R}^3$ to L.

We need also the concept of *enveloping surface* of a sphere congruence S. This is a map $f : \Sigma \to \mathbb{R}^3$ such that for all $s \in \Sigma$ it holds

$$f(s) \in S(s) \ \text{ and } \ df(s)(T_s\Sigma) \subset T_{f(s)}S(s)\,. \tag{A6}$$

Equivalent relations may be stated in $(\mathbb{R}^5, g)$. Indeed, denoting by $X(s)$ the representative in $\mathbb{R}^5$ of $f(s)$ according to (A5), the formulas in (A6) are equivalent to

$$g(X(s), Y(s)) = 0 \ \text{ and } \ g(X(s), dY(s)) = 0\,. \tag{A7}$$

In the proof of the classification theorem of Bryant in Appendix 4 we will see that if f is a Willmore surface and a certain holomorphic differential is identically zero, then f is an enveloping surface for its own conformal Gauss map.

For more informations on sphere congruence and conditions on the existence of a enveloping surface we refer to [11] and the references therein.

B A holomorphic differential for Willmore surfaces

The results we collect here are due to Thomsen [19] and Bryant [2]. We follow the presentation in [9].

Let $f : \Sigma \to \mathbb{R}^3$ (with the standard scalar product) be a smooth immersion of an orientable surface. We have thus fixed a conformal structure on Σ. Locally there exists conformal coordinates. Let denote this conformal coordinates by u and v. We associate a complex coordinate to this conformal structure by considering $z = u + iv$. The first fundamental form of f is given by $I = e^{\mu} dz d\bar{z}$ with e^{μ} the conformal factor. Let n be a unit normal field along the surface. For the second fundamental form we have the representation

$$II = \mathrm{Re}\{\varphi dz^2 + He^{\mu} dz d\bar{z}\}$$

with H the mean curvature of f, e^{μ} the conformal factor and φ the Hopf differential given by

$$\varphi = \frac{1}{2}((f_{uu}, n) - (f_{vv}, n) - 2i(f_{uv}, n)) = 2(f_{zz}, n)\,. \tag{B1}$$

Notice that $\partial_z = \frac{1}{2}(\partial_u - i\partial_v)$ and $\partial_{\bar{z}} = \frac{1}{2}(\partial_u + i\partial_v)$.

We also have

$$\begin{aligned} f_{zz} = \mu_z f_z + \tfrac{1}{2}\varphi n\,, \quad f_{z\bar{z}} = \tfrac{1}{2} He^{\mu} n\,, \\ \text{and} \quad n_z = -Hf_z - \varphi e^{-\mu} f_{\bar{z}}\,, \end{aligned} \tag{B2}$$

and the integrability conditions

$$\begin{aligned} \varphi_{\bar{z}} &= e^{\mu} H_z \quad \text{(Equation of Codazzi)}, \\ |\varphi|^2 e^{-2\mu} &= H^2 - K \quad \text{(Equation of Gauss)}, \end{aligned} \tag{B3}$$

with K the Gaussian curvature of f.

With the same choice of complex coordinate, we find for the conformal Gauss map associated to f as given in (A3) that

$$\begin{aligned} & Y_z = H_z X - \varphi e^{-\mu} X_{\bar{z}}, \\ & g(Y_z, Y_z) = 0 \text{ and } g(Y_z, Y_{\bar{z}}) = (H^2 - K)(f_z, f_{\bar{z}})\,, \end{aligned} \tag{B4}$$

with g the metric given in (A2). Here we have used the formula for n_z in (B2) and (B3). The induced metric is given by $ds_Y^2 = (H^2 - K) ds_f^2$. Thus Y is a conformal map (with degeneracies at the umbilic points of f) with respect to the conformal structure induced on Σ by f and an immersion away from the umbilic points of f.

For Willmore immersions (i.e. solutions to (1.1)) the formulas in (B4) imply immediately the following.

Proposition B.1. *Let $f : \Sigma \to \mathbb{R}^3$ be a Willmore surface and $Y : \Sigma \to \mathbb{S}^4_1$ be the conformal Gauss map associated to f. Then,*

$$Area(Y) = \int_\Sigma ds_Y^2 = \int_\Sigma (H^2 - K)\, ds_f^2\,.$$

Moreover, if Y is a minimal surface, then $f : \Sigma \to \mathbb{R}^3$ is a Willmore immersion.

Remark B.2. We call Willmore surface a solution to equation (1.1). Notice that these are also critical points for the functional $\int (H^2 - K)\, dS$ with respect to interior variations. In our setting, $\int K\, dS$ is equal to a constant. See the discussion in the introduction.

Further, the converse of Proposition B.1 is also true.

Proposition B.3. *An immersion $f : \Sigma \to \mathbb{R}^3$ is a Willmore immersion if and only if the associated conformal Gauss map is an harmonic map.*

Idea of the proof. One first shows that

$$\Delta Y + 2(H^2 - K)Y = (\Delta H + 2(H^2 - K)H)X\,. \tag{B5}$$

with X as defined in (A3). Since $Y \in \mathbb{S}^4_1$, Y is normal to $\mathbb{S}^4_1$ and therefore taking the tangential component in (B5) we find

$$(\Delta Y)^{TQ} = [(\Delta H + 2(H^2 - K)H)X]^{TQ}\,.$$

If f is Willmore, we directly get $(\Delta Y)^{TQ} = 0$ and so Y is a harmonic map. On the other hand if Y is an harmonic map, Y is a critical point for the Dirichlet energy. Being Y conformal, it is also a critical point for the area functional. Proposition B.1 yields that f is a Willmore immersion. □

We consider now the quartic differential

$$Q: \quad g(Y_{zz}, Y_{zz})dz^4\,.$$

Lemma B.4. *The quartic differential $g(Y_{zz}, Y_{zz})dz^4$ can be written as qdz^4 with*

$$q = \begin{cases} \frac{1}{4}\varphi^2(H^2 + \Delta_f \log\varphi) & \text{where } \varphi \neq 0\,, \\ -\varphi_z H_z & \text{where } \varphi = 0, \end{cases}$$

with $\Delta_f = 4e^{-\mu}\partial_z\partial_{\bar z}$ and φ the Hopf differential given in (B1)*.*

Proof. Starting from the formula for Y_z given in (B4) and differentiating it once again we find

$$Y_{zz} = H_{zz}X + H_z X_z - (\varphi e^{-\mu})_z X_{\bar z} - \varphi e^{-\mu} X_{z\bar z}\,. \tag{B6}$$

For the last term starting from the formula for X given in (A3) and using (B2) one gets

$$X_{z\bar z} = \frac{1}{2}He^{\mu}T + \frac{e^{\mu}}{2}(0,1,1)\,. \tag{B7}$$

Using that $g(X,X) = 0$, $g(X,X_z) = 0$, $g(X_z,X_z) = 0$, $g(X_z,X_{\bar z}) = \frac{1}{2}e^{\mu}$, $g(X,T) = 0$ and $g(X_z,T) = 0$, formulas (B6) and (B7) yield

$$g(Y_{zz}, Y_{zz}) = \varphi H_{zz} - H_z(\varphi e^{-\mu})_z e^{\mu} + \frac{1}{4}H^2\varphi^2\,.$$

The claim follows using the equation of Codazzi (B3). □

Proposition B.5. *If $f : \Sigma \to \mathbb{R}^3$ is a Willmore surface, then Q is a holomorphic quartic differential.*

Proof. Let $Y : M \to \mathbb{S}^4_1$ be the conformal Gauss map associated to f. Recalling (B4) we have

$$g(Y_z, Y_z) = 0 \quad\text{and}\quad g(Y_z, Y_{\bar z}) = \frac{1}{2}(H^2 - K)e^{\mu}\,.$$

Let α denote the second fundamental form of Y, i.e. $\alpha_{ij} = (Y_{ij})^{\perp}$ and η denote the mean curvature vector, i.e.

$$\eta = \frac{\alpha_{11} + \alpha_{22}}{2E} \quad\text{with}\quad E = (H^2 - K)e^{\mu}\,.$$

Being f a Willmore immersion, Proposition B.3 gives us that Y is an harmonic map. On the other hand,

$$Y_{z\bar z} = \frac{1}{2}E\eta$$

and so we get that the mean curvature vector η is normal to $\mathbb{S}^4_1 \subset \mathbb{R}^5$. Since $\mathbb{S}^4_1$ is the unit sphere in $(\mathbb{R}^5, g)$, $\eta = \beta Y$ for some $\beta \in \mathbb{R}$ and, by a direct computation, one finds $\eta = -Y$. Therefore, we have

$$Y_{z\bar{z}} = -\frac{1}{2} E Y \,.$$

This is the crucial information for showing that Q is holomorphic. Indeed,

$$\begin{aligned} \partial_{\bar{z}} g(Y_{zz}, Y_{zz}) &= 2g((Y_{z\bar{z}})_z, Y_{zz}) \\ &= -E_z g(Y, Y_{zz}) - E g(Y_z, Y_{zz}) = 0 \,, \end{aligned}$$

since $g(Y, Y_z) = 0$ and $g(Y_z, Y_z) = 0$. □

C The classification theorem of Bryant

We follow once again the presentation in [9].

Let $f : \Sigma \to \mathbb{R}^3$ be a Willmore surface that is not totally umbilic. By Theorem C in [2] the set of umbilic points of f is closed and it has no interior. Let $\Sigma \setminus \Sigma'$ be the preimages of the umbilic points of f. Eschenburg, Tribuzy [10] prove that one can smoothly define on each point of $Y(\Sigma)$ the tangent space. More precisely, the map $\Sigma' \ni s \mapsto dY_s(T_s\Sigma)$ can be smoothly extended to all of Σ. Therefore the normal bundle is defined everywhere. The induced metric on the normal bundle has signature $(+,-)$ and so we may find two real normal vectors N_1 and N_2 such that

$$g(N_i, N_i) = 0 \,,\; i = 1, 2, \text{ and } g(N_1, N_2) = 1 \,. \tag{C1}$$

Lemma C.1. *One has*

$$\begin{aligned} g(Y_{zz}, Y_{zz}) &= 2g(Y_{zz}, N_1) g(Y_{zz}, N_2) \,, \\ \textit{and } \partial_{\bar{z}} g(Y_{zz}, N_i) &= (-1)^{i-1} g(N_{1,\bar{z}}, N_2) g(Y_{zz}, N_i) \,, \end{aligned} \tag{C2}$$

for $i = 1, 2$.

Proof. Since $g(Y_z, Y) = 0$ and $g(Y_z, Y_z) = 0$ one sees that Y_{zz} lies in the span of Y_z, N_1 and N_2. The first claim follows from (B4) and (C1).

For the second equality one first notices that

$$\partial_{\bar{z}} g(Y_{zz}, N_i) = g(Y_{zz}, N_{i,\bar{z}}) \,,$$

and that $N_{i,\bar{z}}$ lies in the span of Y_z and N_i. □

Notice that this lemma gives another proof of Proposition B.5. The next result gives a crucial observation for the proof of Bryant's classification theorem.

Proposition C.2. *If* $g(Y_{zz}, Y_{zz}) \equiv 0$*, then* $g(Y_{zz}, N_j) \equiv 0$ *and* $N_{jz} = \lambda(z) N_j$ *for* $j = 1$ *or* 2 *and some scalar function* λ*.*

Proof. Since the functions $g(Y_{zz}, N_j)$ satisfy the differential equation given in (C2) and $g(N_{1,\bar{z}}, N_2)$ is bounded on compact subsets of Σ, it follows from Carleman's theorem [5] that each $g(Y_{zz}, N_j)$ has isolated zeroes or it is identically zero. Therefore from the first equality in Lemma C.1 and $g(Y_{zz}, Y_{zz}) \equiv 0$, we infer that $g(Y_{zz}, N_j) \equiv 0$ for $j = 1$ or 2. This implies that $g(Y_z, N_{j,z}) = 0$. Further, $g(Y, N_{j,z}) = 0$, $g(N_{j,z}, Y_{\bar{z}}) = 0$ and $g(N_j, N_{j,z}) = 0$. The claim follows. □

We are now ready to state the classification theorem of Bryant.

Theorem C.3.(Bryant classification theorem) *Let $f : \Sigma \to \mathbb{R}^3$ be a Willmore immersion and $Y : \Sigma \to \mathbb{S}^4_1$ the associated conformal Gauss map. Assume further that $g(Y_{zz}, Y_{zz}) \equiv 0$. Then f is either totally umbilic or f is the Möbius transform of a minimal immersion.*

Proof. If f is not totally umbilic, by the discussion at the beginning of the section we have two real normal vectors N_1 and N_2 such that $g(N_i, N_i) = 0$, $g(N_i, Y) = 0$, $g(N_i, Y_z) = 0 = g(N_i, Y_{\bar{z}})$, for $i = 1, 2$, and $g(N_1, N_2) = 1$. According to the definition given in Remark 5.2 and the characterisation in (A7) $[N_1]$ and $[N_2]$ ($[N_i] \in \mathbb{RP}^4$) are enveloping surfaces for the conformal Gauss map associated to f. Even more, we may choose

$$N_1(s) = X(s) = (f(s), \frac{1}{2}(\|f(s)\|^2 - 1), \frac{1}{2}(\|f(s)\|^2 + 1)) .$$

That is, one of the enveloping surfaces is the Willmore immersion itself. The other normal direction $N_2 = \hat{X}$ is called the conformal transform of X.

Since $g(Y_{zz}, Y_{zz}) \equiv 0$, $N_{2,z} = \lambda(z) N_2$ by Proposition C.2. This differential equation and the fact that N_2 is a real vector imply that $[N_2]$ is a well defined fixed vector. Therefore $[N_2] = [\hat{X}]$ can be identified with a point in $\mathbb{S}^3$ and as such it is the image of a fixed point $\hat{x}$ in $\mathbb{R}^3 \cup \{\infty\}$. Via an inversion h in $\mathbb{R}^3$ we can send $\hat{x}$ to infinity. Accordingly all the spheres that passes through $\hat{x}$ are sent to planes. These planes are, by construction, the central spheres of the immersion $h \circ f : \Sigma \to \mathbb{R}^3$. Therefore $h \circ f$ is a minimal immersion. □

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Part 2

Hartree-Fock theory of pseudo-relativistic atoms

This part consists of the following three papers.

- A. Dall'Acqua, T. Østergaard Sørensen, E. Stockmeyer, Hartree-Fock theory for pseudorelativistic atoms, *Ann. Henri Poincaré* **9** (2008), no. 4, 711–742.
- A. Dall'Acqua, S. Fournais, T. Østergaard Sørensen, E. Stockmeyer, Real Analyticity away from the nucleus of pseudorelativistic Hartree-Fock orbitals, Preprint Nr. 9/2011, Universität Magdeburg, submitted.
- A. Dall'Acqua, J.P. Solovej, Excess charge for pseudo-relativistic atoms in Hartree-Fock theory, *Doc. Math.* **15** (2010) 285–345.

Hartree-Fock theory for pseudorelativistic atoms[1]

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Abstract

We study the Hartree-Fock model for pseudorelativistic atoms, that is, atoms where the kinetic energy of the electrons is given by the pseudorelativistic operator $\sqrt{(|\mathbf{p}|c)^2 + (mc^2)^2} - mc^2$. We prove the existence of a Hartree-Fock minimizer, and prove regularity away from the nucleus and pointwise exponential decay of the corresponding orbitals.

1 Introduction and results

We consider a model for an atom with N electrons and nuclear charge Z, where the kinetic energy of the electrons is described by the expression $\sqrt{(|\mathbf{p}|c)^2 + (mc^2)^2} - mc^2$. This model takes into account some (kinematic) relativistic effects; in units where $\hbar = e = m = 1$, the Hamiltonian becomes

$$\begin{aligned} H = H_{\mathrm{rel}}(N, Z, \alpha) &= \sum_{j=1}^{N} \Big\{ \sqrt{-\alpha^{-2}\Delta_j + \alpha^{-4}} - \alpha^{-2} - \frac{Z}{|\mathbf{x}_j|} \Big\} + \sum_{1 \le i < j \le N} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|} \\ &= \sum_{j=1}^{N} \alpha^{-1} \Big\{ T(-\mathrm{i}\nabla_j) - V(\mathbf{x}_j) \Big\} + \sum_{1 \le i < j \le N} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|}\,, \end{aligned} \tag{1}$$

with $T(\mathbf{p}) = E(\mathbf{p}) - \alpha^{-1} = \sqrt{|\mathbf{p}|^2 + \alpha^{-2}} - \alpha^{-1}$ and $V(\mathbf{x}) = Z\alpha/|\mathbf{x}|$. Here, α is Sommerfeld's fine structure constant; physically, $\alpha \simeq 1/137.036$.

The operator H acts on a dense subspace of the N-particle Hilbert space $\mathcal{H}_F = \wedge_{i=1}^{N} L^2(\mathbb{R}^3; \mathbb{C}^q)$ of antisymmetric functions, where q is the number of spin states. It is bounded from below on this subspace (more details below).

The *(quantum) ground state energy* is the infimum of the spectrum of H considered as an operator acting on $\mathcal{H}_F$:

$$E^{\mathrm{QM}}(N, Z, \alpha) := \inf \sigma_{\mathcal{H}_F}(H) = \inf\{\, \mathfrak{q}(\Psi, \Psi) \,|\, \Psi \in \mathcal{Q}(H), \langle \Psi, \Psi \rangle = 1 \}\,,$$

where $\mathfrak{q}$ is the quadratic form defined by H, and $\mathcal{Q}$ the corresponding form domain (see below); $\langle\ ,\ \rangle$ is the scalar product in $\mathcal{H}_F \subset L^2(\mathbb{R}^{3N}; \mathbb{C}^{q^N})$.

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In the Hartree-Fock approximation, instead of minimizing the functional $\mathfrak{q}$ in the entire N-particle space $\mathcal{H}_F$, one restricts to wavefunctions Ψ which are pure wedge products, also called Slater determinants:

$$\Psi(\mathbf{x}_1,\sigma_1;\mathbf{x}_2,\sigma_2;\ldots;\mathbf{x}_N,\sigma_N) = \frac{1}{\sqrt{N!}}\,\det(u_i(\mathbf{x}_j,\sigma_j))_{i,j=1}^N\,, \tag{2}$$

with $\{u_i\}_{i=1}^N$ orthonormal in $L^2(\mathbb{R}^3;\mathbb{C}^q)$ (called *orbitals*). Notice that this way, $\Psi\in\mathcal{H}_F$ and $\|\Psi\|_{L^2(\mathbb{R}^{3N};\mathbb{C}^{q^N})}=1$.

The *Hartree-Fock ground state energy* is the infimum of the quadratic form $\mathfrak{q}$ defined by H over such Slater determinants:

$$E^{\mathrm{HF}}(N,Z,\alpha) := \inf\{\,\mathfrak{q}(\Psi,\Psi)\,|\,\Psi \text{ Slater determinant}\}\,. \tag{3}$$

For the non-relativistic Hamiltonian,

$$H_{\mathrm{cl}}(N,Z)=\sum_{j=1}^N\Big\{-\frac{1}{2}\Delta_j-\frac{Z}{|\mathbf{x}_j|}\Big\}+\sum_{1\le i<j\le N}\frac{1}{|\mathbf{x}_i-\mathbf{x}_j|}\,, \tag{4}$$

the mathematical theory of this approximation has been much studied, the groundbreaking work being that of Lieb and Simon [19]; see also [21] for work on excited states. For a comprehensive discussion of Hartree-Fock (and other) approximations in quantum chemistry, and an extensive literature list, we refer to [16].

The aim of the present paper is to study the Hartree-Fock approximation for the pseudorelativistic operator H in (1).

We turn to the precise description of the problem. The one-particle operator $h_0=T(-\mathrm{i}\nabla)-V(\mathbf{x})$ is bounded from below (by $\alpha^{-1}[(1-(\pi Z\alpha/2)^2)^{1/2}-1]$) if and only if $Z\alpha\le 2/\pi$ (see [13], [15, 5.33 p. 307], and [33]; we shall have nothing further to say on the critical case $Z\alpha=2/\pi$). More precisely, if $Z\alpha<1/2$, then V is a small *operator* pertubation of T. In fact [13, Theorem 2.1 c)], $\big\||\mathbf{x}|^{-1}(T(-\mathrm{i}\nabla)+1)^{-1}\big\|_{\mathcal{B}(L^2(\mathbb{R}^3))}=2$. As a consequence, h_0 is selfadjoint with $\mathcal{D}(h_0)=H^1(\mathbb{R}^3;\mathbb{C}^q)$ when $Z\alpha<1/2$. It is essentially selfadjoint on $C_0^\infty(\mathbb{R}^3;\mathbb{C}^q)$ when $Z\alpha\le 1/2$.

If, on the other hand, $1/2\le Z\alpha<2/\pi$, then V is only a small *form* pertubation of T: Indeed [15, 5.33 p. 307],

$$\int_{\mathbb{R}^3}\frac{|f(\mathbf{x})|^2}{|\mathbf{x}|}\,d\mathbf{x}\le\frac{\pi}{2}\int_{\mathbb{R}^3}|\mathbf{p}||\hat f(\mathbf{p})|^2\,d\mathbf{p}\ \text{ for }\ f\in H^{1/2}(\mathbb{R}^3)\,, \tag{5}$$

where $\hat f$ denotes the Fourier transform of f. Hence, the quadratic form $\mathfrak{v}$ given by

$$\mathfrak{v}[u,v]:=(V^{1/2}u,V^{1/2}v)\ \text{ for }\ u,v\in H^{1/2}(\mathbb{R}^3;\mathbb{C}^q) \tag{6}$$

(multiplication by $V^{1/2}$ in each component) is well defined (for all values of $Z\alpha$). Here, $(\ ,\ )$ denotes the scalar product in $L^2(\mathbb{R}^3;\mathbb{C}^q)$. Let $\mathfrak{e}$ be the quadratic form with domain $H^{1/2}(\mathbb{R}^3;\mathbb{C}^q)$ given by

$$\mathfrak{e}[u,v]:=(E(\mathbf{p})^{1/2}u,E(\mathbf{p})^{1/2}v)\ \text{ for }\ u,v\in H^{1/2}(\mathbb{R}^3;\mathbb{C}^q)\,. \tag{7}$$

By abuse of notation, we write $E(\mathbf{p})$ for the (strictly positive) operator $E(-\mathrm{i}\nabla)=\sqrt{-\Delta+\alpha^{-2}}$. Then, using (5) and that $|\mathbf{p}|\le E(\mathbf{p})$,

$$\mathfrak{v}[u,u]<\mathfrak{e}[u,u]\ \text{ for }\ u\in H^{1/2}(\mathbb{R}^3;\mathbb{C}^q)\ \text{ if }\ Z\alpha<2/\pi\,. \tag{8}$$

Hence, by the KLMN theorem [25, Theorem X.17], there exists a unique self-adjoint operator h_0 whose quadratic form domain is $H^{1/2}(\mathbb{R}^3;\mathbb{C}^q)$ such that (with $\mathfrak{t} = \mathfrak{e} - \alpha^{-1}$)

$$(u, h_0 v) = \mathfrak{t}[u,v] - \mathfrak{v}[u,v] \quad \text{for} \quad u, v \in H^{1/2}(\mathbb{R}^3;\mathbb{C}^q)\,, \tag{9}$$

and h_0 is bounded below by $-\alpha^{-1}$. Moreover, if $Z\alpha < 2/\pi$ then the spectrum of h_0 is discrete in $[-\alpha^{-1}, 0)$ and absolutely continuous in $[0,\infty)$ [13, Theorems 2.2 and 2.3].

As for the N-particle operator in (1), when $Z\alpha < 2/\pi$, (5) implies that the quadratic form

$$\mathfrak{q}(\Psi,\Phi) = \sum_{j=1}^{N} \Big\{ \langle\, E(\mathbf{p}_j)^{1/2}\Psi, E(\mathbf{p}_j)^{1/2}\Phi\,\rangle - \alpha^{-1}\langle \Psi,\Phi\rangle - \langle\, V(\mathbf{x}_j)^{1/2}\Psi, V(\mathbf{x}_j)^{1/2}\Phi\,\rangle \Big\}$$

$$+ \sum_{1\le i<j\le N} \langle\, |\mathbf{x}_i - \mathbf{x}_j|^{-1/2}\Psi, |\mathbf{x}_i - \mathbf{x}_j|^{-1/2}\Phi\rangle\;, \quad \Psi,\Phi \in \bigwedge_{i=1}^{N} H^{1/2}(\mathbb{R}^3;\mathbb{C}^q)\,,$$

is well-defined, closed, and bounded from below. The operator H can then be defined as the corresponding (unique) self-adjoint operator. It satisfies

$$\bigwedge_{i=1}^{N} H^{1}(\mathbb{R}^3;\mathbb{C}^q) \subset \mathcal{D}(H) \subset \mathcal{Q}(H) = \bigwedge_{i=1}^{N} H^{1/2}(\mathbb{R}^3;\mathbb{C}^q)\,,$$
$$\mathfrak{q}(\Psi,\Phi) = \langle \Psi, H\Phi\rangle\,, \quad \Phi \in \mathcal{D}(H)\,, \quad \Psi \in \mathcal{Q}(H)\,.$$

For $Z\alpha < 1/2$, $\mathcal{D}(H) = \wedge_{i=1}^{N} H^1(\mathbb{R}^3;\mathbb{C}^q)$. All this follows from (the statements and proofs of) [25, Theorem X.17] and [24, Theorem VIII.15]. See [20] for further references on H. We shall not have anything further to say on H in this paper, however, but will only study the Hartree-Fock problem mentioned above. We now discuss this in more detail.

It is convenient to use the one-to-one correspondence between Slater determinants and projections onto finite dimensional subspaces of $L^2(\mathbb{R}^3;\mathbb{C}^q)$. Indeed, if Ψ is given by (2) with $\{u_i\}_{i=1}^N \subset H^{1/2}(\mathbb{R}^3;\mathbb{C}^q)$, orthonormal in $L^2(\mathbb{R}^3;\mathbb{C}^q)$, and γ is the projection onto the subspace spanned by $u_1,\ldots,u_N$, then the kernel of γ is given by

$$\gamma(\mathbf{x},\sigma;\mathbf{y},\tau) = \sum_{j=1}^{N} u_j(\mathbf{x},\sigma)\overline{u_j(\mathbf{y},\tau)}\,. \tag{10}$$

Let $\rho_\gamma \in L^1(\mathbb{R}^3)$ denote the 1-particle density associated to γ given by

$$\rho_\gamma(\mathbf{x}) = \sum_{\sigma=1}^{q} \gamma(\mathbf{x},\sigma;\mathbf{x},\sigma) = \sum_{\sigma=1}^{q}\sum_{j=1}^{N} |u_j(\mathbf{x},\sigma)|^2\,.$$

Then the energy expectation of Ψ depends only on γ, more precisely,

$$\mathfrak{q}(\Psi,\Psi) = \langle \Psi, H\Psi\rangle = \mathcal{E}^{\mathrm{HF}}(\gamma)\,,$$

where $\mathcal{E}^{\mathrm{HF}}$ is the Hartree-Fock energy functional defined by

$$\mathcal{E}^{\mathrm{HF}}(\gamma) = \alpha^{-1}\big\{\operatorname{Tr}[E(\mathbf{p})\gamma] - \alpha^{-1}\operatorname{Tr}[\gamma] - \operatorname{Tr}[V\gamma]\big\} + \mathcal{D}(\gamma) - \mathcal{E}x(\gamma)\,. \tag{11}$$

Here,

$$\operatorname{Tr}[E(\mathbf{p})\gamma] := \sum_{j=1}^{N} \mathfrak{e}[u_j,u_j]\;, \quad \operatorname{Tr}[V\gamma] := \sum_{j=1}^{N} \mathfrak{v}[u_j,u_j] = Z\alpha \int_{\mathbb{R}^3} \frac{\rho_\gamma(\mathbf{x})}{|\mathbf{x}|}\,d\mathbf{x}\,,$$

$\mathcal{D}(\gamma)$ is the *direct* Coulomb energy,

$$\mathcal{D}(\gamma) = \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\rho_\gamma(\mathbf{x})\rho_\gamma(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}\,d\mathbf{y}\,, \tag{12}$$

and $\mathcal{E}x(\gamma)$ is the *exchange* Coulomb energy,

$$\mathcal{E}x(\gamma) = \frac{1}{2}\sum_{\sigma,\tau=1}^{q}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|\gamma(\mathbf{x},\sigma;\mathbf{y},\tau)|^2}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}\,d\mathbf{y}\,.$$

This way,

$$\begin{aligned} E^{\mathrm{HF}}(N,Z,\alpha) &= \inf\{\,\mathcal{E}^{\mathrm{HF}}(\gamma)\,|\,\gamma\in\mathcal{P}\,\}\,, \\ \mathcal{P} &= \{\gamma: L^2(\mathbb{R}^3;\mathbb{C}^q)\to L^2(\mathbb{R}^3;\mathbb{C}^q)\,|\,\gamma \text{ projection onto } \mathrm{span}\{u_1,\dots,u_N\}, \\ &\qquad\qquad u_i\in H^{1/2}(\mathbb{R}^3;\mathbb{C}^q), (u_i,u_j)=\delta_{i,j}\}\,. \end{aligned} \tag{13}$$

(Notice that if one of the orbitals u_i of γ is not in $H^{1/2}(\mathbb{R}^3;\mathbb{C}^q)$, then $\mathcal{E}^{\mathrm{HF}}(\gamma) = +\infty$ (since $Z\alpha < 2/\pi$).)

We now extend the definition of the Hartree-Fock energy functional $\mathcal{E}^{\mathrm{HF}}$, in order to turn the minimization problem (13) (that is, (3)) into a convex problem.

A *density matrix* $\gamma : L^2(\mathbb{R}^3;\mathbb{C}^q)\to L^2(\mathbb{R}^3;\mathbb{C}^q)$ is a self-adjoint trace class operator that satisfies the operator inequality $0\le\gamma\le\mathrm{Id}$. A density matrix γ has the integral kernel

$$\gamma(\mathbf{x},\sigma;\mathbf{y},\tau) = \sum_j \lambda_j u_j(\mathbf{x},\sigma)\overline{u_j(\mathbf{y},\tau)}\,, \tag{14}$$

where λ_j, u_j are the eigenvalues and corresponding eigenfunctions of γ. We choose the u_j's to be orthonormal in $L^2(\mathbb{R}^3;\mathbb{C}^q)$. As before, let $\rho_\gamma\in L^1(\mathbb{R}^3)$ denote the 1-particle density associated to γ given by

$$\rho_\gamma(\mathbf{x}) = \sum_{\sigma=1}^{q}\sum_j \lambda_j\,|u_j(\mathbf{x},\sigma)|^2\,. \tag{15}$$

Define

$$\mathcal{A} := \big\{\gamma \text{ density matrix}\;\big|\;\mathrm{Tr}\,\big[E(\mathbf{p})\gamma\big] < +\infty\,\big\}\,, \tag{16}$$

where, by definition, for γ written as in (14),

$$\mathrm{Tr}[E(\mathbf{p})\gamma] := \sum_j \lambda_j\mathfrak{e}[u_j,u_j]\,. \tag{17}$$

Notice that if $\gamma\in\mathcal{A}$ then all the terms in $\mathcal{E}^{\mathrm{HF}}(\gamma)$ (see (11)) are finite. Indeed, for $\gamma\in\mathcal{A}$ and written as in (14),

$$\mathrm{Tr}[V\gamma] := \sum_j \lambda_j\mathfrak{v}[u_j,u_j] = Z\alpha\int_{\mathbb{R}^3}\frac{\rho_\gamma(\mathbf{x})}{|\mathbf{x}|}\,d\mathbf{x} \tag{18}$$

is finite, due to (8). In particular,

$$u_j\in H^{1/2}(\mathbb{R}^3;\mathbb{C}^q)\subset L^3(\mathbb{R}^3;\mathbb{C}^q)\,, \tag{19}$$

the last inclusion by Sobolev's inequality [18, Theorem 8.4].

On the other hand, if $\gamma \in \mathcal{A}$ then

$$\rho_\gamma \in L^1(\mathbb{R}^3) \cap L^{4/3}(\mathbb{R}^3)\,. \tag{20}$$

This follows from Daubechies' inequality, see [6, pp. 519–520]. By Hölder's inquality, $\rho_\gamma \in L^{6/5}(\mathbb{R}^3)$. The Hardy-Littlewood-Sobolev inequality [18, Theorem 4.3] then implies that $\mathcal{D}(\gamma)$ (see (12)) is finite. Finally, $\mathcal{E}x(\gamma) \leq \mathcal{D}(\gamma)$, since

$$\begin{aligned}&\mathcal{D}(\gamma) - \mathcal{E}x(\gamma)\\ &\quad= \frac{1}{2}\sum_{i,j} \lambda_i\lambda_j \sum_{\sigma,\tau=1}^{q} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|u_i(\mathbf{x},\sigma)u_j(\mathbf{y},\tau) - u_j(\mathbf{x},\sigma)u_i(\mathbf{y},\tau)|^2}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}d\mathbf{y} \geq 0\,.\end{aligned}$$

Therefore, $\mathcal{E}^{\mathrm{HF}}$ defined by (11) extends to $\gamma \in \mathcal{A}$. This way, with h_0 defined as in (9),

$$\mathrm{Tr}[h_0\gamma] = \mathrm{Tr}[E(\mathbf{p})\gamma] - \alpha^{-1}\,\mathrm{Tr}[\gamma] - \mathrm{Tr}[V\gamma]\,,$$

and so

$$\mathcal{E}^{\mathrm{HF}}(\gamma) = \alpha^{-1}\,\mathrm{Tr}[h_0\gamma] + \mathcal{D}(\gamma) - \mathcal{E}x(\gamma)\,,\ \gamma \in \mathcal{A}\,. \tag{21}$$

Consider $\gamma \in \mathcal{A}$ and define, with ρ_γ as in (15),

$$R_\gamma(\mathbf{x}) := \int_{\mathbb{R}^3} \frac{\rho_\gamma(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{y}\,. \tag{22}$$

We have that

$$R_\gamma \in L^\infty(\mathbb{R}^3) \cap L^3(\mathbb{R}^3)\,. \tag{23}$$

This follows from (8) (for L^∞), and (20) and the weak Young inequality [18, p. 107] (for L^3). Next, define the operator K_γ with integral kernel

$$K_\gamma(\mathbf{x},\sigma;\mathbf{y},\tau) := \frac{\gamma(\mathbf{x},\sigma;\mathbf{y},\tau)}{|\mathbf{x}-\mathbf{y}|}\,. \tag{24}$$

The operator K_γ is Hilbert-Schmidt; we prove this fact in Lemma 2 below.

Note that, using (14) and the Cauchy-Schwarz inequality, $(u, R_\gamma u) \geq (u, K_\gamma u)$ (multiplication by R_γ is in each component). Denote by $\mathfrak{b}_\gamma$ the (non-negative) quadratic form given by

$$\mathfrak{b}_\gamma[u,v] := \alpha(u, R_\gamma v) - \alpha(u, K_\gamma v) \quad \text{for} \quad u,v \in H^{1/2}(\mathbb{R}^3;\mathbb{C}^q)\,.$$

Then, using $(u, K_\gamma u) \geq 0$ and (8),

$$0 \leq \mathfrak{b}_\gamma[u,u] \leq \alpha(u, R_\gamma u) = \alpha \sum_{\sigma=1}^{q} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\rho_\gamma(\mathbf{y})|u(\mathbf{x},\sigma)|^2}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}\,d\mathbf{y} \leq \alpha\frac{2}{\pi}\,\mathrm{Tr}[\gamma]\,\mathfrak{e}[u,u]\,.$$

Therefore (by the statements and proofs of [25, Theorem X.17] and [24, Theorem VIII.15]), there exists a unique self-adjoint operator h_γ (called the *Hartree-Fock operator associated to* γ), which is bounded below (by $-\alpha^{-1}$), with quadratic form domain $H^{1/2}(\mathbb{R}^3;\mathbb{C}^q)$ and such that

$$(u, h_\gamma v) = \mathfrak{t}[u,v] - \mathfrak{v}[u,v] + \mathfrak{b}_\gamma[u,v] \quad \text{for} \quad u,v \in H^{1/2}(\mathbb{R}^3;\mathbb{C}^q)\,. \tag{25}$$

The operator h_γ has infinitely many eigenvalues in $[-\alpha^{-1}, 0)$ (when $N < Z$), and $\sigma_{\mathrm{ess}}(h_\gamma) = [0,\infty)$; both of these facts will be proved in Lemma 2 below.

The main result of this paper is the following theorem.

Theorem 1. *Let $Z\alpha < 2/\pi$, and let $N \geq 2$ be a positive integer such that $N < Z+1$. Then there exists an N-dimensional projection $\gamma^{\mathrm{HF}} = \gamma^{\mathrm{HF}}(N,Z,\alpha)$ minimizing the Hartree-Fock energy functional $\mathcal{E}^{\mathrm{HF}}$ given by* (11)*, that is, $E^{\mathrm{HF}}(N,Z,\alpha)$ in* (13) *(and therefore, in* (3)*) is attained. In fact,*

$$\begin{aligned}\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) = E^{\mathrm{HF}}(N,Z,\alpha) &= \inf\left\{\mathcal{E}^{\mathrm{HF}}(\gamma)\,\middle|\,\gamma\in\mathcal{A}, \gamma^2=\gamma, \mathrm{Tr}[\gamma]=N\right\}\\ &= \inf\left\{\mathcal{E}^{\mathrm{HF}}(\gamma)\,\middle|\,\gamma\in\mathcal{A},\ \ \mathrm{Tr}[\gamma]=N\right\}\\ &= \inf\left\{\mathcal{E}^{\mathrm{HF}}(\gamma)\,\middle|\,\gamma\in\mathcal{A},\ \ \mathrm{Tr}[\gamma]\leq N\right\}.\end{aligned} \tag{26}$$

Moreover, one can write

$$\gamma^{\mathrm{HF}}(\mathbf{x},\sigma;\mathbf{y},\tau) = \sum_{i=1}^{N}\varphi_i(\mathbf{x},\sigma)\overline{\varphi_i(\mathbf{y},\tau)}\,, \tag{27}$$

with $\varphi_i \in H^{1/2}(\mathbb{R}^3;\mathbb{C}^q), i=1,\dots,N$, ortnonormal, such that the Hartree-Fock orbitals $\{\varphi_i\}_{i=1}^N$ *satisfy:*

(i) *With $h_{\gamma^{\mathrm{HF}}}$ as defined in* (25)*,*

$$h_{\gamma^{\mathrm{HF}}}\varphi_i = \varepsilon_i\varphi_i\ ,\ i=1,\dots,N\,, \tag{28}$$

with $0 > \varepsilon_N \geq \ldots \geq \varepsilon_1 > -\alpha^{-1}$ the N lowest eigenvalues of $h_{\gamma^{\mathrm{HF}}}$.

(ii) *For $i=1,\dots,N$,*

$$\varphi_i \in C^\infty(\mathbb{R}^3\setminus\{0\};\mathbb{C}^q)\,. \tag{29}$$

(iii) *For all $R>0$ and $\beta < \nu_{\varepsilon_N} := \sqrt{-\varepsilon_N(2\alpha^{-1}+\varepsilon_N)}$, there exists $C=C(R,\beta)>0$ such that for $i=1,\dots,N$,*

$$|\varphi_i(\mathbf{x})| \leq C\,e^{-\beta|\mathbf{x}|} \quad \text{for} \quad |\mathbf{x}|\geq R\,. \tag{30}$$

Remark 1.

(i) *In fact, we prove that* (29) *holds for* any *eigenfunction φ of $h_{\gamma^{\mathrm{HF}}}$, and* (30) *for those corresponding to negative eigenvalues ε. More precisely, if $h_{\gamma^{\mathrm{HF}}}\varphi = \varepsilon\varphi$ for some $\varepsilon\in[\varepsilon_N,0)$, then* (30) *holds for φ for all $\beta<\nu_\varepsilon := \sqrt{-\varepsilon(2\alpha^{-1}+\varepsilon)}$ for some $C=C(R,\beta)>0$.*

(ii) *Note that, in general, eigenfunctions of $h_{\gamma^{\mathrm{HF}}}$ can be unbounded at $\mathbf{x}=0$; therefore* (29) *and* (30) *can only be expected to hold away from the origin.*

(iii) *Both the regularity and the exponential decay above are similar to the results in the non-relativistic case (i.e., for the operator in* (4)*; see [19]). However, the proof of Theorem 1 is considerably more complicated due to, on one hand, the non-locality of the kinetic energy operator $E(\mathbf{p})$, and, on the other hand, the fact that the Hartree-Fock operator $h_{\gamma^{\mathrm{HF}}}$ is only given as a* form *sum for $Z\alpha\in[1/2,2/\pi)$.*

(iv) *We show the existence of the Hartree-Fock minimizer by solving the minimization problem on the set of density matrices. This method was introduced in [30]. The same method was used in [5] in the Dirac-Fock case (see Remark 2 below).*

(v) *Notice that nothing is known on the question of uniqueness of the minimizer of the Hartree-Fock functional defined on density matrices (up to the trivial invariance properties of the HartreeFock energy functional) [16]. The Hartree-Fock functional is not convex. This is a major difference compared to the reduced (restricted) HartreeFock theory. The reduced HartreeFock functional has no exchange term and so the uniqueness of the minimizer is assured by the convexity of the functional; see [30].*

(vi) *For any eigenfunction of the HartreeFock operator that is orthogonal to the HartreeFock orbitals $\varphi_1, \ldots, \varphi_N$ the corresponding eigenvalue ε satisfies $\varepsilon > \varepsilon_i$, $i = 1, \ldots, N$. In other words, there are no unfilled shells. This follows from the result in [4] since the only crucial assumption is that the two-body interaction is repulsive (i.e., positive definite). The particular choice of the one-particle operator does not play any role.*

(vii) *As mentioned earlier, we have to assume that $Z\alpha < 2/\pi$; the reason is that our proof that $\mathrm{Tr}[E(\mathbf{p})\gamma_n]$ is uniformly bounded for a minimizing sequence $\{\gamma_n\}_{n\in\mathbb{N}}$ does not work in the critical case $Z\alpha = 2/\pi$.*

(viii) *For simplicity of notation, we give the proof of Theorem 1 only in the spinless case. It will be obvious that the proof also works in the general case.*

(ix) *As will be clear from the proofs, the statements of Theorem 1 (appropriately modified) also hold for molecules. More explicitely, for a molecule with K nuclei of charges $Z_1, \ldots, Z_K$, fixed at $R_1, \ldots, R_K \in \mathbb{R}^3$, replace $\mathfrak{v}$ in (6) by*

$$\mathfrak{v}[u, v] := \sum_{k=1}^{K} (V_k^{1/2} u, V_k^{1/2} v) \quad \text{for} \quad u, v \in H^{1/2}(\mathbb{R}^3; \mathbb{C}^q)\,, \tag{31}$$

with $V_k(\mathbf{x}) = Z_k\alpha/|\mathbf{x} - R_k|$, $Z_k\alpha < 2/\pi$. Then, for $N < 1 + \sum_{k=1}^{K} Z_k$, there exists a Hartree-Fock minimizer, and the corresponding Hartree-Fock orbitals have the regularity and decay properties as stated in Theorem 1, away from each nucleus.

Remark 2. *In our model the kinetic energy of the (relativistic) electrons is given by a non-local operator. Another choice would be to consider the Dirac operator: $D_0 = \boldsymbol{\alpha} \cdot (i\nabla) + \boldsymbol{\beta}\alpha^{-1}$ with $\boldsymbol{\alpha} = (\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \boldsymbol{\alpha}_3), \boldsymbol{\beta}$ the Dirac matrices (α is still the fine structure constant); see [32]. The Dirac operator is local but it has a negative continuous spectrum which is not bounded from below. The analogue of the HartreeFock approximation in this model is called the Dirac-Fock model. Esteban and Séré in [7] proved that the Dirac-Fock functional has infinitely many critical points, giving rise to infinitely many solutions to the Dirac-Fock equations; see also [23]. In this model the rigorous definition of a ground state is a delicate problem since the energy functional is not bounded from below; see [8, 9]. Nevertheless, there are HartreeFock-type models, coming from the Dirac operator, that do have a minimizer. We refer to [5, 11, 12], and the references therein, for the description of these models.*

2 Proof of Theorem 1

2.1 Existence of the Hartree-Fock minimizer

The proof of the existence of an N-dimensional projection γ^{HF} minimizing $\mathcal{E}^{\mathrm{HF}}$, the equalities in (26), and that the corresponding Hartree-Fock orbitals $\{\varphi_i\}_{i=1}^N$ solve the Hartree-Fock equations (28), will be a consequence of the following two lemmas.

Lemma 1. *Let $Z\alpha < 2/\pi$ and $N \in \mathbb{N}$. Then*

$$E_{\leq}^{\mathrm{HF}}(N, Z, \alpha) := \inf \left\{ \mathcal{E}^{\mathrm{HF}}(\gamma) \,\middle|\, \gamma \in \mathcal{A}, \mathrm{Tr}[\gamma] \leq N \right\}$$

is attained.

Lemma 2. *Let $\gamma \in \mathcal{A}$. Then the operator K_γ, defined by (24), is Hilbert-Schmidt. If $Z\alpha < 2/\pi$ then the operator h_γ, defined in (25), satisfies $\sigma_{\mathrm{ess}}(h_\gamma) = [0, \infty)$. If furthermore $\mathrm{Tr}[\gamma] < Z$, then h_γ has infinitely many eigenvalues in $[-\alpha^{-1}, 0)$.*

Before proving these two lemmas, we use them to prove the parts of Theorem 1 mentioned above.

Proof. For computational reasons we first state and prove a lemma in the spirit of [3, Lemma 1].

Lemma 3. *Let $\gamma \in \mathcal{A}$, $u_1, u_2 \in H^{1/2}(\mathbb{R}^3)$, and let $\epsilon_1, \epsilon_2 \in \mathbb{R}$ be such that $\tilde{\gamma}$ given by*

$$\tilde{\gamma}(\mathbf{x}, \mathbf{y}) := \gamma(\mathbf{x}, \mathbf{y}) + \gamma_u(\mathbf{x}, \mathbf{y}) \,, \tag{32}$$

$$\gamma_u(\mathbf{x}, \mathbf{y}) := \gamma_{u_1,u_2}(\mathbf{x}, \mathbf{y}) = \epsilon_1 u_1(\mathbf{x}) \overline{u_1(\mathbf{y})} + \epsilon_2 u_2(\mathbf{x}) \overline{u_2(\mathbf{y})} \tag{33}$$

is again an element of $\mathcal{A}$.

Then we have that

$$\mathcal{E}^{\mathrm{HF}}(\tilde{\gamma}) = \mathcal{E}^{\mathrm{HF}}(\gamma) + \alpha^{-1}\epsilon_1 (u_1, h_\gamma u_1) + \alpha^{-1}\epsilon_2 (u_2, h_\gamma u_2) + \epsilon_1\epsilon_2 R_u \,, \tag{34}$$

where h_γ is given in (25), and

$$R_u := R_{u_1,u_2} = \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|u_1(\mathbf{x}) u_2(\mathbf{y}) - u_2(\mathbf{x}) u_1(\mathbf{y})|^2}{|\mathbf{x} - \mathbf{y}|} \, d\mathbf{x} d\mathbf{y} \,. \tag{35}$$

Proof of Lemma 3. We have that

$$\begin{aligned}
\mathcal{E}^{\mathrm{HF}}(\tilde{\gamma}) &= \mathcal{E}^{\mathrm{HF}}(\gamma) + \alpha^{-1} \mathrm{Tr}[h_0 \gamma_u] + \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho_\gamma(\mathbf{x}) \rho_{\gamma_u}(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|} \, d\mathbf{x} d\mathbf{y} \\
&\quad - \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\gamma(\mathbf{x}, \mathbf{y}) \overline{\gamma_u(\mathbf{x}, \mathbf{y})}}{|\mathbf{x} - \mathbf{y}|} \, d\mathbf{x} d\mathbf{y} + \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho_{\gamma_u}(\mathbf{x}) \rho_{\gamma_u}(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|} \, d\mathbf{x} d\mathbf{y} \\
&\quad - \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\gamma_u(\mathbf{x}, \mathbf{y}) \overline{\gamma_u(\mathbf{x}, \mathbf{y})}}{|\mathbf{x} - \mathbf{y}|} \, d\mathbf{x} d\mathbf{y} \\
&= \mathcal{E}^{\mathrm{HF}}(\gamma) + \alpha^{-1}\epsilon_1 (u_1, h_\gamma u_1) + \alpha^{-1}\epsilon_2 (u_2, h_\gamma u_2) \\
&\quad + \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho_{\gamma_u}(\mathbf{x}) \rho_{\gamma_u}(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|} \, d\mathbf{x} d\mathbf{y} - \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\gamma_u(\mathbf{x}, \mathbf{y}) \overline{\gamma_u(\mathbf{x}, \mathbf{y})}}{|\mathbf{x} - \mathbf{y}|} \, d\mathbf{x} d\mathbf{y} \,.
\end{aligned} \tag{36}$$

Using (33), that $\rho_{\gamma_u}(\mathbf{x}) = \epsilon_1 |u_1(\mathbf{x})|^2 + \epsilon_2 |u_2(\mathbf{x})|^2$, and (35), we obtain (34). □

By Lemma 1 a minimizer $\gamma^{\mathrm{HF}} \in \mathcal{A}$, with $\mathrm{Tr}[\gamma^{\mathrm{HF}}] \leq N$, exists. We may write

$$\gamma^{\mathrm{HF}}(\mathbf{x}, \mathbf{y}) = \sum_k \lambda_k \varphi_k(\mathbf{x}) \overline{\varphi_k(\mathbf{y})} \,, \tag{37}$$

with $1 \geq \lambda_1 \geq \cdots \geq 0$ and $\{\varphi_k\}_k \subset H^{1/2}(\mathbb{R}^3)$ an orthonormal (in $L^2(\mathbb{R}^3)$) system (it might be finite). Extend $\{\varphi_k\}_k$ to an orthonormal basis $\{\varphi_k\}_k \cup \{u_\ell\}_{\ell \in \mathbb{N}}$ for $L^2(\mathbb{R}^3)$, with $u_\ell \in H^{1/2}(\mathbb{R}^3)$.

Let $K+1$ be the first index such that $\lambda_{K+1} < 1$. Fix $j \in \{1, \ldots, K\}$, choose $u \in \{\varphi_k\}_{k \geq K+1} \cup \{u_\ell\}_{\ell \in \mathbb{N}}$, and consider, for ϵ to be chosen,

$$\gamma_\epsilon^{(j)}(\mathbf{x}, \mathbf{y}) := \sum_{k \neq j} \lambda_k \varphi_k(\mathbf{x}) \varphi_k^*(\mathbf{y}) + \frac{1}{1 + m\epsilon^2} \big(\varphi_j(\mathbf{x}) + \epsilon u(\mathbf{x})\big) \big(\overline{\varphi_j(\mathbf{y})} + \epsilon \overline{u(\mathbf{y})} \big) .$$

Choosing $m \geq 1$ assures that $\mathrm{Tr}[\gamma_\epsilon^{(j)}] \leq N$. Then $0 \leq \gamma_\epsilon^{(j)} \leq \mathrm{Id}$ for $|\epsilon|$ small enough (depending on u). Since γ^{HF} minimizes $\mathcal{E}^{\mathrm{HF}}$, and $\gamma_0^{(j)} = \gamma^{\mathrm{HF}}$,

$$0 = \frac{d}{d\epsilon} (\mathcal{E}^{\mathrm{HF}}) \big(\gamma_\epsilon^{(j)}\big) \bigg|_{\epsilon = 0} = \alpha^{-1} (\varphi_j, h_{\gamma^{\mathrm{HF}}} u) + \alpha^{-1} (u, h_{\gamma^{\mathrm{HF}}} \varphi_j) .$$

Repeating the computation for iu we get that $(u, h_{\gamma^{\mathrm{HF}}} \varphi_j) = 0$, from which it follows that $h_{\gamma^{\mathrm{HF}}}$ maps $\mathrm{span}\{\varphi_1, \ldots, \varphi_K\}$ into itself. Diagonalising the restriction of $h_{\gamma^{\mathrm{HF}}}$ to $\mathrm{span}\{\varphi_1, \ldots, \varphi_K\}$, we can choose $\varphi_1, \ldots, \varphi_K$ to be eigenfunctions of $h_{\gamma^{\mathrm{HF}}}$ with eigenvalues $\varepsilon_{n_1}, \ldots, \varepsilon_{n_K}$, $n_j \in \mathbb{N}$ (numbering the eigenvalues of $h_{\gamma^{\mathrm{HF}}}$ in increasing order, $-\alpha^{-1} < \varepsilon_1 \leq \varepsilon_2 \leq \cdots$). Since $\lambda_1 = \cdots = \lambda_K = 1$, this does not change (37).

To show that, for $j > K$, φ_j is also an eigenfunction of $h_{\gamma^{\mathrm{HF}}}$ (corresponding to an eigenvalue ε_{n_j}) one repeats the argument above, with $u \in \{\varphi_k\}_{k \neq 1, \ldots, K, j} \cup \{u_\ell\}_{\ell \in \mathbb{N}}$, and

$$\gamma_\epsilon^{(j)}(\mathbf{x}, \mathbf{y}) = \sum_{k \neq j} \lambda_k \varphi_k(\mathbf{x}) \overline{\varphi_k(\mathbf{y})} + \frac{\lambda_j}{1 + m\epsilon^2} \big(\varphi_j(\mathbf{x}) + \epsilon u(\mathbf{x})\big) \big(\overline{\varphi_j(\mathbf{y})} + \epsilon \overline{u(\mathbf{y})} \big) .$$

Moreover, the eigenvalues ε_{n_k} (of $h_{\gamma^{\mathrm{HF}}}$) corresponding to the eigenfunctions φ_k are non-positive. In fact, if $\varepsilon_{n_k} > 0$, then we could lower the energy: Define $\tilde{\gamma}(\mathbf{x}, \mathbf{y}) = \gamma^{\mathrm{HF}}(\mathbf{x}, \mathbf{y}) - \lambda_k \varphi_k(\mathbf{x}) \overline{\varphi_k(\mathbf{y})}$, then, using Lemma 3, we get that $\mathcal{E}^{\mathrm{HF}}(\tilde{\gamma}) = \mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) - \alpha^{-1} \lambda_k \varepsilon_{n_k} < \mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}})$.

It remains to show that $\mathrm{Tr}[\gamma^{\mathrm{HF}}] = N$, that γ^{HF} is a projection, and that the $\{\varphi_j\}_{j=1}^N$ are eigenfunctions corresponding to the *lowest* (negative) eigenvalues of $h_{\gamma^{\mathrm{HF}}}$ (that is, to $\varepsilon_1 \leq \varepsilon_2 \leq \cdots \leq \varepsilon_N < 0$).

Consider first the case $N < Z$. Assume, for contradiction, that $\mathrm{Tr}[\gamma^{\mathrm{HF}}] < N$. Let $K \in \mathbb{N}$ be the multiplicity of the eigenvalue 1 in (37). Since (by Lemma 2), for $N < Z$, $h_{\gamma^{\mathrm{HF}}}$ has infinitely many eigenvalues in $[-\alpha^{-1}, 0)$ we can find a (normalized) eigenfunction u, corresponding to a negative eigenvalue of $h_{\gamma^{\mathrm{HF}}}$, and orthogonal to $\varphi_1, \ldots, \varphi_K$. Let $\epsilon > 0$ be sufficiently small that $\gamma(\mathbf{x}, \mathbf{y}) := \gamma^{\mathrm{HF}}(\mathbf{x}, \mathbf{y}) + \epsilon u(\mathbf{x}) \overline{u(\mathbf{y})}$ defines a density matrix satisfying $\mathrm{Tr}[\gamma] \leq N$. By Lemma 3 (with $u_1 = u, \epsilon_1 = \epsilon$ and $\epsilon_2 = 0$) we get that

$$\mathcal{E}^{\mathrm{HF}}(\gamma) = \mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) + \epsilon \alpha^{-1} (u, h_{\gamma^{\mathrm{HF}}} u) < \mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) , \tag{38}$$

leading to a contradiction. Hence, $\mathrm{Tr}[\gamma^{\mathrm{HF}}] = N$. That γ^{HF} is a projection follows from Lieb's Variational Principle (see [17]) which we prove for completeness. If this is not the case, there exist indices p, q such that $0 < \lambda_p, \lambda_q < 1$. Consider $\tilde{\gamma}(\mathbf{x}, \mathbf{y}) := \gamma^{\mathrm{HF}}(\mathbf{x}, \mathbf{y}) + \epsilon \varphi_q(\mathbf{x}) \overline{\varphi_q(\mathbf{y})} - \epsilon \varphi_p(\mathbf{x}) \overline{\varphi_p(\mathbf{y})}$ with ϵ such that $0 \leq \tilde{\gamma} \leq \mathrm{Id}$. Choose $\epsilon > 0$ if $\varepsilon_{n_q} \leq \varepsilon_{n_p}$ and $\epsilon < 0$ otherwise. By Lemma 3, we get that $\mathcal{E}^{\mathrm{HF}}(\tilde{\gamma}) < \mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}})$.

Consider now the case $Z \leq N < Z + 1$ (and $N \geq 2$), so that $N - 1 < Z$. Let $\gamma_{N-1}^{\mathrm{HF}}$ denote the density matrix where

$$\inf \big\{ \mathcal{E}^{\mathrm{HF}}(\gamma) \,\big|\, \gamma \in \mathcal{A},\ \mathrm{Tr}[\gamma] \leq N - 1 \big\}$$

is attained. By the above, $\mathrm{Tr}[\gamma_{N-1}^{\mathrm{HF}}] = N - 1$ and $\gamma_{N-1}^{\mathrm{HF}}$ is a projection, so its integral kernel is given by

$$\gamma_{N-1}^{\mathrm{HF}}(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^{N-1} \phi_i(\mathbf{x}) \overline{\phi_i(\mathbf{y})} ,$$

where the ϕ_i's are eigenfunctions of $h_{\gamma_{N-1}^{\mathrm{HF}}}$.

We first prove that

$$\inf\left\{\mathcal{E}^{\mathrm{HF}}(\gamma)\,\middle|\,\gamma\in\mathcal{A},\ \ \mathrm{Tr}[\gamma]\le N\right\} \tag{39}$$

is not attained at the density matrix $\gamma_{N-1}^{\mathrm{HF}}$ by constructing a density matrix $\tilde{\gamma}$ with $\mathrm{Tr}[\tilde{\gamma}]\le N$ such that $\mathcal{E}^{\mathrm{HF}}(\tilde{\gamma})<\mathcal{E}^{\mathrm{HF}}(\gamma_{N-1}^{\mathrm{HF}})$. Indeed, since $h_{\gamma_{N-1}^{\mathrm{HF}}}$ has infinitely many strictly negative eigenvalues (by Lemma 2; $N-1<Z$) there exists a (normalized) eigenfunction u of $h_{\gamma_{N-1}^{\mathrm{HF}}}$ corresponding to a negative eigenvalue, and orthogonal to $\mathrm{span}\{\phi_1,\dots,\phi_{N-1}\}$. Let $\tilde{\gamma}$ be defined by

$$\tilde{\gamma}(\mathbf{x},\mathbf{y})=\gamma_{N-1}^{\mathrm{HF}}(\mathbf{x},\mathbf{y})+u(\mathbf{x})\overline{u(\mathbf{y})}\,.$$

Then $\mathrm{Tr}[\tilde{\gamma}]=N$ and, by a computation like in (38),

$$\mathcal{E}^{\mathrm{HF}}(\tilde{\gamma})=\mathcal{E}^{\mathrm{HF}}(\gamma_{N-1}^{\mathrm{HF}})+\alpha^{-1}(u,h_{\gamma_{N-1}^{\mathrm{HF}}}u)<\mathcal{E}^{\mathrm{HF}}(\gamma_{N-1}^{\mathrm{HF}})\,.$$

Hence,

$$\inf\left\{\mathcal{E}^{\mathrm{HF}}(\gamma)\,\middle|\,\gamma\in\mathcal{A},\mathrm{Tr}[\gamma]\le N\right\}<\inf\left\{\mathcal{E}^{\mathrm{HF}}(\gamma)\,\middle|\,\gamma\in\mathcal{A},\mathrm{Tr}[\gamma]\le N-1\right\}. \tag{40}$$

Let γ_N be a density matrix where (39) is attained (the existence of such a minimizer follows, as before, from Lemma 1). By the above it follows that $N-1<\mathrm{Tr}[\gamma_N]\le N$. We now show that there exists a minimizer γ^{HF} with $\mathrm{Tr}[\gamma^{\mathrm{HF}}]=N$.

The integral kernel of γ_N is given by

$$\gamma_N(\mathbf{x},\mathbf{y})=\sum_j\lambda_j\varphi_j(\mathbf{x})\overline{\varphi_j(\mathbf{y})}\,,$$

where $1\ge\lambda_1\ge\cdots\ge 0$ and the φ_j's are (orthonormal) eigenfunctions of h_{γ_N}. If $\mathrm{Tr}[\gamma_N]<N$ we can define a new density matrix $\tilde{\gamma}$ with $\mathrm{Tr}[\tilde{\gamma}]\le N$ and $\mathcal{E}^{\mathrm{HF}}(\tilde{\gamma})\le\mathcal{E}^{\mathrm{HF}}(\gamma_N)$. Indeed, if $\mathrm{Tr}[\gamma_N]<N$ (and bigger than $N-1$) then there exists a (first) j_0 such that $0<\lambda_{j_0}<1$. We define $\tilde{\gamma}$ with integral kernel

$$\tilde{\gamma}(\mathbf{x},\mathbf{y})=\gamma_N(\mathbf{x},\mathbf{y})+r\varphi_{j_0}(\mathbf{x})\overline{\varphi_{j_0}(\mathbf{y})}\,, \tag{41}$$

with $r=\min\{1-\lambda_{j_0},N-\mathrm{Tr}[\gamma_N]\}>0$. Recall that $h_{\gamma_N}\varphi_j=\varepsilon_{n_j}\varphi_j$, $\varepsilon_{n_j}\le 0$, for all j. By Lemma 3 we have that

$$\mathcal{E}^{\mathrm{HF}}(\tilde{\gamma})=\mathcal{E}^{\mathrm{HF}}(\gamma_N)+\alpha^{-1}r\varepsilon_{n_{j_0}}\,.$$

If $\varepsilon_{n_{j_0}}<0$, it follows that $\mathcal{E}^{\mathrm{HF}}(\tilde{\gamma})<\mathcal{E}^{\mathrm{HF}}(\gamma_N)$. On the other hand, if $\varepsilon_{n_{j_0}}=0$, then $\mathcal{E}^{\mathrm{HF}}(\tilde{\gamma})=\mathcal{E}^{\mathrm{HF}}(\gamma_N)$, and $\mathrm{Tr}[\gamma_N]<\mathrm{Tr}[\tilde{\gamma}]\le N$. Either $\mathrm{Tr}[\tilde{\gamma}]=N$, in which case we let $\gamma^{\mathrm{HF}}:=\tilde{\gamma}$, and, as above, we are done. Or, we repeat all of the above argument on

$$\tilde{\gamma}(\mathbf{x},\mathbf{y})=\sum_{j=1}^{j_0}\varphi_j(\mathbf{x})\overline{\varphi_j(\mathbf{y})}+\sum_{j>j_0}\lambda_j\varphi_j(\mathbf{x})\overline{\varphi_j(\mathbf{y})}\,.$$

Since the trace stays bounded by N, this procedure has to stop eventually. Hence, with γ^{HF} the resulting density matrix, $\mathrm{Tr}[\gamma^{\mathrm{HF}}]=N$ and by Lieb's Variational Principle it follows (as above) that γ^{HF} is a projection.

Finally, let $\{\varphi_j\}$ be the eigenfunctions of $h_{\gamma^{\mathrm{HF}}}$, now numbered corresponding to the eigenvalues $\varepsilon_1\le\varepsilon_2\le\cdots$, where ε_1 is the lowest eigenvalue of $h_{\gamma^{\mathrm{HF}}}$. We know that, for some $j_1,\dots,j_N\in\mathbb{N}$,

$$\gamma^{\mathrm{HF}}(\mathbf{x},\mathbf{y})=\sum_{k=1}^{N}\varphi_{j_k}(\mathbf{x})\overline{\varphi_{j_k}(\mathbf{y})}\,.$$

Suppose for contradiction that $\{\varepsilon_{j_1}, \ldots, \varepsilon_{j_N}\} \neq \{\varepsilon_1, \ldots, \varepsilon_N\}$. Then there exists a $k \in \{1, \ldots, N\}$ with $\varepsilon_{j_k} > \varepsilon_k$. For $\delta \in (0,1)$ define

$$\tilde{\gamma}(\mathbf{x}, \mathbf{y}) = \gamma^{\mathrm{HF}}(\mathbf{x}, \mathbf{y}) + \delta\varphi_k(\mathbf{x})\overline{\varphi_k(\mathbf{y})} - \delta\varphi_{j_k}(\mathbf{x})\overline{\varphi_{j_k}(\mathbf{y})}\,.$$

By Lemma 3,

$$\mathcal{E}^{\mathrm{HF}}(\tilde{\gamma}) = \mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) + \delta\alpha^{-1}(\varepsilon_k - \varepsilon_{j_k}) - \delta^2 R_{\varphi_j, \varphi_{j_k}} < \mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}})\,,$$

where the last inequality follows by choosing δ small enough.

It remains to prove that $\varepsilon_1, \ldots, \varepsilon_N$ are strictly negative. For $N < Z$ this follows directly from Lemma 2. In the case $Z \leq N < Z + 1$, assume, for contradiction, that $\varepsilon_N = 0$; then the density matrix

$$\tilde{\gamma}(\mathbf{x}, \mathbf{y}) := \gamma^{\mathrm{HF}}(\mathbf{x}, \mathbf{y}) - \varphi_N(\mathbf{x})\overline{\varphi_N(\mathbf{y})}$$

satisfies $\mathcal{E}^{\mathrm{HF}}(\tilde{\gamma}) = \mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}})$ (by Lemma 3) and $\mathrm{Tr}[\tilde{\gamma}] = N - 1$. This is a contradiction to (40).

This finishes the proof of the first part of Theorem 1. □

It remains to prove Lemma 1 and Lemma 2.

Proof of Lemma 1. We minimize on density matrices following the method in [30]. In the pseudorelativistic context one faces the problem that the Coulomb potential is not relatively compact with respect to the kinetic energy. This problem has been adressed in [5] and we follow the idea therein.

The quantity $E^{\mathrm{HF}}_{\leq}(N, Z, \alpha)$ is finite since for any density matrix γ, with $\mathrm{Tr}[\gamma] \leq N$,

$$\mathcal{E}^{\mathrm{HF}}(\gamma) \geq \alpha^{-1}\big\{\,\mathrm{Tr}[E(\mathbf{p})\gamma] - \alpha^{-1}N - \mathrm{Tr}[V\gamma]\big\} \geq\, -\alpha^{-2}N\,.$$

Here we used that $\mathcal{D}(\gamma) - \mathcal{E}x(\gamma) \geq 0$, and (8) (see also (17) and (18)).

Let $\{\gamma_n\}_{n=1}^{\infty}$ be a minimizing sequence for $E^{\mathrm{HF}}_{\leq}(N, Z, \alpha)$, more precisely, $\gamma_n \in \mathcal{A}$ (with $\mathcal{A}$ as defined in (16)), $\mathrm{Tr}[\gamma_n] \leq N$, and $\mathcal{E}^{\mathrm{HF}}(\gamma_n) \leq E^{\mathrm{HF}}_{\leq}(N, Z, \alpha) + 1/n$.

The sequence $\mathrm{Tr}[E(\mathbf{p})\gamma_n]$ is uniformly bounded. Indeed, for every $n \in \mathbb{N}$, using (8),

$$\begin{aligned} E^{\mathrm{HF}}(N, Z, \alpha) + 1 \geq \mathcal{E}^{\mathrm{HF}}(\gamma_n) &\geq \alpha^{-1}\big\{\,\mathrm{Tr}[E(\mathbf{p})\gamma_n] - \alpha^{-1}N - \mathrm{Tr}[V\gamma_n]\big\} \\ &\geq \alpha^{-1}(1 - Z\alpha\frac{\pi}{2})\,\mathrm{Tr}[E(\mathbf{p})\gamma_n] - \alpha^{-2}N\,. \end{aligned}$$

The claim follows since $Z\alpha < 2/\pi$. It is this argument that prevents us from proving Theorem 1 for the critical case $Z\alpha = 2/\pi$.

Define $\tilde{\gamma}_n := E(\mathbf{p})^{1/2}\gamma_n E(\mathbf{p})^{1/2}$. Then, by the above, $\{\tilde{\gamma}_n\}_{n\in\mathbb{N}}$ is a sequence of Hilbert-Schmidt operators with uniformly bounded Hilbert-Schmidt norm. Hence, by Banach-Alaoglu's theorem, there exist a subsequence, which we denote again by $\tilde{\gamma}_n$, and a Hilbert-Schmidt operator $\tilde{\gamma}_{(\infty)}$, such that for every Hilbert-Schmidt operator W,

$$\mathrm{Tr}[W\tilde{\gamma}_n] \to \mathrm{Tr}[W\tilde{\gamma}_{(\infty)}]\;,\; n \to \infty\,.$$

Let $\gamma_{(\infty)} := E(\mathbf{p})^{-1/2}\tilde{\gamma}_{(\infty)}E(\mathbf{p})^{-1/2}$. We are going to show that $\gamma_{(\infty)}$ is a minimizer of $\mathcal{E}^{\mathrm{HF}}$ (in fact, of $\alpha\mathcal{E}^{\mathrm{HF}}$, which is equivalent). We first prove that $\gamma_{(\infty)} \in \mathcal{A}$, then that $\mathcal{E}^{\mathrm{HF}}$ is weak lower semicontinuous on $\mathcal{A}$.

Let $\{\psi_k\}_{k\in\mathbb{N}}$ be a basis of $L^2(\mathbb{R}^3)$ with $\psi_k \in H^{1/2}(\mathbb{R}^3)$. Then, for all $k \in \mathbb{N}$,

$$\begin{aligned} \lim_{n\to\infty}(\psi_k, \gamma_n\psi_k) &= \lim_{n\to\infty}(\psi_k, E(\mathbf{p})^{-1/2}\tilde{\gamma}_n E(\mathbf{p})^{-1/2}\psi_k) \\ &= (\psi_k, \gamma_{(\infty)}\psi_k)\,. \end{aligned}$$

From this follows, by Fatou's lemma, that

$$\mathrm{Tr}[\gamma_{(\infty)}] = \sum_k (\psi_k, \gamma_{(\infty)}\psi_k) \le \liminf_{n\to\infty} \sum_k (\psi_k, \gamma_n \psi_k) = \liminf_{n\to\infty} \mathrm{Tr}[\gamma_n] \le N\,,$$

and

$$\mathrm{Tr}[E(\mathbf{p})^{1/2}\gamma_{(\infty)}E(\mathbf{p})^{1/2}] \le \liminf_{n\to\infty} \mathrm{Tr}[E(\mathbf{p})^{1/2}\gamma_n E(\mathbf{p})^{1/2}] < \infty\,.$$

Since also $0 \le \gamma_{(\infty)} \le \mathrm{Id}$ we see that $\gamma_{(\infty)} \in \mathcal{A}$.

To reach the claim it remains to show the weak lower semicontinuity of the functional $\mathcal{E}^{\mathrm{HF}}$. As mentioned in the introduction, the spectrum of the one-particle operator h_0, defined in (9), is discrete in $[-\alpha^{-1}, 0)$ and purely absolutely continuous in $[0,\infty)$. Let $\Lambda_-(\alpha)$ denote the projection on the pure point spectrum of h_0 and $\Lambda_+(\alpha) := \mathrm{Id} - \Lambda_-(\alpha)$. We write

$$\alpha\mathcal{E}^{\mathrm{HF}}(\gamma_n) = T_1(\gamma_n) + T_2(\gamma_n) + \alpha T_3(\gamma_n)\,, \tag{42}$$

with

$$\begin{aligned} &T_1(\gamma_n) = \mathrm{Tr}[\Lambda_+(\alpha)h_0\Lambda_+(\alpha)\gamma_n]\ , \quad T_2(\gamma_n) = \mathrm{Tr}[\Lambda_-(\alpha)h_0\Lambda_-(\alpha)\gamma_n]\,, \\ &T_3(\gamma_n) = \mathcal{D}(\gamma_n) - \mathcal{E}x(\gamma_n)\,. \end{aligned}$$

We consider these three terms separately.

For the first term in (42), fix (as above) a basis $\{\psi_k\}_{k\in\mathbb{N}}$ of $L^2(\mathbb{R}^3)$, with $\{\psi_k\}_{k\in\mathbb{N}} \subset H^{1/2}(\mathbb{R}^3)$. Defining

$$f_k := \big(\Lambda_+(\alpha)h_0\Lambda_+(\alpha)\big)^{1/2}\psi_k\,,$$

we have that

$$\begin{aligned} T_1(\gamma_n) &= \mathrm{Tr}\left[\big(\Lambda_+(\alpha)h_0\Lambda_+(\alpha)\big)^{1/2}\gamma_n\big(\Lambda_+(\alpha)h_0\Lambda_+(\alpha)\big)^{1/2}\right] \\ &= \sum_k (f_k, \gamma_n f_k) = \sum_k (E(\mathbf{p})^{-1/2}f_k, \tilde\gamma_n E(\mathbf{p})^{-1/2}f_k)\,. \end{aligned}$$

Since the projection

$$H_k := \big|E(\mathbf{p})^{-1/2}f_k\big\rangle\,\big\langle E(\mathbf{p})^{-1/2}f_k\big|$$

is a non-negative Hilbert-Schmidt operator, we find, by Fatou's lemma, that

$$\liminf_{n\to\infty} T_1(\gamma_n) = \liminf_{n\to\infty}\sum_k \mathrm{Tr}[H_k\tilde\gamma_n] \ge \sum_k \mathrm{Tr}[H_k\tilde\gamma_{(\infty)}] = T_1(\gamma_{(\infty)})\,.$$

As for the second term in (42), we have $\lim_{n\to\infty} T_2(\gamma_n) = T_2(\gamma_{(\infty)})$ since the operator $\Lambda_-(\alpha)h_0\Lambda_-(\alpha)$ is Hilbert-Schmidt; see Lemma 7 in Appendix A.

Finally, for the last term in (42), following the reasoning in [5, pp.142–143] (here we need that $N \in \mathbb{N}$), we get that

$$\liminf_{n\to\infty} T_3(\gamma_n) \ge T_3(\gamma_{(\infty)})\,.$$

This finishes the proof of Lemma 1. $\square$

Proof of Lemma 2. In order to prove that K_γ is Hilbert-Schmidt it is enough to prove that its integral kernel belongs to $L^2(\mathbb{R}^6)$. We have that (see (24) and (14))

$$\begin{aligned}\int_{\mathbb{R}^6} |K_\gamma(\mathbf{x},\mathbf{y})|^2\, d\mathbf{x}d\mathbf{y} &= \int_{\mathbb{R}^6} \frac{|\gamma(\mathbf{x},\mathbf{y})|^2}{|\mathbf{x}-\mathbf{y}|^2}\, d\mathbf{x}d\mathbf{y} \\ &= \sum_{j,k} \lambda_j\lambda_k \int_{\mathbb{R}^6} \frac{\overline{u_k(\mathbf{x})}u_j(\mathbf{x})u_k(\mathbf{y})\overline{u_j(\mathbf{y})}}{|\mathbf{x}-\mathbf{y}|^2}\, d\mathbf{x}d\mathbf{y} =: \sum_{j,k}\lambda_j\lambda_k I_{j,k}\,.\end{aligned} \tag{43}$$

The last integral can be estimated using the Hardy-Littlewood-Sobolev, Hölder, and Sobolev inequalities (in that order), to get

$$I_{j,k} \le \|u_k u_j\|_{3/2}^2 \le \|u_k\|_3^2\|u_j\|_3^2 \le C\|u_k\|_{H^{1/2}}^2\|u_j\|_{H^{1/2}}^2\,. \tag{44}$$

Inserting (44) in (43) we obtain (since $\gamma \in \mathcal{A}$)

$$\begin{aligned}\int_{\mathbb{R}^6} |K_\gamma(\mathbf{x},\mathbf{y})|^2\, d\mathbf{x}d\mathbf{y} &\le C\sum_{j,k}\lambda_j\lambda_k\|u_k\|_{H^{1/2}}^2\|u_j\|_{H^{1/2}}^2 = C\Big(\sum_j \lambda_j\|u_j\|_{H^{1/2}}^2\Big)^2 \\ &= C\big(\mathrm{Tr}[E(\mathbf{p})\gamma]\big)^2 < \infty\,.\end{aligned}$$

To prove the statement on the essential spectrum, define $\tilde{h}_\gamma := h_\gamma + \alpha K_\gamma$. Since K_γ is Hilbert-Schmidt, and $\sigma_{\mathrm{ess}}(h_0) = [0,\infty)$ (see the introduction), it is enough to prove that $(\tilde{h}_\gamma+\eta)^{-1} - (h_0+\eta)^{-1}$ is compact for some $\eta > 0$ large enough [27, Theorem XIII.14]. Since $\mathcal{D}(h_0) = \mathcal{D}(\tilde{h}_\gamma) \subset \mathcal{D}(R_\gamma)$, we have that

$$(\tilde{h}_\gamma+\eta)^{-1} - (h_0+\eta)^{-1} = \,-\,(\tilde{h}_\gamma+\eta)^{-1}\alpha R_\gamma(h_0+\eta)^{-1}\,. \tag{45}$$

From Tiktopoulos's formula (see [29, (II.8), Section II.3]), it follows that

$$\begin{aligned}&(h_0+\eta)^{-1} \\ &\quad = (T(\mathbf{p})+\eta)^{-1/2}[1-(T(\mathbf{p})+\eta)^{-1/2}V(T(\mathbf{p})+\eta)^{-1/2}]^{-1}(T(\mathbf{p})+\eta)^{-1/2}\,.\end{aligned} \tag{46}$$

Since, by (5), $\|(T(\mathbf{p})+\eta)^{-1/2}V^{1/2}\| < 1$ for $Z\alpha < 2/\pi$ and $\eta > \alpha^{-1}$, the right side of (46) is well defined. Inserting (46) in (45) one sees that it suffices to prove that $R_\gamma(T(\mathbf{p})+\eta)^{-1/2}$ is compact. That this is indeed the case follows by using [26, Theorem XI.20] together with the observation that, for $\varepsilon > 0$ and $\eta > \alpha^{-1}$, R_γ and $(T(\mathbf{p})+\eta)^{-1/2}$ (as a function of $\mathbf{p}$) belong to the space $L^{6+\varepsilon}(\mathbb{R}^3)$ (for R_γ, see (23)).

Finally, we show that if $\mathrm{Tr}[\gamma] = N < Z$ then h_γ has infinitely many eigenvalues in $[-\alpha^{-1},0)$. By the min-max principle [27, Theorem XIII.1] and since $\sigma_{\mathrm{ess}}(h_\gamma) = [0,\infty)$, it is sufficient to show that for every $n \in \mathbb{N}$ we can find n orthogonal functions $u_1,\dots,u_n$ in $L^2(\mathbb{R}^3)$ such that $(u_i, h_\gamma u_i) < 0$ for $i = 1,\dots,n$.

Let $n \in \mathbb{N}$. Fix $\delta := 1 - N/Z$ and let $h_{0,\delta}$ be the unique self-adjoint operator whose quadratic form domain is $H^{1/2}(\mathbb{R}^3)$ such that

$$(u, h_{0,\delta}v) = \mathfrak{t}[u,v] - \delta\,\mathfrak{v}[u,v] \text{ for } u,v \in H^{1/2}(\mathbb{R}^3)\,.$$

By [13, Theorems 2.2 and 2.3], $\sigma_{\mathrm{ess}}(h_{0,\delta}) = [0,\infty)$. Moreover, $h_{0,\delta}$ has infinitely many eigenvalues in $[-\alpha^{-1},0)$. This follows by the min-max principle and the inequality $h_{0,\delta} \le \alpha/2(-\Delta) - \delta Z\alpha/|\mathbf{x}|$. Hence, we can find $u_1,\dots,u_n$ spherically symmetric and orthonormal such that $(u_i, h_{0,\delta}u_i) < 0$ for $i = 1,\dots,n$. Then, by the positivity of K_γ, by Newton's Theorem [18, p. 249], and since $\mathrm{Tr}[\gamma] = N$ we get, for $i = 1,\dots,n$, that

$$\begin{aligned}(u_i, h_\gamma u_i) &\le \mathfrak{t}[u_i,u_i] - \mathfrak{v}[u_i,u_i] + \alpha(u_i, R_\gamma u_i) \\ &\le \mathfrak{t}[u_i,u_i] - \mathfrak{v}[u_i,u_i] + \frac{N}{Z}\,\mathfrak{v}[u_i,u_i] = (u_i, h_{0,\delta}u_i) < 0\,.\end{aligned}$$

The claim follows. □

2.2 Regularity of the Hartree-Fock orbitals

Here we prove that any eigenfunction of $h_{\gamma^{\mathrm{HF}}}$ is in $C^\infty(\mathbb{R}^3 \setminus \{0\})$.

Proof. Let φ be a solution of $h_{\gamma^{\mathrm{HF}}}\varphi = \varepsilon\varphi$ for some $\varepsilon \in \mathbb{R}$. Then φ belongs to the domain of the operator and in particular to $H^{1/2}(\mathbb{R}^3;\mathbb{C}^q)$. We are going to prove that $\varphi \in H^k(\Omega)$ for all bounded smooth $\Omega \subset \mathbb{R}^3 \setminus \{0\}$ and all $k \in \mathbb{N}$. The claim will then follow from the Sobolev imbedding theorem [2, Theorem 4.12]. We will use results on pseudodifferential operators; see Appendix B. We briefly summarize these here.

1) For all $k, \ell \in \mathbb{R}$, $E(\mathbf{p})^\ell$ maps $H^k(\mathbb{R}^3)$ to $H^{k-\ell}(\mathbb{R}^3)$.
2) For all $k, \ell \in \mathbb{R}$, and any $\chi \in C_0^\infty(\mathbb{R}^3)$, the commutator $[\chi, E(\mathbf{p})^\ell]$ maps $H^k(\mathbb{R}^3)$ to $H^{k-\ell+1}(\mathbb{R}^3)$.
3) For all $k, \ell, m \in \mathbb{R}$ and $\chi_1, \chi_2 \in C_0^\infty(\mathbb{R})$ with $\operatorname{supp}\chi_1 \cap \operatorname{supp}\chi_2 = \emptyset$, $\chi_1 E(\mathbf{p})^\ell \chi_2$ maps $H^k(\mathbb{R}^3)$ to $H^m(\mathbb{R}^3)$. Such an operator is called 'smoothing'.

Fix Ω a bounded smooth subset of $\mathbb{R}^3 \setminus \{0\}$. We proceed by induction on $k \in \mathbb{N}$. Assume that $\varphi \in H^k(\Omega)$ for some $k \geq 0$, i.e., $\chi\varphi \in H^k(\mathbb{R}^3)$ for all $\chi \in C_0^\infty(\Omega)$. Notice that $H^k(\mathbb{R}^3) = D(E(\mathbf{p})^k)$.

Since $\chi\varphi \in H^{k+1}(\mathbb{R}^3)$ is equivalent to $\chi\varphi \in D(E(\mathbf{p})^{k+1})$, and $D(E(\mathbf{p})^{k+1}) = D((E(\mathbf{p})^{k+1})^*)$, it is sufficient to prove that $\chi\varphi \in D((E(\mathbf{p})^{k+1})^*)$, or equivalently, that there exists $v \in L^2(\mathbb{R}^3)$ such that

$$(\chi\varphi, E(\mathbf{p})^{k+1} f) = (v, f) \quad \text{for all } f \in H^{k+1}(\mathbb{R}^3)\,.$$

Let $f \in H^{k+1}(\mathbb{R}^3)$. Then

$$\begin{aligned}(\chi\varphi, E(\mathbf{p})^{k+1} f) &= \mathfrak{e}(\varphi, E(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1} f) \\ &= (\varepsilon + \alpha^{-1})(\varphi, E(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1} f) + \mathfrak{v}(\varphi, E(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1} f) \\ &\quad - \mathfrak{b}_{\gamma^{\mathrm{HF}}}(\varphi, E(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1} f)\,, \end{aligned} \tag{47}$$

where we use that $h_{\gamma^{\mathrm{HF}}}\varphi = \varepsilon\varphi$. We study the terms in (47) separately. In the following, $\tilde{\chi}$ denotes a function in $C_0^\infty(\Omega)$ with $\tilde{\chi} \equiv 1$ on $\operatorname{supp}\chi$.

For the first term in (47) we find that

$$\begin{aligned}(\varphi, E(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1} f) &= (\chi E(\mathbf{p})^{-1}\varphi, E(\mathbf{p})^{k+1} f) \\ &= ([\chi, E(\mathbf{p})^{-1}]\varphi, E(\mathbf{p})^{k+1} f) + (E(\mathbf{p})^{-1}\chi\varphi, E(\mathbf{p})^{k+1} f)\,. \end{aligned} \tag{48}$$

Since $\chi\varphi \in H^k(\mathbb{R}^3)$ by the induction hypothesis, we have that $E(\mathbf{p})^{-1}\chi\varphi \in H^{k+1}(\mathbb{R}^3)$ and hence there exists $w_1 \in L^2(\mathbb{R}^3)$ such that

$$(E(\mathbf{p})^{-1}\chi\varphi, E(\mathbf{p})^{k+1} f) = (w_1, f)\,.$$

It remains to study the first term in (48). We have that

$$\begin{aligned}&([\chi, E(\mathbf{p})^{-1}]\varphi, E(\mathbf{p})^{k+1} f) \\ &= ([\chi, E(\mathbf{p})^{-1}]\tilde{\chi}\varphi, E(\mathbf{p})^{k+1} f) + ([\chi, E(\mathbf{p})^{-1}](1-\tilde{\chi})\varphi, E(\mathbf{p})^{k+1} f)\,. \end{aligned}$$

Since $\tilde{\chi}\varphi \in H^k(\mathbb{R}^3)$ by the induction hypothesis, it follows from Proposition 2 that $[\chi, E(\mathbf{p})^{-1}]\tilde{\chi}\varphi$ belongs to $H^{k+2}(\mathbb{R}^3)$. On the other hand since the supports of χ and $\tilde{\chi}$ are disjoint the operator $[\chi, E(\mathbf{p})^{-1}](1-\tilde{\chi})$ is a smoothing operator. Hence there exists a $w_2 \in L^2(\mathbb{R}^3)$ such that

$$([\chi, E(\mathbf{p})^{-1}]\varphi, E(\mathbf{p})^{k+1} f) = (w_2, f)\,.$$

As for the second term in (47), we find, with $\tilde{\chi}$ as before,

$$\begin{aligned}\mathfrak{v}(\varphi, E(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1}f) &= (\varphi, VE(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1}f) \\ &= (\tilde{\chi}\varphi, VE(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1}f) \\ &\quad + ((1-\tilde{\chi})\varphi, VE(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1}f)\,.\end{aligned} \tag{49}$$

Since $\tilde{\chi}$ has support away from zero, $V\tilde{\chi}\varphi \in H^k(\mathbb{R}^3)$ and hence there exists $w_3 \in L^2(\mathbb{R}^3)$ such that

$$(\tilde{\chi}\varphi, VE(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1}f) = (w_3, f)\,.$$

For the second term in (49) we proceed via an approximation. Let $\{\varphi_n\}_{n=1}^{\infty} \subset C_0^{\infty}(\mathbb{R}^3)$ such that $\varphi_n \to \varphi, n \to \infty$, in $L^2(\mathbb{R}^3)$. Since $(1-\tilde{\chi})VE(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1}f$ belongs to $L^2(\mathbb{R}^3)$, we have that

$$(\varphi, (1-\tilde{\chi})VE(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1}f) = \lim_{n\to+\infty}(\varphi_n, (1-\tilde{\chi})VE(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1}f)\,.$$

For each $n \in \mathbb{N}$, $V(1-\tilde{\chi})\varphi_n \in H^m(\mathbb{R}^3)$ for all m, since $\varphi_n \in C_0^{\infty}(\mathbb{R}^3)$, and V maps $H^k(\mathbb{R}^3)$ into $H^{k-1}(\mathbb{R}^3)$ for all k. Therefore, $E(\mathbf{p})^{k+1}\chi E(\mathbf{p})^{-1}V(1-\tilde{\chi})\varphi_n \in L^2(\mathbb{R}^3)$, and so

$$\begin{aligned}&(\varphi_n, (1-\tilde{\chi})VE(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1}f) \\ &\quad = (E(\mathbf{p})^{k+1}\chi E(\mathbf{p})^{-1}V(1-\tilde{\chi})\varphi_n, f) \\ &\quad = (E(\mathbf{p})^{k+1}\chi E(\mathbf{p})^{-1}(1-\tilde{\chi})E(\mathbf{p})E(\mathbf{p})^{-1}V\varphi_n, f)\,.\end{aligned}$$

Here $E(\mathbf{p})^{-1}V$ is bounded by (8), and $\chi E(\mathbf{p})^{-1}(1-\tilde{\chi})$ is a smoothing operator by the choice of the supports of χ and $\tilde{\chi}$. It then follows that $\{E(\mathbf{p})^{k+1}\chi E(\mathbf{p})^{-1}(1-\tilde{\chi})E(\mathbf{p})E(\mathbf{p})^{-1}V\varphi_n\}_{n\in\mathbb{N}}$ is a uniformly bounded sequence in $L^2(\mathbb{R}^3)$ and hence there exists $w_4 \in L^2(\mathbb{R}^3)$ such that

$$\lim_{n\to+\infty}(\varphi_n, ((1-\tilde{\chi})VE(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1}f) = (w_4, f)\,.$$

For the third term in (47), we have to separate the cases $k=0$ and $k \geq 1$.

Let $k=0$. The terms $R_{\gamma^{\mathrm{HF}}}\varphi$ and $K_{\gamma^{\mathrm{HF}}}\varphi$ belong to $L^2(\mathbb{R}^3)$, since $R_{\gamma^{\mathrm{HF}}} \in L^{\infty}(\mathbb{R}^3)$ (see (23)) and $K_{\gamma^{\mathrm{HF}}}$ is Hilbert-Schmidt (see Lemma 2), and therefore

$$\mathfrak{b}_{\gamma^{\mathrm{HF}}}(\varphi, E(\mathbf{p})^{-1}\chi E(\mathbf{p})f) = \alpha\,(E(\mathbf{p})\chi E(\mathbf{p})^{-1}(R_{\gamma^{\mathrm{HF}}} - K_{\gamma^{\mathrm{HF}}})\varphi, f)\,.$$

Assume now $k \geq 1$. With $\tilde{\chi}$ as before,

$$\begin{aligned}\mathfrak{b}_{\gamma^{\mathrm{HF}}}(\varphi, E(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1}f) &= \alpha\,(\tilde{\chi}(R_{\gamma^{\mathrm{HF}}} - K_{\gamma^{\mathrm{HF}}})\varphi, E(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1}f) \\ &\quad + \alpha\,((1-\tilde{\chi})(R_{\gamma^{\mathrm{HF}}} - K_{\gamma^{\mathrm{HF}}})\varphi, E(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1}f)\,.\end{aligned} \tag{50}$$

By the induction hypothesis and Lemma 6 (see Appendix A) we have that $\tilde{\chi}R_{\gamma^{\mathrm{HF}}}\varphi$ and $\tilde{\chi}K_{\gamma^{\mathrm{HF}}}\varphi$ belong to $H^k(\mathbb{R}^3)$. Therefore there exists $w_5 \in L^2(\mathbb{R}^3)$ such that

$$(\tilde{\chi}(R_{\gamma^{\mathrm{HF}}} - K_{\gamma^{\mathrm{HF}}})\varphi, E(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1}f) = (w_5, f)\,.$$

For the second term in (50) we find, since $R_{\gamma^{\mathrm{HF}}}\varphi$, $K_{\gamma^{\mathrm{HF}}}\varphi \in L^2(\mathbb{R}^3)$, that

$$\begin{aligned}&((1-\tilde{\chi})(R_{\gamma^{\mathrm{HF}}} - K_{\gamma^{\mathrm{HF}}})\varphi, E(\mathbf{p})^{-1}\chi E(\mathbf{p})^{k+1}f) \\ &\qquad = (\chi E(\mathbf{p})^{-1}(1-\tilde{\chi})(R_{\gamma^{\mathrm{HF}}} - K_{\gamma^{\mathrm{HF}}})\varphi, E(\mathbf{p})^{k+1}f)\,,\end{aligned}$$

and the result follows since $\chi E(\mathbf{p})^{-1}(1-\tilde{\chi})$ is a smoothing operator. $\square$

2.3 Exponential decay of the Hartree-Fock orbitals

The pointwise exponential decay (30) will be a consequence of Proposition 1 and Lemma 4 below.

Proposition 1. *Let γ^{HF} be a Hartree-Fock minimizer, let $h_{\gamma^{\mathrm{HF}}}$ be the corresponding Hartree-Fock operator as defined in (25), and let $\{\varphi_i\}_{i=1}^N$ be the Hartree-Fock orbitals, such that*

$$h_{\gamma^{\mathrm{HF}}}\varphi_i = \varepsilon_i\varphi_i \ , \ i = 1, \ldots, N \,,$$

with $0 > \varepsilon_N \geq \ldots \geq \varepsilon_1 > -\alpha^{-1}$ the N lowest eigenvalues of $h_{\gamma^{\mathrm{HF}}}$.

(i) *Let $\nu_{\varepsilon_N} := \sqrt{-\varepsilon_N(2\alpha^{-1}+\varepsilon_N)}$. Then $\varphi_i \in \mathcal{D}(e^{\beta|\cdot|})$ for every $\beta < \nu_{\varepsilon_N}$ and $i \in \{1, \ldots, N\}$.*

(ii) *Assume $h_{\gamma^{\mathrm{HF}}}\varphi = \varepsilon\varphi$ for some $\varepsilon \in [\varepsilon_N, 0)$, and let $\nu_\varepsilon := \sqrt{-\varepsilon(2\alpha^{-1}+\varepsilon)}$. Then $\varphi \in \mathcal{D}(e^{\beta|\cdot|})$ for every $\beta < \nu_\varepsilon$.*

Lemma 4. *Let $E < 0$ and $\nu_E := \sqrt{|-E(2\alpha^{-1}+E)|} = \sqrt{|\alpha^{-2} - (E+\alpha^{-1})^2|}$.*

Then the operator $T(-\mathrm{i}\nabla) - E = \sqrt{-\Delta + \alpha^{-2}} - \alpha^{-1} - E$ is invertible and the integral kernel of its inverse is given by

$$\begin{aligned}(T-E)^{-1}(\mathbf{x},\mathbf{y}) = G_E(\mathbf{x}-\mathbf{y}) &= \frac{(E+\alpha^{-1})e^{-\nu_E|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} + \frac{\alpha^{-1}}{2\pi^2}\frac{K_1(\alpha^{-1}|\mathbf{x}-\mathbf{y}|)}{|\mathbf{x}-\mathbf{y}|} \\ &+ (\alpha^{-2}-\nu_E^2)\frac{\alpha^{-1}}{2\pi^2}\Big[\frac{K_1(\alpha^{-1}|\cdot|)}{|\cdot|} * \frac{e^{-\nu_E|\cdot|}}{4\pi|\cdot|}\Big](\mathbf{x}-\mathbf{y})\,, \end{aligned} \tag{51}$$

where K_1 is a modified Bessel function of the second kind [1].

Moreover,

$$0 \leq G_E(\mathbf{x}) \leq C_{\alpha,E}\frac{e^{-\nu_E|\mathbf{x}|}}{4\pi|\mathbf{x}|} + \frac{\alpha^{-1}}{2\pi^2}\frac{K_1(\alpha^{-1}|\mathbf{x}|)}{|\mathbf{x}|}\,, \tag{52}$$

$$e^{\beta|\cdot|}G_E \in L^q(\mathbb{R}^3) \ \text{ for all } \ \beta < \nu_E \ \text{ and } \ q \in [1, 3/2)\,. \tag{53}$$

Proof of Lemma 4. The formula (51) for the kernel of $(T-E)^{-1}$ can be found in [22, eq. (35)].

The estimate (52) is a consequence of the bound

$$\frac{K_1(\alpha^{-1}|\cdot|)}{|\cdot|} * \frac{e^{-\nu_E|\cdot|}}{4\pi|\cdot|}(\mathbf{x}) \leq C_{\alpha,E}\frac{e^{-\nu_E|\mathbf{x}|}}{4\pi|\mathbf{x}|}\,.$$

This estimate, on the other hand, follows from Newton's theorem (see e. g. [18]),

$$\begin{aligned}&\int_{\mathbb{R}^3}\frac{K_1(\alpha^{-1}|\mathbf{x}-\mathbf{y}|)}{|\mathbf{x}-\mathbf{y}|}\,\frac{e^{-\nu_E|\mathbf{y}|}}{4\pi|\mathbf{y}|}\,d\mathbf{y} \\ &\leq e^{-\nu_E|\mathbf{x}|}\int_{\mathbb{R}^3}\frac{K_1(\alpha^{-1}|\mathbf{x}-\mathbf{y}|)}{|\mathbf{x}-\mathbf{y}|}\,\frac{e^{\nu_E|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{y}|}\,d\mathbf{y} \leq \frac{e^{-\nu_E|\mathbf{x}|}}{4\pi|\mathbf{x}|}\int_{\mathbb{R}^3}\frac{K_1(\alpha^{-1}|\mathbf{z}|)}{|\mathbf{z}|}\,e^{\nu_E|\mathbf{z}|}\,d\mathbf{z}\,.\end{aligned}$$

The last integral is finite since $\nu_E < \alpha^{-1}$, using the following properties of K_1 (see [10, 8.446, 8.451.6]):

$$K_1(t) \leq \frac{1}{|t|} \ \text{ for all } \ t > 0\,, \tag{54}$$

and for every $r > 0$ there exists c_r such that

$$K_1(t) \leq c_r\frac{e^{-t}}{\sqrt{t}} \ \text{ for all } \ t \geq r\,. \tag{55}$$

The estimate (53) is a consequence of (52), (54), and (55). □

Before proving Proposition 1, we apply it, and Lemma 4, to prove the pointwise exponential decay, i.e., the estimate in (30).

Proof of Theorem 1 (iii). Fix $i \in \{1, \dots, N\}$. If $Z\alpha < 1/2$ we can rewrite the Hartree-Fock equation (28) as

$$\big(\sqrt{-\Delta + \alpha^{-2}} - \alpha^{-1}\big)\varphi_i = \varepsilon_i \varphi_i + \frac{Z\alpha}{|\mathbf{x}|}\,\varphi_i - \alpha R_{\gamma^{\mathrm{HF}}}\varphi_i + \alpha K_{\gamma^{\mathrm{HF}}}\varphi_i\,. \tag{56}$$

The idea of the proof is to study the elliptic regularity of the corresponding parametrix. By Lemma 4 we find that

$$\varphi_i(\mathbf{x}) = \int_{\mathbb{R}^3} (T - \varepsilon_N)^{-1}(\mathbf{x},\mathbf{y})\big[(\varepsilon_i - \varepsilon_N)\varphi_i + \frac{Z\alpha}{|\cdot|}\,\varphi_i - \alpha R_{\gamma^{\mathrm{HF}}}\varphi_i + \alpha K_{\gamma^{\mathrm{HF}}}\varphi_i\big](\mathbf{y})\,d\mathbf{y}\,.$$

In the case $1/2 \le Z\alpha < 2/\pi$, on the other hand, the operator of which we are studying the eigenfunctions cannot be written as a sum of operators acting on $L^2(\mathbb{R}^3)$ and hence we cannot write directly the equation (28) as in (56). However, since the eigenfunctions are smooth away from the origin we are able to write a pointwise equation for a localized version of φ_i. In fact, let $\chi \in C^\infty(\mathbb{R}^3)$ be such that $0 \le \chi \le 1$ and

$$\chi(\mathbf{x}) = \begin{cases} 1 & \text{if } |\mathbf{x}| \ge 1, \\ 0 & \text{if } |\mathbf{x}| \le 1/2\,, \end{cases}$$

and let, for $R > 0$, $\chi_R(\mathbf{x}) = \chi(\mathbf{x}/R)$. We will derive an equation (similar to (56)) for $T(-\mathrm{i}\nabla)(\chi_R\varphi_i)$. Indeed, for every $u \in H^{1/2}(\mathbb{R}^3)$ we have that

$$\begin{aligned}(u, h_{\gamma^{\mathrm{HF}}}(\chi_R\varphi_i)) &= \mathfrak{e}(u,\chi_R\varphi_i) - \alpha^{-1}(u,\chi_R\varphi_i) - \mathfrak{v}(u,\chi_R\varphi_i) + \mathfrak{b}_{\gamma^{\mathrm{HF}}}(u,\chi_R\varphi_i)\\ &= (\chi_R u, h_{\gamma^{\mathrm{HF}}}\varphi_i) + \mathfrak{e}(u,\chi_R\varphi_i) - \mathfrak{e}(\chi_R u,\varphi_i)\\ &\quad + \mathfrak{b}_{\gamma^{\mathrm{HF}}}(u,\chi_R\varphi_i) - \mathfrak{b}_{\gamma^{\mathrm{HF}}}(\chi_R u,\varphi_i)\,.\end{aligned}$$

Note that

$$\mathfrak{e}(u,\chi_R\varphi_i) - \mathfrak{e}(\chi_R u,\varphi_i) = (u, [E(\mathbf{p}),\chi_R]\varphi_i)\,,$$

where $[E(\mathbf{p}),\chi_R]$ is a bounded operator in $L^2(\mathbb{R}^3)$ (see Appendix B), and

$$\mathfrak{b}_{\gamma^{\mathrm{HF}}}(u,\chi_R\varphi_i) - \mathfrak{b}_{\gamma^{\mathrm{HF}}}(\chi_R u,\varphi_i) = (u, \mathcal{K}\varphi_i)\,,$$

with $\mathcal{K}$ the bounded operator on $L^2(\mathbb{R}^3)$ given by the kernel

$$\mathcal{K}(\mathbf{x},\mathbf{y}) = \alpha \sum_{j=1}^N \varphi_j(\mathbf{x})\overline{\varphi_j(\mathbf{y})}\,\frac{\chi_R(\mathbf{x}) - \chi_R(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,. \tag{57}$$

Therefore there exists $w \in L^2(\mathbb{R}^3)$ such that

$$\begin{aligned}\mathfrak{e}(u,\chi_R\varphi_i) &= (\varepsilon_i + \alpha^{-1})(u,\chi_R\varphi_i) + \mathfrak{v}(u,\chi_R\varphi_i) - \mathfrak{b}_{\gamma^{\mathrm{HF}}}(u,\chi_R\varphi_i)\\ &\quad + (u,[E(\mathbf{p}),\chi_R]\varphi_i) + (u,\mathcal{K}\varphi_i) = (u,w)\,.\end{aligned}$$

Hence $\chi_R\varphi_i \in H^1(\mathbb{R}^3)$ and we can write the pointwise equation

$$\begin{aligned}(\sqrt{-\Delta + \alpha^{-2}} - \alpha^{-1})\chi_R\varphi_i &= \varepsilon_i\chi_R\varphi_i + \frac{Z\alpha}{|\mathbf{x}|}\chi_R\varphi_i - \alpha R_{\gamma^{\mathrm{HF}}}\chi_R\varphi_i\\ &\quad + \alpha K_{\gamma^{\mathrm{HF}}}(\chi_R\varphi_i) + [E(\mathbf{p}),\chi_R]\varphi_i + \mathcal{K}\varphi_i\,.\end{aligned} \tag{58}$$

This is the substitute for (56) in the case $1/2 \le Z\alpha < 2/\pi$; if $Z\alpha < 1/2$, the proof below simplifies somewhat, using (56) directly.

By Lemma 4, (58) implies that

$$\chi_R(\mathbf{x})\varphi_i(\mathbf{x}) = \int_{\mathbb{R}^3} (T-\varepsilon_N)^{-1}(\mathbf{x},\mathbf{y})\big[\frac{Z\alpha}{|\cdot|}\chi_R\varphi_i - \alpha R_{\gamma^{\rm HF}}\chi_R\varphi_i + \alpha K_{\gamma^{\rm HF}}(\chi_R\varphi_i) \\ + (\varepsilon_i-\varepsilon_N)\chi_R\varphi_i + [E(\mathbf{p}),\chi_R]\varphi_i + \mathcal{K}\varphi_i\big](\mathbf{y})\,d\mathbf{y}\,. \tag{59}$$

We will first show that, for all $R>0$ and $\beta < \nu_{\varepsilon_N}$,

$$\chi_R\varphi_i e^{\beta|\cdot|} \in L^p(\mathbb{R}^3) + L^\infty(\mathbb{R}^3) \quad \text{for } p \in [2,6)\,, \tag{60}$$

and then, by a bootstrap argument, that $\chi_R\varphi_i e^{\beta|\cdot|} \in L^\infty(\mathbb{R}^3)$, which is the claim of Theorem 1 (iii).

We multiply (59) by $\chi_{R/2}(\mathbf{x})e^{\beta|\mathbf{x}|}$. Using that $|(Z\alpha/|\mathbf{y}|)\chi_R(\mathbf{y})| \le (Z\alpha)/R$ for all $\mathbf{y}\in\mathbb{R}^3$, (23), (24), and (57) (recall (27), that $\varphi_j \in H^{1/2}(\mathbb{R}^3)$, and (5)) we get, for some constant $C = C_{R,\alpha} > 0$, that

$$\big|\chi_R(\mathbf{x})\varphi_i(\mathbf{x})e^{\beta|\mathbf{x}|}\big| \le C\chi_{R/2}(\mathbf{x})e^{\beta|\mathbf{x}|}\int_{\mathbb{R}^3}(T-\varepsilon_N)^{-1}(\mathbf{x},\mathbf{y})\big[|\varphi_i(\mathbf{y})| + \sum_{j=1}^N |\varphi_j(\mathbf{y})|\big]\,d\mathbf{y} \\ + \chi_{R/2}(\mathbf{x})e^{\beta|\mathbf{x}|}\Big|\int_{\mathbb{R}^3}(T-\varepsilon_N)^{-1}(\mathbf{x},\mathbf{y})\big([E(\mathbf{p}),\chi_R]\varphi_i\big)(\mathbf{y})\,d\mathbf{y}\Big|\,. \tag{61}$$

We will show that the first term on the right side of (61) belongs to $L^p(\mathbb{R}^3)$ for $p\in[2,6)$, and that the second belongs to $L^\infty(\mathbb{R}^3)$. This will prove (60).

The first term on the right side of (61) is a sum of terms of the form

$$h_f(\mathbf{x}) := \chi_{R/2}(\mathbf{x})e^{\beta|\mathbf{x}|}\int_{\mathbb{R}^3}(T-\varepsilon_N)^{-1}(\mathbf{x},\mathbf{y})\,|f(\mathbf{y})|\,d\mathbf{y}\,, \tag{62}$$

with f such that, by Proposition 1, $fe^{\beta|\cdot|} \in L^2(\mathbb{R}^3)$. By Lemma 4 we have, using $e^{|\mathbf{x}|-|\mathbf{y}|} \le e^{|\mathbf{x}-\mathbf{y}|}$, that

$$|h_f(\mathbf{x})| \le C\int_{\mathbb{R}^3} e^{\beta|\mathbf{x}-\mathbf{y}|}G_{\varepsilon_N}(\mathbf{x}-\mathbf{y})e^{\beta|\mathbf{y}|}|f(\mathbf{y})|\,d\mathbf{y}\,.$$

From Young's inequality it follows that $h_f \in L^p(\mathbb{R}^3)$ for all $p\in[2,6)$, since $\beta < \nu_{\varepsilon_N}$, so (by Proposition 1) $fe^{\beta|\cdot|}\in L^2(\mathbb{R}^3)$ and (by Lemma 4) $e^{\beta|\cdot|}G_{\varepsilon_N} \in L^q(\mathbb{R}^3)$ for all $q \in [1,3/2)$.

We now prove that the second term on the right side of (61) is in $L^\infty(\mathbb{R}^3)$. This follows from Young's inequality once we have proved that

$$e^{\beta|\cdot|}[E(\mathbf{p}),\chi_R]\varphi_i \in L^p(\mathbb{R}^3) \quad \text{for } p\in[2,\infty)\,, \tag{63}$$

since

$$e^{\beta|\mathbf{x}|}\Big|\int_{\mathbb{R}^3}(T-\varepsilon_N)^{-1}(\mathbf{x},\mathbf{y})\big([E(\mathbf{p}),\chi_R]\varphi_i\big)(\mathbf{y})\,d\mathbf{y}\Big| \\ \le \int_{\mathbb{R}^3} e^{\beta|\mathbf{x}-\mathbf{y}|}G_{\varepsilon_N}(\mathbf{x}-\mathbf{y})e^{\beta|\mathbf{y}|}\big|[E(\mathbf{p}),\chi_R]\varphi_i\big|(\mathbf{y})\,d\mathbf{y}\,,$$

and $e^{\beta|\cdot|}G_{\varepsilon_N} \in L^q(\mathbb{R}^3)$ for $q\in[1,3/2)$.

To prove (60) it therefore remains to prove (63). To do so, we consider a new localization function. Let $\eta \in C_0^\infty(\mathbb{R}^3)$ be such that $0 \le \eta \le 1$ and

$$\eta(\mathbf{x}) = \begin{cases} 1 & \text{if } R/4 \le |\mathbf{x}| \le 3R/2 \\ 0 & \text{if } |\mathbf{x}| \le R/8 \text{ or } |\mathbf{x}| \ge 2R\,, \end{cases}$$

and consider the following splitting

$$\begin{aligned} e^{\beta|\cdot|}[E(\mathbf{p}),\chi_R]\varphi_i &= e^{\beta|\cdot|}\eta[E(\mathbf{p}),\chi_R](\eta\varphi_i) + e^{\beta|\cdot|}\eta[E(\mathbf{p}),\chi_R]((1-\eta)\varphi_i) \\ &\quad + e^{\beta|\cdot|}(1-\eta)[E(\mathbf{p}),\chi_R](\eta\varphi_i) + e^{\beta|\cdot|}(1-\eta)[E(\mathbf{p}),\chi_R](1-\eta)\varphi_i\,. \end{aligned} \tag{64}$$

Since $\eta\varphi_i \in H^k(\mathbb{R}^3)$ for all $k \in \mathbb{N}$ (as proved earlier), $[E(\mathbf{p}),\chi_R](\eta\varphi_i)$ belongs to $H^k(\mathbb{R}^3)$ for all $k \in \mathbb{N}$. Hence, since η has compact support away from $\mathbf{x} = 0$, the first term on the right side of (64) is in $L^p(\mathbb{R}^3)$ for $p \in [1,\infty]$ by Sobolev's imbedding theorem (the term is smooth).

For the second term in (64) we proceed by duality: We will prove that

$$\psi(\mathbf{x}) := \big(e^{\beta|\cdot|}\eta[E(\mathbf{p}),\chi_R]((1-\eta)\varphi_i)\big)(\mathbf{x})$$

defines a bounded linear functional on $L^q(\mathbb{R}^3)$ for any $q \in (1,2]$. It then follows that $\psi \in L^p(\mathbb{R}^3)$ for all $p \in [2,\infty)$.

Note that [18, 7.12 Theorem (iv)]

$$\begin{aligned} &(g,[\sqrt{-\Delta+\alpha^{-2}} - \alpha^{-1}]g) \\ &\quad = \frac{\alpha^{-2}}{4\pi^2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{|g(\mathbf{x})-g(\mathbf{y})|^2}{|\mathbf{x}-\mathbf{y}|^2}K_2(\alpha^{-1}|\mathbf{x}-\mathbf{y}|)\,d\mathbf{x}d\mathbf{y} \quad \text{for } g \in \mathcal{S}(\mathbb{R}^3)\,, \end{aligned} \tag{65}$$

where K_2 is a modified Bessel function of the second kind (in fact, $K_2(t) = -t\frac{d}{dt}[t^{-1}K_1(t)]$), satisfying [1]

$$K_2(t) \le Ct^{-1}e^{-t} \quad \text{for} \quad t \ge 1\,. \tag{66}$$

Let $f \in C_0^\infty(\mathbb{R}^3)$. Using (65) and polarization, we have that

$$\begin{aligned} &\int_{\mathbb{R}^3}\overline{f(\mathbf{x})}\psi(\mathbf{x})\,d\mathbf{x} = (f, e^{\beta|\cdot|}\eta[E(\mathbf{p}),\chi_R]((1-\eta)\varphi_i)) \\ &= \frac{\alpha^{-2}}{4\pi^2}\iint_{|\mathbf{x}-\mathbf{y}|\ge R/4}\frac{\chi_R(\mathbf{x})-\chi_R(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^2}\,K_2(\alpha^{-1}|\mathbf{x}-\mathbf{y}|) \\ &\qquad \times \big[\,\overline{f(\mathbf{x})}e^{\beta|\mathbf{x}|}\eta(\mathbf{x})(1-\eta(\mathbf{y}))\varphi_i(\mathbf{y}) - \overline{f(\mathbf{y})}e^{\beta|\mathbf{y}|}\eta(\mathbf{y})(1-\eta(\mathbf{x}))\varphi_i(\mathbf{x})\big]\,d\mathbf{x}d\mathbf{y}\,, \end{aligned}$$

by the properties of χ and η. Hence,

$$\begin{aligned} &\Big|\int_{\mathbb{R}^3}\overline{f(\mathbf{x})}\psi(\mathbf{x})\,d\mathbf{x}\Big| \\ &\qquad \le C_R\iint_{|\mathbf{x}-\mathbf{y}|\ge R/4}|f(\mathbf{x})|e^{\beta|\mathbf{x}-\mathbf{y}|}K_2(\alpha^{-1}|\mathbf{x}-\mathbf{y}|)e^{\beta|\mathbf{y}|}|\varphi_i(\mathbf{y})|\,d\mathbf{x}d\mathbf{y}\,, \\ &\qquad \le C_R\iint|f(\mathbf{x})|e^{\beta|\mathbf{x}-\mathbf{y}|}K_2(\alpha^{-1}|\mathbf{x}-\mathbf{y}|)\chi_{R/4}(|\mathbf{x}-\mathbf{y}|)e^{\beta|\mathbf{y}|}|\varphi_i(\mathbf{y})|\,d\mathbf{x}d\mathbf{y}\,. \end{aligned} \tag{67}$$

Note that, since $\beta < \nu_{\varepsilon_N} < \alpha^{-1}$, (66) implies that $e^{\beta|\cdot|}K_2(\alpha^{-1}|\cdot|)\chi_{R/4}$ is in $L^r(\mathbb{R}^3)$ for all $r \ge 1$. Since (by Proposition 1) $e^{\beta|\cdot|}\varphi_i \in L^2(\mathbb{R}^3)$, Young's inequality therefore gives that

$$(e^{\beta|\cdot|}K_2(\alpha^{-1}|\cdot|)\chi_{R/4}) * (e^{\beta|\cdot|}|\varphi_i|) \in L^s(\mathbb{R}^3) \quad \text{for all } s \in [2,\infty)\,.$$

This, (67), and Hölder's inequality (with $1/q + 1/s = 1$) imply that, for all $f \in C_0^\infty(\mathbb{R}^3)$ and all $q \in (1, 2]$

$$\Big| \int_{\mathbb{R}^3} \overline{f(\mathbf{x})}\psi(\mathbf{x})\, d\mathbf{x} \Big| \leq C_R \big\| (e^{\beta|\cdot|} K_2(\alpha^{-1}|\cdot|)\chi_{R/4}) * (e^{\beta|\cdot|}|\varphi_i|) \big\|_s \, \|f\|_q \, .$$

By density of $C_0^\infty(\mathbb{R}^3)$ in $L^q(\mathbb{R}^3)$, it follows that ψ defines a bounded linear functional on $L^q(\mathbb{R}^3)$ for any $q \in (1, 2]$, and therefore, that $\psi \in L^p(\mathbb{R}^3)$ for all $p \in [2, \infty)$.

Proceeding similarly one shows that the two remaining terms in (64) are also in $L^p(\mathbb{R}^3)$ for all $p \in [2, \infty)$.

This finishes the proof of (63), and therefore of (60).

Finally we prove that $\chi_R \varphi_i e^{\beta|\cdot|} \in L^\infty(\mathbb{R}^3)$. We start again from (61). We already know that the second term is in $L^\infty(\mathbb{R}^3)$. The first term is a sum of terms of the form (see also (62))

$$h_f(\mathbf{x}) = \chi_{R/2}(\mathbf{x}) e^{\beta|\mathbf{x}|} \int_{\mathbb{R}^3} (T - \varepsilon_N)^{-1}(\mathbf{x}, \mathbf{y}) |f(\mathbf{y})| \, d\mathbf{y} \, ,$$

with $f \in L^2(\mathbb{R}^3)$ and $\chi_{R/4} e^{\beta|\cdot|} f \in L^p(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ for $p \in [2, 6)$ by what just proved, replacing R by $R/4$ in (60). We find that

$$\begin{aligned} h_f(\mathbf{x}) \leq{}& \chi_{R/2}(\mathbf{x}) \int_{\mathbb{R}^3} e^{\beta|\mathbf{x}-\mathbf{y}|} (T - \varepsilon_N)^{-1}(\mathbf{x}, \mathbf{y}) e^{\beta|\mathbf{y}|} \chi_{R/4}(\mathbf{y}) |f(\mathbf{y})| \, d\mathbf{y} \\ &+ \chi_{R/2}(\mathbf{x}) \int_{\mathbb{R}^3} e^{\beta|\mathbf{x}-\mathbf{y}|} (T - \varepsilon_N)^{-1}(\mathbf{x}, \mathbf{y}) e^{\beta|\mathbf{y}|} (1 - \chi_{R/4})(\mathbf{y}) |f(\mathbf{y})| \, d\mathbf{y} \, , \end{aligned}$$

and, again by Young's inequality, we see that both terms are in $L^\infty(\mathbb{R}^3)$. Notice that in the second integrand $|\mathbf{x} - \mathbf{y}| > R/4$.

This finishes the proof of Theorem 1 (iii). □

It therefore remains to prove Proposition 1.

Proof of Proposition 1. We start by proving (i). It will be convenient to write the Hartree-Fock equations $h_{\gamma^{\mathrm{HF}}} \varphi_i = \varepsilon_i \varphi_i$, $i = 1, \ldots, N$, (see (28)) as a system.

Let $\mathtt{t}$ be the quadratic form with domain $[H^{1/2}(\mathbb{R})]^N$ defined by

$$\mathtt{t}(\mathrm{u}, \mathrm{v}) = \sum_{i=1}^{N} \mathfrak{t}(\mathrm{u}_i, \mathrm{v}_i) \text{ for all } \mathrm{u}, \mathrm{v} \in [H^{1/2}(\mathbb{R}^3)]^N \, ,$$

where u_i denotes the i-th component of $\mathrm{u} \in [H^{1/2}(\mathbb{R}^3)]^N$ and $\mathfrak{t}$ is the quadratic form defined in (7). Similarly we define the quadratic forms $\mathtt{v}$, $\mathtt{r}_\gamma$ and $\mathtt{k}_\gamma$, all with domain $[H^{1/2}(\mathbb{R}^3)]^N$, by

$$\mathtt{v}(\mathrm{u}, \mathrm{v}) = \sum_{i=1}^{N} \mathfrak{v}(\mathrm{u}_i, \mathrm{v}_i) \, , \quad \mathtt{r}_\gamma(\mathrm{u}, \mathrm{v}) = \alpha \sum_{i=1}^{N} (\mathrm{u}_i, R_\gamma \mathrm{v}_i) \, , \quad \mathtt{k}_\gamma(\mathrm{u}, \mathrm{v}) = \alpha \langle \mathrm{u}, \mathrm{K}_\gamma \mathrm{v} \rangle \, ,$$

with $\mathfrak{v}$ defined in (6), R_γ defined in (22), and K_γ the $N \times N$-matrix given by

$$(\mathrm{K}_\gamma)_{i,j} = \int_{\mathbb{R}^3} \frac{\varphi_i(\mathbf{y}) \overline{\varphi_j(\mathbf{y})}}{|\mathbf{x} - \mathbf{y}|} \, d\mathbf{y} \, .$$

The effect of writing the Hartree-Fock equations as a system is that K_γ is a (non-diagonal) multiplication operator. This idea was already used in [19]. Note that $(\mathrm{K}_\gamma)_{i,j} \in L^3(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$; the argument is the same as for (22).

Let finally $\mathtt{E}$ be the $N \times N$ matrix defined by $(\mathtt{E})_{i,j} = -\varepsilon_i \delta_{i,j}$.

We then define the quadratic form $\mathtt{q}$ by

$$\mathtt{q}(\mathrm{u}, \mathrm{v}) = \mathtt{t}(\mathrm{u}, \mathrm{v}) - \mathtt{v}(\mathrm{u}, \mathrm{v}) + \mathtt{r}_\gamma(\mathrm{u}, \mathrm{v}) - \mathtt{k}_\gamma(\mathrm{u}, \mathrm{v}) + \langle \mathrm{u}, \mathtt{E}\mathrm{v} \rangle \,. \tag{68}$$

One sees that the quadratic form domain of $\mathtt{q}$ is $[H^{1/2}(\mathbb{R}^3)]^N$, that $\mathtt{q}$ is closed (since $\mathtt{t}$ is closed), and that there exists a unique selfadjoint operator $\mathtt{H}$ with $\mathcal{D}(\mathtt{H}) \subset [H^{1/2}(\mathbb{R}^3)]^N$ such that

$$\langle \mathrm{u}, \mathtt{H}\mathrm{v} \rangle = \mathtt{q}(\mathrm{u}, \mathrm{v}) \quad \text{for all} \quad \mathrm{u} \in [H^{1/2}(\mathbb{R}^3)]^N \,, \ \mathrm{v} \in \mathcal{D}(\mathtt{H}) \,.$$

Notice that the vector $\Phi = (\varphi_1, \ldots, \varphi_N)$ satisfies $\mathtt{H}\Phi = 0$.

Let $W(\kappa)$, $\kappa \in \mathbb{C}^3$, denote the multiplication operator from a subset of $[L^2(\mathbb{R}^3)]^N$ to $[L^2(\mathbb{R}^3)]^N$ given by $f(\mathbf{x}) \mapsto e^{i\kappa \cdot \mathbf{x}} f(\mathbf{x})$. Instead of proving directly the claim of the proposition, we are going to prove the following statement, which implies the proposition:

$$\Phi \in \mathcal{D}(W(\kappa)) \quad \text{for} \quad \|\mathrm{Im}(\kappa)\|_{\mathbb{R}^3} < \nu_{\varepsilon_N} \,, \tag{69}$$

where $\Phi = (\varphi_1, \ldots, \varphi_N)$. Here, $\kappa = \mathrm{Re}(\kappa) + i\mathrm{Im}(\kappa)$ with $\mathrm{Re}(\kappa), \mathrm{Im}(\kappa) \in \mathbb{R}^3$.

We know that $W(\kappa)\Phi$ is well defined on $[L^2(\mathbb{R}^3)]^N$ for $\kappa \in \mathbb{R}^3$ and we need to show that it has a continuation into the 'strip' $\Sigma_{\nu_{\varepsilon_N}}$, where

$$\Sigma_t := \{\kappa \in \mathbb{C}^3 \,|\, \|\mathrm{Im}(\kappa)\|_{\mathbb{R}^3} < t\} \,.$$

We shall also need $\Sigma_{\alpha^{-1}}$; note that $\Sigma_{\alpha^{-1}} \supset \Sigma_{\nu_{\varepsilon_N}}$. The idea is to use O'Connor's Lemma (see Lemma 5 below).

Starting from the quadratic form $\mathtt{q}$ defined in (68) we define the following family of quadratic forms on $[H^{1/2}(\mathbb{R}^3)]^N$:

$$\mathtt{q}(\kappa)(\mathrm{u}, \mathrm{u}) := \mathtt{q}(W(-\kappa)\mathrm{u}, W(-\kappa)\mathrm{u}) \,,$$

depending on the *real* parameter $\kappa \in \mathbb{R}^3$. From the definition,

$$\mathtt{q}(\kappa)(\mathrm{u}, \mathrm{u}) = \mathtt{t}(\kappa)(\mathrm{u}, \mathrm{u}) - \mathtt{v}(\mathrm{u}, \mathrm{u}) + \mathtt{r}_\gamma(\mathrm{u}, \mathrm{u}) - \mathtt{k}_\gamma(\mathrm{u}, \mathrm{u}) + \langle \mathrm{u}, \mathtt{E}\mathrm{u} \rangle \,,$$

where

$$\mathtt{t}(\kappa)(\mathrm{u}, \mathrm{u}) = \sum_{i=1}^{N} \int_{\mathbb{R}^3} \big(\alpha^{-2} + \sum_{j=1}^{3} (p_j - \kappa_j)^2\big)^{1/2} |\hat{\mathrm{u}}_i(\mathbf{p})|^2 \, d\mathbf{p} - \alpha^{-1} \langle \mathrm{u}, \mathrm{u} \rangle \,. \tag{70}$$

One sees that $\mathtt{q}(\kappa)$ extends to a family of sectorial forms with angle $\theta < \frac{\pi}{4}$, and that $\mathtt{q}(\kappa)$ is holomorphic in the strip $\Sigma_{\alpha^{-1}}$ (indeed, $\|\mathrm{Im}(\kappa)\|_{\mathbb{R}^3} < \alpha^{-1}$ is needed to assure that the complex number under the square root in (70) has non-negative real part for all $\mathbf{p} \in \mathbb{R}^3$). Moreover, $\mathtt{q}(\kappa)$ is closed. Indeed, it is sufficient to prove that the real part of $\mathtt{q}(\kappa)$ is closed, which will follow from

$$\mathtt{v}(\mathrm{u}, \mathrm{u}) + \mathtt{r}_\gamma(\mathrm{u}, \mathrm{u}) + \mathtt{k}_\gamma(\mathrm{u}, \mathrm{u}) + \langle \mathrm{u}, \mathtt{E}\mathrm{u} \rangle \leq b \, \mathrm{Re}(\mathtt{t}(\kappa))(\mathrm{u}, \mathrm{u}) + K \langle \mathrm{u}, \mathrm{u} \rangle \,, \tag{71}$$

with $b < 1$, $K > 0$ and $\mathrm{Re}(\mathtt{t}(\kappa))$ closed. We now prove (71). We already know that

$$\mathtt{r}_\gamma(\mathrm{u}, \mathrm{u}) + \mathtt{k}_\gamma(\mathrm{u}, \mathrm{u}) + \langle \mathrm{u}, \mathtt{E}\mathrm{u} \rangle \leq K' \langle \mathrm{u}, \mathrm{u} \rangle \text{ for } K' > 0 \,. \tag{72}$$

By (8) we find

$$\begin{aligned} \mathtt{v}(\mathrm{u}, \mathrm{u}) &\leq (Z\alpha) \frac{\pi}{2} \sum_{i=1}^{N} \int_{\mathbb{R}^3} |\mathbf{p}| \, |\hat{\mathrm{u}}_i(\mathbf{p})|^2 \, d\mathbf{p} \\ &\leq (Z\alpha) \frac{\pi}{2} R \sum_{i=1}^{N} \Big[\int_{|\mathbf{p}| \leq R} |\hat{\mathrm{u}}_i(\mathbf{p})|^2 \, d\mathbf{p} + \int_{|\mathbf{p}| \geq R} |\mathbf{p}| \, |\hat{\mathrm{u}}_i(\mathbf{p})|^2 \, d\mathbf{p} \Big] \,. \end{aligned} \tag{73}$$

Let $\delta > 0$ be such that $Z\alpha\frac{\pi}{2}(1-\delta)^{-1} < 1$. Since

$$\begin{aligned}\mathrm{Re}(\mathtt{t}(\kappa))(\mathrm{u},\mathrm{u}) = \sum_{i=1}^{N}\int_{\mathbb{R}^3}\Big|\alpha^{-2}+\sum_{j=1}^{3}(p_j-\kappa_j)^2\Big|^{1/2}\cos(\theta(\mathbf{p},\kappa))\,|\hat{\mathrm{u}}_i(\mathbf{p})|^2\,d\mathbf{p}\\ -\alpha^{-1}\langle \mathrm{u},\mathrm{u}\rangle\,,\end{aligned}$$

with

$$2\cos^2(\theta(\mathbf{p},\kappa))-1 = \frac{\alpha^{-2}+\sum_{j=1}^{3}(p_j-\mathrm{Re}(\kappa_j))^2-(\mathrm{Im}(\kappa_j))^2)}{|\alpha^{-2}+\sum_{j=1}^{3}(p_j-\kappa_j)^2|}\,,$$

there exists $R > 0$ such that $\cos(\theta(\mathbf{p},\kappa)) \geq (1-\delta)$ for $|\mathbf{p}| > R$. Hence we find that

$$\begin{aligned}\mathrm{Re}(\mathtt{t}(\kappa))(\mathrm{u},\mathrm{u}) &\geq (1-\delta)\sum_{i=1}^{N}\int_{|\mathbf{p}|>R}\Big|\alpha^{-2}+\sum_{j=1}^{3}(p_j-\kappa_j)^2\Big|^{1/2}|\hat{\mathrm{u}}_i(\mathbf{p})|^2\,d\mathbf{p}\\ &\quad -\alpha^{-1}\langle \mathrm{u},\mathrm{u}\rangle\\ &\geq (1-\delta)\sum_{i=1}^{N}\int_{|\mathbf{p}|>R}(|\mathbf{p}|-C)|\,\hat{\mathrm{u}}_i(\mathbf{p})|^2\,d\mathbf{p}-\alpha^{-1}\langle \mathrm{u},\mathrm{u}\rangle\,,\end{aligned} \tag{74}$$

with $C > \|\mathrm{Re}(\kappa)\|_{\mathbb{R}^3}$. The estimate in (71) follows combining (72) with (73) and (74).

The fact that $\mathrm{Re}(\mathtt{t}(\kappa))$ is closed follows from

$$\frac{1}{\sqrt{2}}\sum_{i=1}^{N}\int(|\mathbf{p}|-C)\,|\hat{\mathrm{u}}_i(\mathbf{p})|^2\,d\mathbf{p} \leq \mathrm{Re}(\mathtt{t}(\kappa))(\mathrm{u},\mathrm{u}) \leq \sum_{i=1}^{N}\int(|\mathbf{p}|+C)|\hat{\mathrm{u}}_i(\mathbf{p})|^2\,d\mathbf{p}\,,$$

with $C \geq 2\alpha^{-1}+\mathrm{Re}(\kappa)$.

Hence, $\mathtt{q}(\kappa)$ is an analytic family of forms of type (a) ([15, p. 395]). The associated family $\mathtt{H}(\kappa)$ of sectorial operators is a holomorphic family of operators of type (B) and has domain in a subset of $[H^{1/2}(\mathbb{R}^3)]^N$.

We are interested now in locating the essential spectrum of $\mathtt{H}(\kappa)$. Since K_γ is a Hilbert-Schmidt operator, the essential spectrum of $\mathtt{H}(\kappa)$ coincides with the essential spectrum of the operator associated to

$$\mathtt{t}(\kappa)(\mathrm{u},\mathrm{u})-\mathtt{v}(\mathrm{u},\mathrm{u})+\alpha\,\mathtt{r}_\gamma(\mathrm{u},\mathrm{u})+\langle \mathrm{u},\mathtt{E}\mathrm{u}\rangle\,.$$

Notice that the operator associated to this quadratic form is diagonal. Proceeding as in the proof of $\sigma_{\mathrm{ess}}(h_\gamma) = [0,\infty)$ (Lemma 2), one sees that $\sigma_{\mathrm{ess}}(\mathtt{H}(\kappa)) \subset \sigma_{\mathrm{ess}}(T(\kappa)-\varepsilon_N)$ with $T(\kappa) := \sqrt{\alpha^{-2}+\sum_{j=1}^{3}(p_j-\kappa_j)^2}-\alpha^{-1}$. Hence we find that

$$\sigma_{\mathrm{ess}}(\mathtt{H}(\kappa)) \subset \big\{z\in\mathbb{C}\,\big|\,\mathrm{Re}(z)\geq\sqrt{\alpha^{-2}-\|\mathrm{Im}(\kappa)\|^2_{\mathbb{R}^3}}-\alpha^{-1}-\varepsilon_N\big\}\,.$$

Hence 0, eigenvalue of $\mathtt{H}(0)$, remains disjoint from the essential spectrum of $\mathtt{H}(\kappa)$ for all $\kappa\in\Sigma_{\nu_{\varepsilon_N}}$ (recall that $\Sigma_{\nu_{\varepsilon_N}}\subset\Sigma_{\alpha^{-1}}$) .

Since $\mathtt{H}(\kappa)$ is an analytic family of type (B) [27, p.20] in Σ_{ν_ε}, 0 is an eigenvalue of $\mathtt{H}(0)$ and moreover, 0 remains disjoint from the essential spectrum of $\mathtt{H}(\kappa)$, it follows that 0 is an eigenvalue in the pure point spectrum of $\mathtt{H}(\kappa)$ for all $\kappa\in\Sigma_{\nu_{\varepsilon_N}}$ (reasoning as in [27, page 187]). Let $\mathtt{P}(\kappa)$ be the projection onto the eigenspace corresponding to the eigenvalue 0 of the operator $\mathtt{H}(\kappa)$. Then $\mathtt{P}(\kappa)$ is an analytic function in $\Sigma_{\nu_{\varepsilon_N}}$ and for $\kappa\in\Sigma_{\nu_{\varepsilon_N}}$ and $\kappa_0\in\mathbb{R}$ we have

$$\mathtt{P}(\kappa+\kappa_0) = W(\kappa_0)\mathtt{P}(\kappa)W(-\kappa_0)\,.$$

Here we used that $W(-\kappa_0)$ is a unitary operator. The result of the lemma follows by applying Lemma 5 below to $\tilde{W}(\theta) := e^{i\theta\kappa\cdot\mathbf{x}}$ with $\kappa \in \mathbb{R}^3$, $\|\kappa\|_{\mathbb{R}^3} = \nu_{\varepsilon_N}$, and $\theta \in \{z \in \mathbb{C} \,|\, |\mathrm{Im}(z)| < 1\}$. Notice that $\tilde{W}(\theta) = W(\theta\kappa)$ and that the projection $\tilde{\mathtt{P}}(\theta) := \mathtt{P}(\theta\kappa)$ is analytic and satisfies $\tilde{\mathtt{P}}(\theta+\theta_0) = \tilde{W}(\theta_0)\tilde{\mathtt{P}}(\theta)\tilde{W}(-\theta_0)$ for $\theta_0 \in \mathbb{R}$.

This finishes the proof of (i).

To prove (ii), we can work directly with the Hartree-Fock equation, since, from (i), the function $K_{\gamma^{\mathrm{HF}}}\varphi$ is exponentially decaying. Therefore, let

$$\mathfrak{q}[u,v] = (u, h_{\gamma^{\mathrm{HF}}}v) - \varepsilon(u,v) \quad \text{for} \quad u,v \in H^{1/2}(\mathbb{R}^3)\,, \tag{75}$$

and note that, by assumption, 0 is an eigenvalue for the corresponding operator (φ is an eigenfunction). Define, for $\kappa \in \mathbb{R}^3$,

$$\begin{aligned}\mathfrak{q}(\kappa)[u,v] &= \mathfrak{q}[W(-\kappa)u, W(-\kappa)v] \\ &= \mathfrak{t}(\kappa)[u,v] - \mathfrak{v}[u,v] + \mathfrak{b}_{\gamma^{\mathrm{HF}}}(\kappa)[u,v] - \varepsilon(u,v)\,,\end{aligned} \tag{76}$$

with $W(\kappa)$ and $\mathfrak{t}(\kappa)$ as before (but now on $H^{1/2}(\mathbb{R}^3)$), see (70), and

$$\mathfrak{b}_{\gamma^{\mathrm{HF}}}(\kappa)[u,v] = \alpha(u, R_{\gamma^{\mathrm{HF}}}v) - \alpha(u, K_{\gamma^{\mathrm{HF}}}(\kappa)v)\,, \tag{77}$$

where

$$K_{\gamma^{\mathrm{HF}}}(\kappa)(\mathbf{x},\mathbf{y}) = \sum_{j=1}^{N} \frac{\varphi_j(\mathbf{x})e^{i\kappa\mathbf{x}}e^{-i\kappa\mathbf{y}}\overline{\varphi_j(\mathbf{y})}}{|\mathbf{x}-\mathbf{y}|}\,. \tag{78}$$

Using (i) of the proposition (exponential decay of the Hartree-Fock orbitals $\{\varphi_j\}_{j=1}^N$) one now proves that (78) extends to a holomorphic family of Hilberts-Schmidt operators in $\Sigma_{\nu_{\varepsilon_N}}$. One can now repeat the reasoning in the proof of (i) to obtain the stated exponential decay of φ. $\square$

Lemma 5. ([27, p. 196]) *Let $W(\kappa) = e^{i\kappa A}$ be a one-parameter unitary group (in particular, A is self-adjoint) and let D be a connected region in $\mathbb{C}$ with $0 \in D$. Suppose that a projection-valued analytic function $P(\kappa)$ is given on D with $P(0)$ of finite rank and so that*

$$W(\kappa_0)P(\kappa)W(\kappa_0)^{-1} = P(\kappa+\kappa_0) \text{ for } \kappa_0 \in \mathbb{R} \text{ and } \kappa, \kappa+\kappa_0 \in D\,.$$

Let $\psi \in \mathrm{Ran}(P(0))$. Then the function $\psi(\kappa) = W(\kappa)\psi$ has an analytic continuation from $D \cap \mathbb{R}$ to D.

A Some useful lemmata

Lemma 6. *Let Ω be an open subset of $\mathbb{R}^3 \setminus \{0\}$ with smooth boundary and let $f_1, f_2 \in H^k(\Omega)$ for some $k \geq 1$.*

Then the function

$$F(\mathbf{x}) := \int_{\mathbb{R}^3} \frac{f_1(\mathbf{y})f_2(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y}$$

belongs to $C^k(\Omega)$ if $k \geq 2$, while if $k = 1$, it belongs to $W^{1,p}(\Omega)$ for all $p \geq 1$, and hence to $C(\Omega)$.

Proof. We are going to prove the following equivalent statement. If $k \geq 2$, $\chi F \in C^k(\mathbb{R}^3)$ for all $\chi \in C_0^\infty(\Omega)$, while if $k = 1$, $\chi F \in W^{1,p}(\mathbb{R}^3)$ for all $p \geq 1$ and $\chi \in C_0^\infty(\Omega)$.

Fix $\chi \in C_0^\infty(\Omega)$ and take $\tilde\chi \in C_0^\infty(\Omega)$ verifying $\tilde\chi \equiv 1$ on $\operatorname{supp}\chi$ and such that there is a strictly positive distance between $\operatorname{supp}\chi$ and $\operatorname{supp}(1-\tilde\chi)$. We write $\chi F(\mathbf{x}) = \chi F_1(\mathbf{x}) + \chi F_2(\mathbf{x})$ with

$$F_1(\mathbf{x}) = \int_{\mathbb{R}^3} \frac{\tilde\chi(\mathbf{y}) f_1(\mathbf{y}) f_2(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y} \quad \text{and} \quad F_2(\mathbf{x}) = \int_{\mathbb{R}^3} (1-\tilde\chi(\mathbf{y})) \frac{f_1(\mathbf{y}) f_2(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y}\,.$$

The term χF_2 is clearly in $C^\infty(\mathbb{R}^3)$. For the other term we use Young's inequality: if $f \in L^p(\mathbb{R}^3)$ and $g \in L^q(\mathbb{R}^3)$ then

$$\|f * g\|_r \le C \|f\|_p \|g\|_q \quad \text{with } 1 + \frac{1}{r} = \frac{1}{p} + \frac{1}{q}\,. \tag{79}$$

Moreover, if $1/p + 1/q = 1$ then $f * g$ is continuous (see [31, Lemma 2.1]). Let $\alpha \in \mathbb{N}_0^3$ with $|\alpha| \le k$. Then

$$|D^\alpha(\chi F_1)(\mathbf{x})| \le \sum_{\substack{\beta_1+\beta_2=\alpha,\\ \beta_1,\beta_2\in\mathbb{N}_0^3}} |D^{\beta_1}\chi(\mathbf{x})| \Big| \int_{\mathbb{R}^3} \frac{1}{|\mathbf{x}-\mathbf{y}|} D^{\beta_2}(\tilde\chi f_1 f_2)(\mathbf{y}) d\mathbf{y} \Big|\,. \tag{80}$$

If $f_1, f_2 \in H^k(\Omega)$, $k \ge 2$, then $D^{\beta_2}(\tilde\chi f_1 f_2) \in L^{5/3}(\mathbb{R}^3)$ for all β_2 as in (80). From (79), (80) and $\tilde\chi/|\cdot| \in L^{5/2}(\mathbb{R}^3)$ it follows that $D^\alpha(\chi F_1)$ is continuous and, since α is arbitrary, that $\chi F \in C^k(\mathbb{R}^3)$.

If $f_1, f_2 \in H^1(\Omega)$ then $\partial(\tilde\chi f_1 f_2) \in L^{3/2}(\mathbb{R}^3)$ and from (79) we get (only) that $\partial(\chi F) \in L^p(\mathbb{R}^3)$ for all $p \ge 1$. It then follows that $F \in W^{1,p}(\Omega)$ for all $p \ge 1$ and therefore (by the Sobolev imbedding theorem) $F \in C(\Omega)$. □

Lemma 7. *Let, for $Z\alpha < 2/\pi$, h_0 be the self-adjoint operator defined in (9), and let $\Lambda_-(\alpha)$ be the projection onto the pure point spectrum of h_0.*

Then the operator $\Lambda_-(\alpha) h_0 \Lambda_-(\alpha)$ is Hilbert-Schmidt.

Proof. Let $\epsilon > 0$ be such that $Z\alpha(1+\epsilon) \le 2/\pi(1-\epsilon)$. We are going to prove that there exists a constant $M = M(\epsilon)$ such that

$$h_0 \ge \frac{1}{M + 2\alpha^{-1}} P(-\Delta - \frac{C}{|\cdot|})P\,, \tag{81}$$

with $C = Z\alpha(M + 2\alpha^{-1})(1 + 1/\epsilon)$ and $P = \chi_{[0,M]}(T(\mathbf{p}))$. The claim will then follow from (81) since

$$\operatorname{Tr}\big([h_0]_-\big)^2 \le \frac{1}{(M+2\alpha^{-1})^2} \operatorname{Tr}\big([-\Delta - \frac{C}{|\cdot|}]_-\big)^2 < \infty\,.$$

The last inequality follows since the eigenvalues of $-\Delta - C/|\cdot|$ are $-C^2/4n^2, n \in \mathbb{N}$, with multiblicity n^2.

We now prove (81). For $\epsilon > 0$ and any projection P (with $P^\perp = \mathbf{1} - P$), we have that

$$\begin{aligned} h_0 &= P h_0 P + P^\perp h_0 P^\perp - P \frac{Z\alpha}{|\cdot|} P^\perp - P^\perp \frac{Z\alpha}{|\cdot|} P \\ &\ge P(h_0 - \frac{1}{\epsilon}\frac{Z\alpha}{|\cdot|})P + P^\perp(h_0 - \epsilon \frac{Z\alpha}{|\cdot|})P^\perp\,. \end{aligned} \tag{82}$$

By a direct computation one sees that there exists a constant $M = M(\epsilon)$ such that $T(\mathbf{p}) \ge M$ implies $T(\mathbf{p}) \ge (1-\epsilon)|\mathbf{p}|$ and $T(\mathbf{p}) \le M$ implies $T(\mathbf{p}) \ge \frac{1}{M+2\alpha^{-1}}(-\Delta)$. Hence, with this choice of M and $P = \chi_{[0,M]}(T(\mathbf{p}))$, (82) implies that

$$h_0 \ge P\big[\frac{1}{M+2\alpha^{-1}}(-\Delta) - (1+\epsilon^{-1})\frac{Z\alpha}{|\cdot|}\big]P + P^\perp\big[(1-\epsilon)\sqrt{-\Delta} - (1+\epsilon)\frac{Z\alpha}{|\cdot|}\big]P^\perp\,.$$

The inequality (81) follows directly by the choice of ϵ. □

B Pseudodifferential operators

In this appendix we collect facts needed from the calculus of pseudodifferential operators (ψdo's) (for references, see e.g. [14] or [28]).

Define the standard (Hörmander) symbol class $S^\mu(\mathbb{R}^n)$, $\mu \in \mathbb{R}$, to be the set of functions $a \in C^\infty(\mathbb{R}^n_x \times \mathbb{R}^n_\xi)$ satisfying

$$\left|\partial_x^\alpha \partial_\xi^\beta a(x,\xi)\right| \le C_{\alpha,\beta}(1+|\xi|^2)^{(\mu-|\beta|)/2} \text{ for all } (x,\xi) \in \mathbb{R}^n_x \times \mathbb{R}^n_\xi \,. \tag{83}$$

Here, $\alpha, \beta \in \mathbb{N}^n$ and $|\alpha| = \alpha_1 + \cdots + \alpha_n$. Furthermore, $S^\mu(\mathbb{R}^n) \subset S^{\mu'}(\mathbb{R}^n)$ for $\mu \le \mu'$. We denote $S^\infty(\mathbb{R}^n) = \cup_{\mu\in\mathbb{R}} S^\mu(\mathbb{R}^n)$ and $S^{-\infty}(\mathbb{R}^n) = \cap_{\mu\in\mathbb{R}} S^\mu(\mathbb{R}^n)$. Finally, note that $ab \in S^{\mu_1+\mu_2}(\mathbb{R}^n)$, $\partial_x^\alpha \partial_\xi^\beta a \in S^{\mu_1-|\beta|}(\mathbb{R}^n)$ when $a \in S^{\mu_1}(\mathbb{R}^n), b \in S^{\mu_2}(\mathbb{R}^n)$.

A symbol $a \in S^\mu(\mathbb{R}^n)$ defines a linear operator $A = \mathrm{Op}(a) \in: \Psi^\mu$ ('pseudodifferential operator of order μ') by

$$[\mathrm{Op}(a)u](x) = (2\pi)^{-n} \int_{\mathbb{R}^n} e^{ix\cdot\xi} a(x,\xi)\hat{u}(\xi)\, d\xi \,, \tag{84}$$

where $\hat{u}$ is the Fourier-transform of u. The operator A is well-defined on the space $\mathcal{S}(\mathbb{R}^n)$ of Schwartz-functions; it extends by duality to $\mathcal{S}'(\mathbb{R}^n)$, the space of tempered distributions. Note that for

$$a(x,\xi) = \sum_{0\le|\alpha|\le\mu} a_\alpha(x)\xi^\alpha \tag{85}$$

(with a_α smooth and with all derivatives bounded, i.e., $a_\alpha \in \mathcal{B}(\mathbb{R}^n)$), $A = \mathrm{Op}(a) \in \Psi^\mu$ is the partial differential operator given by

$$[\mathrm{Op}(a)u](x) = \sum_{0\le|\alpha|\le\mu} a_\alpha(x) D^\alpha u(x) \,. \tag{86}$$

Note also that, with $a = a(x)$ and $b = b(\xi)$,

$$[\mathrm{Op}(a)u](x) = a(x)u(x) \text{ and } [\widehat{\mathrm{Op}(b)u}](\xi) = b(\xi)\hat{u}(\xi) \,.$$

If $a \in S^\mu(\mathbb{R}^n)$, then $\mathrm{Op}(a)$, defined this way, maps $H^k(\mathbb{R}^n)$ continuously into $H^{k-\mu}(\mathbb{R}^n)$ for all $k \in \mathbb{R}$. Here, $H^k(\mathbb{R}^n)$ is the Sobolev-space of order k, consisting of $u \in \mathcal{S}'(\mathbb{R}^n)$ for which

$$\|u\|^2_{H^k(\mathbb{R}^n)} := \int_{\mathbb{R}^n} |\hat{u}(\xi)|^2 (1+|\xi|^2)^k \, d\xi \tag{87}$$

is finite; this defines the norm on $H^k(\mathbb{R}^n)$. We denote

$$H^\infty(\mathbb{R}^n) = \bigcap_{k\in\mathbb{R}} H^k(\mathbb{R}^n) \,, \quad H^{-\infty}(\mathbb{R}^n) = \bigcup_{k\in\mathbb{R}} H^k(\mathbb{R}^n) \,.$$

In particular, symbols in $S^0(\mathbb{R}^n)$ define bounded operators on $L^2(\mathbb{R}^n) = H^0(\mathbb{R}^n)$. Furthermore, operators defined by symbols in $S^{-\infty}(\mathbb{R}^n)$ maps any $H^k(\mathbb{R}^n)$ into $H^\infty(\mathbb{R}^n)$; such operators are called 'smoothing'.

We need to compose ψdo's. There exists a composition $\#$ of symbols,

$$\# : S^{\mu_1}(\mathbb{R}^n) \times S^{\mu_2}(\mathbb{R}^n) \to S^{\mu_1+\mu_2}(\mathbb{R}^n) \tag{88}$$

$$(a,b) \mapsto a\#b \,, \tag{89}$$

such that $\mathrm{Op}(a)\mathrm{Op}(b) = \mathrm{Op}(a\#b)$. It is given by

$$(a\#b)(x,\xi) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n\times\mathbb{R}^n} e^{-iy\cdot\xi} a(x,\xi-\eta) b(x-y,\eta)\, dy d\eta\,. \tag{90}$$

Here, the integral is to be understood as an oscillating integral.

The symbol $a\#b$ has the expansion

$$a\#b \sim \sum_{\alpha} \frac{i^{-|\alpha|}}{\alpha!} (\partial_x^\alpha a)(\partial_\xi^\alpha b)\,. \tag{91}$$

Here, '$\sim$' means that for all $j \in \mathbb{N}$,

$$a\#b - \sum_{|\alpha|<j} \frac{i^{-|\alpha|}}{\alpha!} (\partial_x^\alpha a)(\partial_\xi^\alpha b) \in S^{\mu_1+\mu_2-j}(\mathbb{R}^n) \tag{92}$$

(recall that $(\partial_x^\alpha a)(\partial_\xi^\alpha b) \in S^{\mu_1+\mu_2-|\alpha|}$). One easily sees that the composition is associative.

Proposition 2. *If $a \in S^{m_1}(\mathbb{R}^n)$, $b \in S^{m_2}(\mathbb{R}^n)$ then the symbol associated to $[\mathrm{Op}(a), \mathrm{Op}(b)]$ belongs to $S^{m_1+m_2-1}(\mathbb{R}^n)$.*

In particular, if $\phi_1, \phi_2 \in \mathcal{B}^\infty(\mathbb{R}^n)$ (the smooth functions with bounded derivatives) with $\mathrm{supp}\,\phi_1 \cap \mathrm{supp}\,\phi_2 = \emptyset$ and $a \in S^\mu(\mathbb{R}^n)$, $a(x,\xi) = a(\xi)$, then $\phi_1\#a\#\phi_2 \sim 0$, and so, with $A := \mathrm{Op}(a)$,

$$\phi_1 A \phi_2 = \mathrm{Op}(\phi_1)\mathrm{Op}(a)\mathrm{Op}(\phi_2)$$

is smoothing.

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Real analyticity away from the nucleus of pseudorelativistic Hartree-Fock orbitals

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Abstract

We prove that the Hartree-Fock orbitals of pseudorelativistic atoms, that is, atoms where the kinetic energy of the electrons is given by the pseudorelativistic operator $\sqrt{-\Delta+1}-1$, are real analytic away from the origin.

Our proof is inspired by the classical proof of analyticity by nested balls of Morrey and Nirenberg [27]. However, the technique has to be adapted to take care of the non-local pseudodifferential operator, the singularity of the potential at the origin, and the non-linear terms in the equation.

1 Introduction and results

In a recent paper [5], three of the present authors studied the Hartree-Fock model for pseudorelativistic atoms, and proved the existence of Hartree-Fock minimizers. Furthermore, they proved that the corresponding Hartree-Fock orbitals (solutions to the associated Euler-Lagrange equation) are smooth away from the nucleus, and that they decay exponentially. In this paper we prove that all of these orbitals are, in fact, real analytic away from the origin. Apart from intrinsic mathematical interest, analyticity of solutions has important consequences. For example, in the non-relativistic case, the analyticity of the orbitals and the regularity properties of the true quantum mechanical eigenfunction was used in [14] to prove that the quantum mechanical ground state is never a Hartree-Fock state. Our proof also shows that any $H^{1/2}$-solution $\varphi:\mathbb{R}^3\to\mathbb{C}$ to the non-linear equation

$$(\sqrt{-\Delta+1})\varphi-\frac{Z}{|\cdot|}\varphi\pm\big(|\varphi|^2*|\cdot|^{-1}\big)\varphi=\lambda\varphi \tag{1}$$

which is smooth away from $\mathbf{x}=0$, is in fact real analytic there. As will be clear from the proof, our method yields the same result for solutions to equations of the form

$$(-\Delta+m)^s\varphi+V\varphi+|\varphi|^k\varphi=\lambda\varphi\,, \tag{2}$$

where V has a finite number of point singularities (but is analytic elsewhere), under certain conditions on m, s, V, and k (see Remark 1.2 below). We believe this result is of independent interest,

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but stick concretely to the case of pseudorelativistic Hartree-Fock orbitals, since this was the original motivation for the present work.

We consider a model for an atom with N electrons and nuclear charge Z (fixed at the origin), where the kinetic energy of the electrons is described by the expression $\sqrt{(|\mathbf{p}|c)^2+(mc^2)^2}-mc^2$. This model takes into account some (kinematic) relativistic effects; in units where $\hbar = e = m = 1$, the Hamiltonian becomes

$$H=\sum_{j=1}^{N}\alpha^{-1}\Big\{T(-\mathrm{i}\nabla_j)-V(\mathbf{x}_j)\Big\}+\sum_{1\le i<j\le N}\frac{1}{|\mathbf{x}_i-\mathbf{x}_j|}\,, \tag{3}$$

with $T(\mathbf{p})=E(\mathbf{p})-\alpha^{-1}=\sqrt{|\mathbf{p}|^2+\alpha^{-2}}-\alpha^{-1}$ and $V(\mathbf{x})=Z\alpha/|\mathbf{x}|$. Here, α is Sommerfeld's fine structure constant; physically, $\alpha\simeq 1/137$.

The operator H acts on a dense subspace of the N-particle Hilbert space $\mathcal{H}_F=\wedge_{i=1}^{N}L^2(\mathbb{R}^3)$ of antisymmetric functions. (We will not consider spin since it is irrelevant for our discussion.) It is bounded from below on this subspace if and only if $Z\alpha\le 2/\pi$ (see [25]; for a number of other works on this operator, see [3, 6, 9, 16, 23, 28, 31, 32]).

The *(quantum) ground state energy* is the infimum of the quadratic form $\mathfrak{q}$ defined by H, over the subset of elements of norm 1 of the corresponding form domain. Hence, it coincides with the infimum of the spectrum of H considered as an operator acting in $\mathcal{H}_F$.

In the Hartree-Fock approximation, instead of minimizing the quadratic form $\mathfrak{q}$ in the entire N-particle space $\mathcal{H}_F$, one restricts to wavefunctions Ψ which are pure wedge products, also called Slater determinants:

$$\Psi(\mathbf{x}_1,\dots,\mathbf{x}_N)=\frac{1}{\sqrt{N!}}\,\det(u_i(\mathbf{x}_j))_{i,j=1}^{N}\,, \tag{4}$$

with $\{u_i\}_{i=1}^N$ orthonormal in $L^2(\mathbb{R}^3)$ (called *orbitals*). Notice that this way, $\Psi\in\mathcal{H}_F$ and $\|\Psi\|_{L^2(\mathbb{R}^{3N})}=1$.

The *Hartree-Fock ground state energy* is the infimum of the quadratic form $\mathfrak{q}$ defined by H over such Slater determinants:

$$E^{\mathrm{HF}}(N,Z,\alpha):=\inf\{\,\mathfrak{q}(\Psi,\Psi)\,|\,\Psi\text{ Slater determinant}\,\}\,. \tag{5}$$

Inserting Ψ of the form in (4) into $\mathfrak{q}$ formally yields

$$\begin{aligned}\mathcal{E}^{\mathrm{HF}}(u_1,\dots,u_N)&:=\mathfrak{q}(\Psi,\Psi)\\&=\alpha^{-1}\sum_{j=1}^{N}\int_{\mathbb{R}^3}\big\{\,\overline{u_j(\mathbf{x})}\,[T(-\mathrm{i}\nabla)u_j](\mathbf{x})-V(\mathbf{x})|u_j(\mathbf{x})|^2\big\}\,d\mathbf{x}\\&\quad+\frac12\sum_{1\le i,j\le N}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{|u_i(\mathbf{x})|^2|u_j(\mathbf{y})|^2}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}d\mathbf{y}\\&\quad-\frac12\sum_{1\le i,j\le N}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\overline{u_j(\mathbf{x})}u_i(\mathbf{x})\overline{u_i(\mathbf{y})}u_j(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}d\mathbf{y}\,.\end{aligned} \tag{6}$$

In fact, $u_i\in H^{1/2}(\mathbb{R}^3)$, $1\le i\le N$, is needed for this to be well-defined (see Section 3 for a detailed discussion), and so (5)–(6) can be written

$$E^{\mathrm{HF}}(N,Z,\alpha)=\inf\{\,\mathcal{E}^{\mathrm{HF}}(u_1,\dots,u_N)\,|\,(u_1,\dots,u_N)\in\mathcal{M}_N\}\,, \tag{7}$$

$$\mathcal{M}_N=\big\{\,(u_1,\dots,u_N)\in[H^{1/2}(\mathbb{R}^3)]^N\;\big|\;(u_i,u_j)=\delta_{ij}\,\big\}\,. \tag{8}$$

Here, (,) denotes the scalar product in $L^2(\mathbb{R}^3)$. The existence of minimizers for the problem (7)–(8) was proved in [5] when $Z > N-1$ and $Z\alpha < 2/\pi$. (Note that such minimizers are generally not unique since $\mathcal{E}^{\mathrm{HF}}$ is not convex; see [10]). The existence of infinitely many distinct critical points of the functional $\mathcal{E}^{\mathrm{HF}}$ on $\mathcal{M}_N$ was proved recently (under the same conditions) in [7].

The Euler–Lagrange equations of the problem (7)–(8) are the *Hartree–Fock equations*,

$$\begin{aligned} \big[\big(T(-\mathrm{i}\nabla) - V\big)\varphi_i\big](\mathbf{x}) &+ \alpha\Big(\sum_{j=1}^{N}\int_{\mathbb{R}^3}\frac{|\varphi_j(\mathbf{y})|^2}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{y}\Big)\varphi_i(\mathbf{x}) \\ &- \alpha\sum_{j=1}^{N}\Big(\int_{\mathbb{R}^3}\frac{\overline{\varphi_j(\mathbf{y})}\varphi_i(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{y}\Big)\varphi_j(\mathbf{x}) = \varepsilon_i\varphi_i(\mathbf{x})\ , \quad 1 \le i \le N\,. \end{aligned} \tag{9}$$

Here, the ε_i's are the Lagrange multipliers of the orthonormality constraints in (8). (Note that the naive Euler–Lagrange equations are more complicated than (9), but can be transformed to (9); see [10].) Note that (9) can be re-formulated as

$$h_{\boldsymbol{\varphi}}\varphi_i = \varepsilon_i\varphi_i\ , \quad 1 \le i \le N\,, \tag{10}$$

with $h_{\boldsymbol{\varphi}}$ the *Hartree-Fock operator associated to* $\boldsymbol{\varphi} = \{\varphi_1, \dots, \varphi_N\}$, formally given by

$$h_{\boldsymbol{\varphi}}u = [T(-\mathrm{i}\nabla) - V]u + \alpha R_{\boldsymbol{\varphi}}u - \alpha K_{\boldsymbol{\varphi}}u\,, \tag{11}$$

where $R_{\boldsymbol{\varphi}}u$ is the *direct interaction*, given by the multiplication operator defined by

$$R_{\boldsymbol{\varphi}}(\mathbf{x}) := \sum_{j=1}^{N}\int_{\mathbb{R}^3}\frac{|\varphi_j(\mathbf{y})|^2}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{y} \tag{12}$$

and $K_{\boldsymbol{\varphi}}u$ is the *exchange term*, given by the integral operator

$$(K_{\boldsymbol{\varphi}}u)(\mathbf{x}) = \sum_{j=1}^{N}\Big(\int_{\mathbb{R}^3}\frac{\overline{\varphi_j(\mathbf{y})}u(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{y}\Big)\varphi_j(\mathbf{x})\,. \tag{13}$$

The equations (9) (or equivalently (10)) are called the *self-consistent Hartree-Fock equations*. One has that $\sigma_{\mathrm{ess}}(h_{\boldsymbol{\varphi}}) = [0,\infty)$ and that, when in addition $N < Z$, the operator $h_{\boldsymbol{\varphi}}$ has infinitely many eigenvalues in $[-\alpha^{-1}, 0)$ (see [5, Lemma 2]; the argument given there holds for any $\boldsymbol{\varphi} = \{\varphi_1, \dots, \varphi_N\}$, $\varphi_i \in H^{1/2}(\mathbb{R}^3)$, as long as $Z\alpha < 2/\pi$). If $(\varphi_1, \dots, \varphi_N) \in \mathcal{M}_N$ is a minimizer for the problem (7)–(8), then the φ_i's solve (10) with $\varepsilon_1 \le \varepsilon_2 \le \dots \le \varepsilon_N < 0$ the N *lowest* eigenvalues of the operator $h_{\boldsymbol{\varphi}}$ [5].

In [5] it was proved that solutions $\{\varphi_1, \dots, \varphi_N\}$ to (9)—and, more generally, all eigenfunctions of the corresponding Hartree-Fock operator $h_{\boldsymbol{\varphi}}$—are smooth away from $\mathbf{x} = 0$ (the singularity of V), and that (for the φ_i's for which $\varepsilon_i < 0$) they decay exponentially. (The solutions studied in [5] came from a minimizer of $\mathcal{E}^{\mathrm{HF}}$, but the proof trivially extends to the solutions $\{\boldsymbol{\varphi}_n\}_{n\in\mathbb{N}} = \big\{\{\varphi_1^n, \dots, \varphi_N^n\}\big\}_{n\in\mathbb{N}}$ to (9) found in [7], and to all the eigenfunctions of the corresponding Hartree-Fock operators mentioned above). The main theorem of this paper is the following, which completely settles the question of regularity away from the origin of solutions to the equations (9).

Theorem 1.1. *Let $Z\alpha < 2/\pi$, and let $N \ge 2$ be a positive integer such that $N < Z+1$. Let $\boldsymbol{\varphi} = \{\varphi_1, \dots, \varphi_N\}$, $\varphi_i \in H^{1/2}(\mathbb{R}^3)$, $i = 1, \dots, N$, be solutions to the pseudorelativistic Hartree-Fock equations in* (9).

Then, for $i = 1, \ldots, N$,

$$\varphi_i \in C^\omega(\mathbb{R}^3 \setminus \{0\}), \tag{14}$$

that is, the Hartree-Fock orbitals are real analytic away from the origin in $\mathbb{R}^3$.

Remark 1.2. *(i) The restrictions $Z\alpha < 2/\pi$, $N < Z+1$, and $N \geq 2$ are only made to ensure existence of $H^{1/2}$-solutions to* (9). *In fact, our proof proves analyticity away from $\mathbf{x} = 0$ for $H^{1/2}$-solutions to* (9) *for any $Z\alpha$. For the case $N = 1$,* (9) *reduces to $(T - V)\varphi = \varepsilon\varphi$ and our result also holds for $H^{1/2}$-solutions to this equation (see also (iv) and (v) below about more general V for which the result also holds for the linear equation). More interestingly, the result also holds for $H^{1/2}$-solutions to* (1) *(which, strictly speaking, cannot be obtained from* (9) *by any choice of N).*

(ii) The statement also holds for any eigenfunction of the associated Hartree-Fock operator given by (11).

(iii) It is obvious from the proof that the theorem holds true if we include spin.

(iv) As will also be clear from the proof, the statement of Theorem 1.1 (appropriately modified) also holds for molecules. More explicitely, for a molecule with K nuclei of charges $Z_1, \ldots, Z_K$, fixed at $R_1, \ldots, R_K \in \mathbb{R}^3$, replace V in (9) *by $\sum_{k=1}^K V_k$ with $V_k(\mathbf{x}) = Z_k\alpha/|\mathbf{x} - R_k|, Z_k\alpha < 2/\pi$. Then, for $N < 1 + \sum_{k=1}^K Z_k$, Hartree-Fock minimizers exist (see [5, Remark 1 (viii)]), and the corresponding Hartree-Fock orbitals are real analytic away from the positions of the nuclei, i.e., belong to $C^\omega(\mathbb{R}^3 \setminus \{R_1, \ldots, R_K\})$.*

(v) In fact, for V we only need the analyticity of V away from finitely many points in $\mathbb{R}^3$, and certain integrability properties of $V\varphi_i$ in the vicinity of each of these points, and at infinity; for more details, see Remark 4.1.

(vi) As will be clear from the proof, the statement of Theorem 1.1 also holds for other non-linearities than the Hartree-Fock term in (9), *namely $|\varphi|^k\varphi$ as in* (2) *(for k even; for k odd, one needs to take φ^{k+1}). The L^p-space in which one needs to study the problem (see Proposition 2.1 and the description of the proof below for details) needs to be chosen depending on k in this case (the larger the k, the larger the p).*

(vii) Also, as will be clear from the proof, the result holds if $T(-\mathrm{i}\nabla) = |\nabla|$ (i.e., $T(\mathbf{p}) = |\mathbf{p}|$) in (9). *In* (35) *below, $E(\mathbf{p})^{-1}$ should then be replaced by $(|\mathbf{p}|+1)^{-1}$ (and '1' added to '$\alpha^{-1}+\varepsilon_i$'). The only properties of $E(\mathbf{p})^{-1}$ used are in Lemmas C.1 and C.2, which follow also for $(|\mathbf{p}|+1)^{-1}$ from the same methods with minor modifications. Similarly, one can replace $T(\mathbf{p})$ with $(-\Delta + \alpha^{-2})^s$, $s \in [1/2, 1]$.*

(viii) The result of Theorem 1.1 in the non-relativistic case ($T(-\mathrm{i}\nabla)$ replaced by $-\alpha\Delta$ in (3)*) was proved in [13, 22]; see also the discussion below. In this case, it is furthermore known [10] that, for $\mathbf{x} \in B_r(0)$ for some $r > 0$, $\varphi_i(\mathbf{x}) = \varphi_i^{(1)}(\mathbf{x}) + |\mathbf{x}|\varphi_i^{(2)}(\mathbf{x})$ with $\varphi_i^{(1)}, \varphi_i^{(2)} \in C^\omega(B_r(0))$.*

Description of the proof: The proof of Theorem 1.1 is inspired by the standard Morrey-Nirenberg [27] proof of analyticity of solutions to general (linear) elliptic partial differential equations with real analytic coefficients by 'nested balls'. A good presentation of this technique can be found in [17]. (Other proofs using a complexification of the coordinates also exist and have been applied to both linear and non-linear equations; see [26] and references therein.)

In [17] one proves L^2-bounds on derivatives of order k of the solution in a ball B_r (of some radius r) around a given point. These bounds should behave suitably in k in order to make the Taylor series of the solution converge locally, thereby proving analyticity.

The proof of these bounds is inductive. In fact, for some ball B_R with $R > r$, one proves the bounds on all balls B_ρ with $r \leq \rho \leq R$, with the appropriate (with respect to k) behaviour in $R - \rho$. The induction basis is provided by standard elliptic estimates. In the induction step, one has to bound $k+1$ derivatives of the solution in the ball B_ρ. To do so, one divides the difference $B_R \setminus B_\rho$ into $k+1$ nested balls using $k+1$ localization functions with successively larger supports. Commuting m of the k derivatives (in the case of an operator of order m) with these localization functions produces (local) differential operators of order $m-1$, with support in a larger ball. These local commutator terms are controlled by the induction hypothesis, since they contain one derivative less. For the last term—the term where no commutators occur—one then uses the equation.

This approach poses new technical difficulties in our case, due to the non-locality of the kinetic energy $T(\mathbf{p}) = \sqrt{-\Delta + \alpha^{-2}} - \alpha^{-1}$ and the non-linearity of the terms $R_{\boldsymbol{\varphi}}\varphi_i$ and $K_{\boldsymbol{\varphi}}\varphi_i$.

The non-locality of the operator $\sqrt{-\Delta + \alpha^{-2}}$ implies that, as opposed to the case of a differential operator, the commutator of the kinetic energy with a localization function is not localized in the support of the localization function. That is, when resorting to proving analyticity by differentiating the equation, the localization argument described above introduces commutators which are (non-local) pseudodifferential operators. Now the induction hypothesis does not provide control of these terms. Furthermore, it is far from obvious that the singularity of the potential V outside B_R does not influence the regularity in B_R of the solution through these operators (or rather, through the non-locality of $\sqrt{-\Delta + \alpha^{-2}}$). Loosely speaking, the singularity of the nuclear potential 'can be felt everywhere'. (Note that if we would not have a (singular) potential V one could proceed as in [11] and prove global analyticity by showing exponential decay of the solutions in Fourier space.)

We overcome this problem by a new localization argument which enable us to capture in more detail the action of high order derivatives on nested balls (manifested in Lemma B.1 in Appendix B below). This, together with very explicit bounds on the (smoothing) operators $\phi E(\mathbf{p})^{-1} D^\beta \chi$ for χ and ϕ with disjoint supports (see Lemma C.2), are the main ingredients in solving the problem of nonlocality. The estimates are on $\phi E(\mathbf{p})^{-1} D^\beta \chi$ (not $\phi E(\mathbf{p}) D^\beta \chi$), since we invert $E(\mathbf{p})$ (turning the equation into an integral operator equation, see (35)). Our method of proof would also work in the non-relativistic case, since the integral operators $(-\Delta + 1)^{-1}$ and $E(\mathbf{p})^{-1}$ enjoy similar properties.

The second major obstacle is the (morally cubic) non-linearity of the terms $R_{\boldsymbol{\varphi}}\varphi_i$ and $K_{\boldsymbol{\varphi}}\varphi_i$.

To illustrate the problem, we discuss proving analyticity by the above method (local L^2-estimates) for solutions u to the equation $\Delta u = u^3$. When differentiating this equation (and therefore u^3), the application of Leibniz' rule introduces a sum of terms. After using Hölder's inequality on each term (the product of three factors, each a number of derivatives on u), one needs to use a Sobolev inequality to 'get back down to L^2' in order to use the induction hypothesis. Summing the many terms, the needed estimate does not come out (in fact, some Gevrey-regularity would follow, but not analyticity).

In the quadratic case this can be done (that is, for the equation $\Delta u = u^2$ this problem does *not* occur), but in the cubic case, one looses too many derivatives.

The second insight of our proof is that this problem of loss of derivatives may be overcome by characterizing analyticity by growth of derivatives in some L^p with $p > 2$. When working in L^p for $p > 2$, the loss of derivatives in the Sobolev inequality mentioned above is less (as seen in Theorem D.1. Choosing p sufficiently large allows us to prove the needed estimate. The operator estimates on $\phi E(\mathbf{p})^{-1} D^\beta \chi$ mentioned above therefore have to be L^p-estimates. In fact, using $L^p - L^q$ estimates, one can also deal with the problem that the singularity of the nuclear potential V 'can be felt everywhere'.

Note that taking $p = \infty$ would avoid using a Sobolev inequality altogether (L^∞ being an algebra), but the needed estimates on $\phi E(\mathbf{p})^{-1} D^\beta \chi$ cannot hold in this case. For local equations an approach to handle the loss of derivatives (due to Sobolev inequalities) exists. This was carried out in [12], where analyticity of solutions to elliptic partial differential equations with general analytic non-linearities was proved. Friedman works in spaces of continuous functions. In this approach, one needs to have a sufficiently high degree of regularity of the solution beforehand (it is not proved along the way). Also, since the elliptic regularity in spaces of continuous functions have an inherent loss of derivative, one needs to work on a sufficiently small domain in order for the method to work. We prefer to work in Sobolev spaces since this is the natural setting for our equation and since the needed estimates on the resolvent are readily obtained in these spaces.

For an alternative method of proof (one *fixed* localization function, to the power k, and estimating in a higher order Sobolev space (instead of in L^2) which is also an algebra), see Kato [19] (for the equation $\Delta u = u^2$) and Hashimoto [15] (for general second order non-linear analytic PDE's).

Additional technical difficulties occur due to the fact that the cubic terms, $R_{\boldsymbol{\varphi}}\varphi_i$ and $K_{\boldsymbol{\varphi}}\varphi_i$, are actually non-local.

Note that in the proof that *non*-relativistic Hartree-Fock orbitals are analytic away from the positions of the nuclei (see [13, 22]), the non-linearities are dealt with by cleverly re-writing the Hartree-Fock equations as a system. One introduces new functions $\phi_{i,j} = [\varphi_i\overline{\varphi_j}] * |\cdot|^{-1}$, which satisfy $-\Delta\phi_{i,j} = 4\pi\varphi_i\overline{\varphi_j}$. This eliminates the terms $R_{\boldsymbol{\varphi}}\varphi_i, K_{\boldsymbol{\varphi}}\varphi_i$, turning these into quadratic products in the functions $\varphi_i, \phi_{i,j}$, hence one obtains a (quadratic and local) non-linear system of elliptic second order equations with coefficients analytic away from the positions of the nuclei. The result now follows from the results cited above [19, 26]. (In fact, this argument extends to solutions of the more general multiconfiguration self-consistent field equations, see [13, 22].)

This idea cannot readily be extended to our case. The operator $E(\mathbf{p})$ is a pseudodifferential operator of first order, so when re-writing the Hartree-Fock equations as described above, one obtains a system of pseudodifferential equations. This system is, as before, of second (differential) order in the auxiliary functions $\phi_{i,j}$, but only of first (pseudodifferential) order in the original functions φ_i. Hence, the leading (second) order matrix is singular elliptic. Hence (even if we ignore the fact that the square root is non-local) the above argument does not apply.

To summarize, our approach is as follows. We invert the kinetic energy in the equation for the orbitals thereby obtaining an integral equation to which we apply successive differentiations. The localization argument of Lemma B.1 together with the smoothing estimates on $\phi E(\mathbf{p})^{-1}D^\beta\chi$ handle the non-locality of this equation. By working in L^p for suitably large p one can afford the necessary loss of derivatives from using Sobolev inequalities when treating the non-linear terms.

2 Proof of analyticity

In order to prove that the φ_i's are real analytic in $\mathbb{R}^3\setminus\{0\}$ it is sufficient [21, Proposition 2.2.10] to prove that for every $\mathbf{x}_0 \in \mathbb{R}^3\setminus\{0\}$ there exists an open set $U \subseteq \mathbb{R}^3\setminus\{0\}$ containing $\mathbf{x}_0$, and constants $\mathcal{C}, \mathcal{R} > 0$, such that

$$|\partial^\beta\varphi_i(\mathbf{x})| \le \mathcal{C}\,\frac{\beta!}{\mathcal{R}^{|\beta|}} \quad \text{for all } \mathbf{x}\in U \text{ and all } \beta\in\mathbb{N}_0^3\,. \tag{15}$$

Let $\mathbf{x}_0 \in \mathbb{R}^3\setminus\{0\}$, and let ω be the ball $B_R(\mathbf{x}_0)$ with center $\mathbf{x}_0$ and radius $R := \min\{1, |\mathbf{x}_0|/4\}$. For $\delta > 0$ we denote by ω_δ the set of points in ω at distance larger than δ from $\partial\omega$, i.e.,

$$\omega_\delta := \{\mathbf{x}\in\omega \,|\, d(\mathbf{x},\partial\omega) > \delta\}\,. \tag{16}$$

By our choice of ω we have $\omega_\delta = B_{R-\delta}(\mathbf{x}_0)$. Therefore $\omega_\delta = \emptyset$ for $\delta \ge R$. In particular, by our choice of R,

$$\omega_\delta = \emptyset \quad \text{for} \quad \delta \ge 1\,. \tag{17}$$

For $\Omega \subseteq \mathbb{R}^n$ and $p \geq 1$ we let $L^p(\Omega)$ denote the usual L^p-space with norm

$$\|f\|_{L^p(\Omega)} = \Big(\int_\Omega |f(\mathbf{x})|^p \, d\mathbf{x}\Big)^{1/p} .$$

We write $\|f\|_p \equiv \|f\|_{L^p(\mathbb{R}^3)}$. In the following we equip the Sobolev space $W^{m,p}(\Omega)$, $\Omega \subseteq \mathbb{R}^n$, $m \in \mathbb{N}$ and $p \in [1, \infty)$, with the norm

$$\|u\|_{W^{m,p}(\Omega)} := \sum_{|\sigma| \leq m} \|D^\sigma u\|_{L^p(\Omega)} . \tag{18}$$

Theorem 1.1 follows from the following proposition.

Proposition 2.1. *Let $Z\alpha < 2/\pi$, and let $N \geq 2$ be a positive integer such that $N < Z + 1$. Let $\boldsymbol{\varphi} = \{\varphi_1, \ldots, \varphi_N\}$, $\varphi_i \in H^{1/2}(\mathbb{R}^3)$, $i = 1, \ldots, N$, be solutions to the pseudorelativistic Hartree-Fock equations in* (9)*. Let $\mathbf{x}_0 \in \mathbb{R}^3 \setminus \{0\}$, $R = \min\{1, |\mathbf{x}_0|/4\}$, and $\omega = B_R(\mathbf{x}_0)$. Define $\omega_\delta = B_{R-\delta}(\mathbf{x}_0)$ for $\delta > 0$.*

Then for all $p \geq 5$ there exist constants $C, B > 1$ such that for all $j \in \mathbb{N}$, for all $\epsilon > 0$ such that $\epsilon j \leq R/2$, and for all $i \in \{1, \ldots, N\}$ we have

$$\epsilon^{|\beta|} \|D^\beta \varphi_i\|_{L^p(\omega_{\epsilon j})} \leq C B^{|\beta|} \ \text{ for all } \ \beta \in \mathbb{N}_0^3 \ \text{ with } \ |\beta| \leq j . \tag{19}$$

Given Proposition 2.1, the proof that the φ_i's are real analytic is standard, using Sobolev embedding. We give the argument here for completeness. We then give the proof of Proposition 2.1 in the next section.

Let $U = B_{R/2}(\mathbf{x}_0) = \omega_{R/2} \subseteq \omega$. Using Theorem D.5 and (19) we have $\varphi_i \in C(\overline{U})$. Therefore it suffices to prove (15) for $|\beta| \geq 1$. Fix $i \in \{1, \ldots, N\}$ and consider $\beta \in \mathbb{N}_0^3 \setminus \{0\}$ an arbitrary multiindex. Setting $j = |\beta|$ and $\epsilon = (R/2)/j$ it follows from Proposition 2.1 (since $\epsilon j = R/2$) that there exists constants $C, B > 1$ such that

$$\|D^\beta \varphi_i\|_{L^p(\omega_{R/2})} \leq C\Big(\frac{B}{\epsilon}\Big)^{|\beta|} = C\Big(\frac{2B}{R}\Big)^{|\beta|} |\beta|^{|\beta|} , \tag{20}$$

with C, B independent of the choice of β. By Theorem D.5 (see also Remark D.6) there exists a constant $K_4 = K_4(p, \mathbf{x}_0)$ such that, for all $\beta' \in \mathbb{N}_0^3 \setminus \{0\}$,

$$\begin{aligned}
\sup_{\mathbf{x} \in U} |D^{\beta'} \varphi_i(\mathbf{x})| &\leq K_4 \sum_{|\sigma| \leq 1} \|D^{\beta' + \sigma} \varphi_i\|_{L^p(\omega_{R/2})} \\
&\leq K_4 \sum_{|\sigma| \leq 1} C\Big(\frac{2B}{R}\Big)^{|\sigma| + |\beta'|} \big(|\sigma| + |\beta'|\big)^{|\sigma| + |\beta'|} ,
\end{aligned}$$

using (20). Using that $R \leq 1 \leq B$, that $\#\{\sigma \in \mathbb{N}_0^3 \,|\, |\sigma| = 1\} = 3$, and that, from (A.7),

$$\big(1 + |\beta'|\big)^{1 + |\beta'|} \leq \frac{\mathrm{e}}{\sqrt{2\pi}} \, \mathrm{e}^{2|\beta'|} \, |\beta'|! ,$$

this implies that for all $\beta' \in \mathbb{N}_0^3 \setminus \{0\}$,

$$\sup_{\mathbf{x} \in U} |D^{\beta'} \varphi_i(\mathbf{x})| \leq \Big(\frac{8\mathrm{e} K_4 C B}{\sqrt{2\pi} R}\Big) \Big(\frac{2\mathrm{e}^2 B}{R}\Big)^{|\beta'|} |\beta'|! . \tag{21}$$

Since $|\sigma|! \leq 3^{|\sigma|} \sigma!$ for all $\sigma \in \mathbb{N}_0^3$ (see (A.4) in Appendix A below), this implies that

$$\sup_{\mathbf{x} \in U} |D^{\beta'} \varphi_i(\mathbf{x})| \leq \mathcal{C} \, \frac{\beta'!}{\mathcal{R}^{|\beta'|}} , \tag{22}$$

for some $\mathcal{C}, \mathcal{R} > 0$. This proves (15). Hence φ_i is real analytic in $\mathbb{R}^3 \setminus \{0\}$. This finishes the proof of Theorem 1.1.

It therefore remains to prove Proposition 2.1.

Remark 2.2. *We here give explicit choices for the constants C and B in Proposition 2.1. Let*

$$C_1 := \max_{1\le a,b\le N} \Big\| \int_{\mathbb{R}^3} \frac{|\varphi_a(\mathbf{y})\varphi_b(\mathbf{y})|}{|\cdot - \mathbf{y}|}\, d\mathbf{y} \Big\|_\infty . \tag{23}$$

Note that by (29) *below, this is finite since $\varphi_i \in H^{1/2}(\mathbb{R}^3)$, $i = 1, \ldots, N$.*

Furthermore, let $A = A(\mathbf{x}_0) \ge 1$ be such that, for all $\sigma \in \mathbb{N}_0^3$,

$$\sup_{\mathbf{x}\in\omega} |D^\sigma V(\mathbf{x})| \le A^{|\sigma|+1}|\sigma|! . \tag{24}$$

The existence of A follows from the real analyticity in $\omega = B_R(\mathbf{x}_0)$ (recall that $R = \min\{1, |\mathbf{x}_0|/4\}$) of $V = Z\alpha|\cdot|^{-1}$ (see e. g. [21, Proposition 2.2.10]). Assume without restriction that $A \ge \alpha^{-1} + \max_{1\le i\le N} |\varepsilon_i|$.

Let $K_1 = K_1(p), K_2 = K_2(p)$, and $K_3 = K_3(p)$ be the constants in Lemma C.1, Corollary D.2, and Corollary D.4, respectively (see Appendices C and D below). Then let

$$C_2 = \max\big\{K_1, 256\sqrt{2}/\pi\big\}, \tag{25}$$

$$C_3 = \max\big\{4\pi(1 + 2C_1/R^2)K_3, 160\pi K_2^2 K_3\big\}. \tag{26}$$

Choose

$$C > \max_{i\in\{1,\ldots,N\}} \big\{1, \|\varphi_i\|_{W^{1,p}(\omega)}, \|\varphi_i\|_{L^{3p}(B_{2R}(\mathbf{x}_0))}, \frac{768}{\pi}|\mathbf{x}_0|^{3(2-p)/(2p)}\|\varphi_i\|_2, \\ \big[\frac{48\sqrt{2}}{\pi}A + 48\sqrt{2}C_1\frac{N}{Z\pi} + \frac{1536\sqrt{2}}{\pi^2|\mathbf{x}_0|}\big]\|\varphi_i\|_3\big\}. \tag{27}$$

That $C < \infty$ follows from the smoothness away from $\mathbf{x} = 0$ of the φ_i's [5, Theorem 1 (ii)] and the fact that, since $\varphi_i \in H^{1/2}(\mathbb{R}^3)$, $1 \le i \le N$, we have $\varphi_i \in L^3(\mathbb{R}^3)$, $1 \le i \le N$, by Sobolev's inequality. Then choose

$$B > \max\big\{48AC_2, C_*, \frac{16}{|\mathbf{x}_0|}, 4C_1^2, (160C^2K_2C_3)^2, (24NC_2/Z)^2, 16K_3\big\}, \tag{28}$$

where C_* is the constant (related to a smooth partition of unity) introduced in (B.3). *In particular, $B > 48$. We will prove Proposition 2.1 with these choices of C and B.*

3 Proof of the main estimate

We first make (6) more precise, thereby also explaining the choice of $\mathcal{M}_N$ in (8). By Kato's inequality [20, (5.33) p. 307],

$$\int_{\mathbb{R}^3} \frac{|f(\mathbf{x})|^2}{|\mathbf{x}|}\, d\mathbf{x} \le \frac{\pi}{2}\int_{\mathbb{R}^3} |\mathbf{p}||\hat{f}(\mathbf{p})|^2\, d\mathbf{p} \quad \text{for} \quad f \in H^{1/2}(\mathbb{R}^3) \tag{29}$$

(where $\hat{f}(\mathbf{p}) = (2\pi)^{-3/2}\int_{\mathbb{R}^3} \mathrm{e}^{-\mathrm{i}\mathbf{x}\cdot\mathbf{p}} f(\mathbf{x})\, d\mathbf{x}$ denotes the Fourier transform of f), and the KLMN theorem [29, Theorem X.17] the operator h_0 given as

$$h_0 = T(-\mathrm{i}\nabla) - V \tag{30}$$

is well-defined on $H^{1/2}(\mathbb{R}^3)$ (and bounded below by $-\alpha^{-1}$) as a form sum when $Z\alpha < 2/\pi$, that is,

$$(u, h_0 v) = (E(\mathbf{p})^{1/2}u, E(\mathbf{p})^{1/2}v) - \alpha^{-1}(u,v) - (V^{1/2}u, V^{1/2}v) \text{ for } u, v \in H^{1/2}(\mathbb{R}^3). \tag{31}$$

By abuse of notation, we write $E(\mathbf{p})$ for the (strictly positive) operator $E(-\mathrm{i}\nabla) = \sqrt{-\Delta + \alpha^{-2}}$. For $(\varphi_1, \dots, \varphi_N) \in \mathcal{M}_N$, the function $R_{\boldsymbol{\varphi}}$ given in (12) belongs to $L^\infty(\mathbb{R}^3)$ (using Kato's inequality above), and the operator $K_{\boldsymbol{\varphi}}$ given in (13) is Hilbert-Schmidt (see [5, Lemma 2]). As a consequence, when $Z\alpha < 2/\pi$, the operator $h_{\boldsymbol{\varphi}}$ in (11) is a well-defined self-adjoint operator with quadratic form domain $H^{1/2}(\mathbb{R}^3)$ such that

$$(u, h_{\boldsymbol{\varphi}} v) = (u, h_0 v) + \alpha(u, R_{\boldsymbol{\varphi}} v) - \alpha(u, K_{\boldsymbol{\varphi}} v) \text{ for } u, v \in H^{1/2}(\mathbb{R}^3). \tag{32}$$

Since $(u, R_{\boldsymbol{\varphi}} u) - (u, K_{\boldsymbol{\varphi}} u) \geq 0$ for any $u \in L^2(\mathbb{R}^3)$, also $h_{\boldsymbol{\varphi}}$ is bounded from below by $-\alpha^{-1}$.

Then, for $(u_1, \dots, u_N) \in \mathcal{M}_N$, the precise version of (6) becomes

$$\begin{aligned} &\mathcal{E}^{\mathrm{HF}}(u_1, \dots, u_N) \\ &\quad = \sum_{j=1}^N \alpha^{-1}(u_j, h_0 u_j) + \frac{1}{2} \sum_{1 \leq i,j \leq N} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|u_i(\mathbf{x})|^2 |u_j(\mathbf{y})|^2}{|\mathbf{x}-\mathbf{y}|} \, d\mathbf{x} d\mathbf{y} \\ &\qquad - \frac{1}{2} \sum_{1 \leq i,j \leq N} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\overline{u_j(\mathbf{x})} u_i(\mathbf{x}) \overline{u_i(\mathbf{y})} u_j(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} \, d\mathbf{x} d\mathbf{y}. \end{aligned} \tag{33}$$

The considerations on $R_{\boldsymbol{\varphi}}$ and $K_{\boldsymbol{\varphi}}$ above imply that also the non-linear terms in (33) are finite for $u_i \in H^{1/2}(\mathbb{R}^3)$, $1 \leq i \leq N$.

If $(\varphi_1, \dots, \varphi_N) \in \mathcal{M}_N$ is a critical point of $\mathcal{E}^{\mathrm{HF}}$ in (33), then $\boldsymbol{\varphi} = \{\varphi_1, \dots, \varphi_N\}$ satisfies the self-consistent HF-equations (10) with the operator $h_{\boldsymbol{\varphi}}$ defined above.

Note that $E(\mathbf{p})$ is a bounded operator from $H^{1/2}(\mathbb{R}^3)$ to $H^{-1/2}(\mathbb{R}^3)$, and recall that (29) shows that V also defines a bounded operator from $H^{1/2}(\mathbb{R}^3)$ to $H^{-1/2}(\mathbb{R}^3)$ (for any $Z\alpha$). As noted above, both $R_{\boldsymbol{\varphi}}$ and $K_{\boldsymbol{\varphi}}$ are bounded operators on $L^2(\mathbb{R}^3)$ when $(\varphi_1, \dots, \varphi_N) \in \mathcal{M}_N$. In particular, this shows that if $(\varphi_1, \dots, \varphi_N) \in \mathcal{M}_N$ solves (10), then

$$E(\mathbf{p})\varphi_i - \alpha^{-1}\varphi_i - V\varphi_i + \alpha R_{\boldsymbol{\varphi}}\varphi_i - \alpha K_{\boldsymbol{\varphi}}\varphi_i = \varepsilon_i \varphi_i \ , \ 1 \leq i \leq N, \tag{34}$$

hold as equations in $H^{-1/2}(\mathbb{R}^3)$. Using that $E(\mathbf{p})^{-1}$ is a bounded operator from $H^{-1/2}(\mathbb{R}^3)$ to $H^{1/2}(\mathbb{R}^3)$, this implies that, as equalities in $H^{1/2}(\mathbb{R}^3)$ (and therefore, in particular, in $L^2(\mathbb{R}^3)$),

$$\begin{aligned} \varphi_i &= E(\mathbf{p})^{-1} V \varphi_i - \alpha E(\mathbf{p})^{-1} R_{\boldsymbol{\varphi}} \varphi_i \\ &\quad + \alpha E(\mathbf{p})^{-1} K_{\boldsymbol{\varphi}} \varphi_i + (\alpha^{-1} + \varepsilon_i) E(\mathbf{p})^{-1} \varphi_i \ , \quad 1 \leq i \leq N, \end{aligned} \tag{35}$$

Proof of Proposition 2.1. The proof of Proposition 2.1 is by induction on $j \in \mathbb{N}_0$. More precisely:

Definition 3.1. *For $p \geq 1$ and $j \in \mathbb{N}_0$, let $\mathcal{P}(p,j)$ be the statement:*
For all $\epsilon > 0$ with $\epsilon j \leq R/2$, and all $i \in \{1, \dots, N\}$ we have

$$\epsilon^{|\beta|} \| D^\beta \varphi_i \|_{L^p(\omega_{\epsilon j})} \leq C\, B^{|\beta|} \ \textit{for all} \ \beta \in \mathbb{N}_0^3 \ \textit{with} \ |\beta| \leq j, \tag{36}$$

with $C, B > 1$ the constants in Remark 2.2.

Then Proposition 2.1 is equivalent to the statement: For all $p \geq 5$, $\mathcal{P}(p,j)$ holds for all $j \in \mathbb{N}_0$. This is the statement we will prove by induction on $j \in \mathbb{N}_0$.

Induction start: For convenience, we prove the induction start for both $j = 0$ and $j = 1$. Note that $\mathcal{P}(p, 0)$ trivially holds since (see Remark 2.2)

$$C = C(p) > \max_{1 \leq i \leq N} \|\varphi_i\|_{L^p(\omega)} . \tag{37}$$

Also $\mathcal{P}(p, 1)$ holds by the choice of C, since

$$C = C(p) > \max_{\substack{1 \leq i \leq N,\\ \nu \in \{1,2,3\}}} \|D_\nu \varphi_i\|_{L^p(\omega)} . \tag{38}$$

Namely, since $\omega_\epsilon \subseteq \omega$, (36) holds for $|\beta| = 0$ (and *all* $\epsilon > 0$) using (37). For $\beta \in \mathbb{N}_0$ with $|\beta| = 1 = j$ (i.e., $\beta = e_\nu$ for some $\nu \in \{1, 2, 3\}$), and all $\epsilon > 0$ with $\epsilon = \epsilon j \leq R/2 < 1$,

$$\begin{aligned} \epsilon^{|\beta|} \|D^\beta \varphi_i\|_{L^p(\omega_{\epsilon j})} &= \epsilon \|D_\nu \varphi_i\|_{L^p(\omega_\epsilon)} \leq \|D_\nu \varphi_i\|_{L^p(\omega)} \\ &\leq C \leq CB = CB^{|\beta|} . \end{aligned} \tag{39}$$

Here we again used that $\omega_\epsilon \subseteq \omega$, (38), and that $B > 1$ (see Remark 2.2).

We move on to the induction step.

Induction hypothesis:

$$\text{Let } p \geq 5 \text{ and } j \in \mathbb{N}_0,\ j \geq 1. \text{ Then } \mathcal{P}(p, \tilde{j}) \text{ holds for all } \tilde{j} \leq j. \tag{40}$$

We now prove that $\mathcal{P}(p, j + 1)$ holds. Note that to prove this, it suffices to study $\beta \in \mathbb{N}_0^3$ with $|\beta| = j + 1$. Namely, assume $\epsilon > 0$ is such that $\epsilon(j + 1) \leq R/2$ and let $\beta \in \mathbb{N}_0^3$ with $|\beta| < j + 1$. Then $|\beta| \leq j$ and $\epsilon j \leq R/2$ so, by the definition of ω_δ and the induction hypothesis,

$$\epsilon^{|\beta|} \|D^\beta \varphi_i\|_{L^p(\omega_{\epsilon(j+1)})} \leq \epsilon^{|\beta|} \|D^\beta \varphi_i\|_{L^p(\omega_{\epsilon j})} \leq CB^{|\beta|} . \tag{41}$$

It therefore remains to prove that

$$\begin{aligned} \epsilon^{|\beta|} \|D^\beta \varphi_i\|_{L^p(\omega_{\epsilon(j+1)})} \leq C\, B^{|\beta|} \quad &\text{for all } \ \epsilon > 0 \ \text{ with } \ \epsilon(j + 1) \leq R/2 \\ &\text{and all } \beta \in \mathbb{N}_0^3 \ \text{ with } \ |\beta| = j + 1 . \end{aligned} \tag{42}$$

Remark 3.2. *To use the induction hypothesis in its entire strength, it is convenient to write, for $\ell > 0$, $\epsilon > 0$ such that $\epsilon\ell \leq R/2$, and $\sigma \in \mathbb{N}_0^3$ with $0 < |\sigma| \leq j$,*

$$\|D^\sigma \varphi_i\|_{L^p(\omega_{\epsilon\ell})} = \|D^\sigma \varphi_i\|_{L^p(\omega_{\tilde{\epsilon}\tilde{j}})} \quad \textit{with} \quad \tilde{\epsilon} = \frac{\epsilon\ell}{|\sigma|},\ \tilde{j} = |\sigma| ,$$

so that, by the induction hypothesis (applied on the term with $\tilde{\epsilon}$ and $\tilde{j}$) we get that

$$\|D^\sigma \varphi_i\|_{L^p(\omega_{\epsilon\ell})} \leq C\Big(\frac{B}{\tilde{\epsilon}}\Big)^{|\sigma|} = C\Big(\frac{|\sigma|}{\ell}\Big)^{|\sigma|}\Big(\frac{B}{\epsilon}\Big)^{|\sigma|} . \tag{43}$$

Compare this with (36)*. With the convention that $0^0 = 1$,* (43) *also holds for $|\sigma| = 0$.*

We choose a function Φ (depending on j) satisfying

$$\Phi \in C_0^\infty(\omega_{\epsilon(j+3/4)}) , \quad 0 \leq \Phi \leq 1 , \quad \text{ with } \ \Phi \equiv 1 \ \text{ on } \ \omega_{\epsilon(j+1)} . \tag{44}$$

Then

$$\|D^\beta \varphi_i\|_{L^p(\omega_{\epsilon(j+1)})} \leq \|\Phi D^\beta \varphi_i\|_p . \tag{45}$$

The estimate (42)–and hence, by induction, the proof of Proposition 2.1—now follows from the equations (35) for the φ_i's, (45) and the following two lemmas.

Lemma 3.3. *Assume* (40) *(the induction hypothesis) holds. Let* Φ *be as in* (44). *Then for all* $i \in \{1, \ldots, N\}$, *all* $\epsilon > 0$ *with* $\epsilon(j+1) \leq R/2$, *and all* $\beta \in \mathbb{N}_0^3$ *with* $|\beta| = j+1$, *both* $\Phi D^\beta E(\mathbf{p})^{-1} V \varphi_i$ *and* $\Phi D^\beta E(\mathbf{p})^{-1} \varphi_i$ *belong to* $L^p(\mathbb{R}^3)$, *and*

$$\|\Phi D^\beta E(\mathbf{p})^{-1} V \varphi_i\|_p \leq \frac{C}{4}\Big(\frac{B}{\epsilon}\Big)^{|\beta|}, \tag{46}$$

$$\|(\alpha^{-1} + \varepsilon_i) \Phi D^\beta E(\mathbf{p})^{-1} \varphi_i\|_p \leq \frac{C}{4}\Big(\frac{B}{\epsilon}\Big)^{|\beta|}, \tag{47}$$

where $C, B > 1$ *are the constants in* (36) *(see also Remark 2.2).*

Lemma 3.4. *Assume* (40) *(the induction hypothesis) holds. Let* Φ *be as in* (44). *Then for all* $i \in \{1, \ldots, N\}$, *all* $\epsilon > 0$ *with* $\epsilon(j+1) \leq R/2$, *and all* $\beta \in \mathbb{N}_0^3$ *with* $|\beta| = j+1$, *both* $\Phi D^\beta E(\mathbf{p})^{-1} R_{\boldsymbol{\varphi}} \varphi_i$ *and* $\Phi D^\beta E(\mathbf{p})^{-1} K_{\boldsymbol{\varphi}} \varphi_i$ *belong to* $L^p(\mathbb{R}^3)$, *and*

$$\|\alpha\, \Phi D^\beta E(\mathbf{p})^{-1} R_{\boldsymbol{\varphi}} \varphi_i\|_p \leq \frac{C}{4}\Big(\frac{B}{\epsilon}\Big)^{|\beta|},$$

$$\|\alpha\, \Phi D^\beta E(\mathbf{p})^{-1} K_{\boldsymbol{\varphi}} \varphi_i\|_p \leq \frac{C}{4}\Big(\frac{B}{\epsilon}\Big)^{|\beta|},$$

where $C, B > 1$ *are the constants in* (36) *(see also Remark 2.2).*

Remark 3.5. *For* $a, b \in \{1, \ldots, N\}$, *let* $U_{a,b}$ *denote the function*

$$U_{a,b}(\mathbf{x}) = \int_{\mathbb{R}^3} \frac{\varphi_a(\mathbf{y})\overline{\varphi_b(\mathbf{y})}}{|\mathbf{x} - \mathbf{y}|}\, d\mathbf{y}\,, \ \ \mathbf{x} \in \mathbb{R}^3\,. \tag{48}$$

In particular, $\|U_{a,b}\|_\infty \leq C_1$ *for all* $a, b \in \{1, \ldots, N\}$ *(see* (23)*). Note that (see* (12) *and* (13)*)*

$$R_{\boldsymbol{\varphi}} \varphi_i = \sum_{\ell=1}^N U_{\ell,\ell} \varphi_i\,, \quad K_{\boldsymbol{\varphi}} \varphi_i = \sum_{\ell=1}^N U_{i,\ell} \varphi_\ell\,. \tag{49}$$

Hence Lemma 3.4 follows from the following lemma and the fact that $Z\alpha < 2/\pi < 1$.

Lemma 3.6. *Assume* (40) *(the induction hypothesis) holds. Let* Φ *be as in* (44). *For* $a, b \in \{1, \ldots, N\}$, *let* $U_{a,b}$ *be given by* (48). *Then for all* $a, b, i \in \{1, \ldots, N\}$, *all* $\epsilon > 0$ *with* $\epsilon(j+1) \leq R/2$, *and all* $\beta \in \mathbb{N}_0^3$ *with* $|\beta| = j+1$, $\Phi D^\beta E(\mathbf{p})^{-1} U_{a,b} \varphi_i$ *belong to* $L^p(\mathbb{R}^3)$, *and*

$$\|\Phi D^\beta E(\mathbf{p})^{-1} U_{a,b} \varphi_i\|_p \leq \frac{CZ}{4N}\Big(\frac{B}{\epsilon}\Big)^{|\beta|}, \tag{50}$$

where $C, B > 1$ *are the constants in* (36) *(see also Remark 2.2).*

It therefore remains to prove Lemmas 3.3 and 3.6. This will be done in the two following sections. $\square$

4 Proof of Lemma 3.3

We prove Lemma 3.3 by proving (46) and (47) separately.

Proof of (46). Let $\sigma \in \mathbb{N}_0^3$ and $\nu \in \{1, 2, 3\}$ be such that $\beta = \sigma + e_\nu$, so that $D^\beta = D_\nu D^\sigma$. Notice that $|\sigma| = j$. Choose localization functions $\{\chi_k\}_{k=0}^j$ and $\{\eta_k\}_{k=0}^j$ as in Appendix B below. Since

$V\varphi_i \in H^{-1/2}(\mathbb{R}^3)$, and $E(\mathbf{p})^{-1}$ maps $H^s(\mathbb{R}^3)$ to $H^{s+1}(\mathbb{R}^3)$ for all $s \in \mathbb{R}$, Lemma B.1 (with $\ell = j$) implies that

$$\begin{aligned}\Phi D^{\beta} E(\mathbf{p})^{-1}[V\varphi_i] &= \sum_{k=0}^{j} \Phi D_\nu E(\mathbf{p})^{-1} D^{\beta_k} \chi_k D^{\sigma-\beta_k}[V\varphi_i] \\ &\quad + \sum_{k=0}^{j-1} \Phi D_\nu E(\mathbf{p})^{-1} D^{\beta_k} [\eta_k, D^{\mu_k}] D^{\sigma-\beta_{k+1}}[V\varphi_i] \\ &\quad + \Phi D_\nu E(\mathbf{p})^{-1} D^{\sigma}[\eta_j V\varphi_i]\,, \end{aligned} \tag{51}$$

as an identity in $H^{-|\beta|+1/2}(\mathbb{R}^3)$ (we have also used that $E(\mathbf{p})^{-1}$ commutes with derivatives on any $H^s(\mathbb{R}^3)$). Here, $[\,\cdot\,,\,\cdot\,]$ denotes the commutator. Also, $|\beta_k| = k$, $|\mu_k| = 1$, and $0 \le \eta_k, \chi_k \le 1$. (For the support properties of η_k, χ_k, see the mentioned appendix.) We will prove that each term on the right side of (51) belong to $L^p(\mathbb{R}^3)$, and bound their norms. The proof of (46) will follow by summing these bounds.

The first sum in (51). Let θ_k be the characteristic function of the support of χ_k (which is contained in ω). Since V is smooth on the closure of ω it follows from the induction hypothesis that the $D^{\sigma-\beta_k}[V\varphi_i]$'s belong to $L^p(\omega')$ for any $\omega' \subset\subset \omega$. Also, the operator $\Phi D_\nu E(\mathbf{p})^{-1} D^{\beta_k}\chi_k$ is bounded on $L^p(\mathbb{R}^3)$ (as we will observe below). Therefore we can estimate, for $k \in \{0, \dots, j\}$,

$$\begin{aligned}&\|\Phi D_\nu E(\mathbf{p})^{-1} D^{\beta_k} \chi_k D^{\sigma-\beta_k}[V\varphi_i]\|_p \\ &\qquad = \|(\Phi E(\mathbf{p})^{-1} D_\nu D^{\beta_k}\chi_k)\theta_k D^{\sigma-\beta_k}[V\varphi_i]\|_p \\ &\qquad \le \|\Phi E(\mathbf{p})^{-1} D_\nu D^{\beta_k}\chi_k\|_{\mathcal{B}_p}\, \|\theta_k D^{\sigma-\beta_k}[V\varphi_i]\|_p\,. \end{aligned} \tag{52}$$

Here, $\|\cdot\|_{\mathcal{B}_p}$ is the operator norm on $\mathcal{B}_p := B(L^p(\mathbb{R}^3))$, the bounded operators on $L^p(\mathbb{R}^3)$.

For $k = 0$, the first factor on the right side of (52) can be estimated using Lemma C.1 (since $|\beta_0| = 0$). This way, since $\|\chi_0\|_\infty = \|\Phi\|_\infty = 1$,

$$\|\Phi E(\mathbf{p})^{-1} D_\nu \chi_0\|_{\mathcal{B}_p} \le K_1\,, \tag{53}$$

with $K_1 = K_1(p)$ the constant in (C.1).

For $k > 0$, the first factor on the right side of (52) can be estimated using (C.4) in Lemma C.2 (with $\mathfrak{r} = 1$, $\mathfrak{q}^* = \mathfrak{p} = p$). Since

$$\operatorname{dist}(\operatorname{supp}\chi_k, \operatorname{supp}\Phi) \ge \epsilon(k - 1 + 1/4)$$

and $\|\chi_k\|_\infty = \|\Phi\|_\infty = 1$, this gives (since $(\beta_k + e_\nu)! \le (|\beta_k| + 1)! = (k+1)!$) that

$$\begin{aligned}\|\Phi E(\mathbf{p})^{-1} D_\nu D^{\beta_k}\chi_k\|_{\mathcal{B}_p} &\le \frac{32\sqrt{2}}{\pi}\frac{(k+1)!}{k}\Big(\frac{8}{\epsilon(k-1+1/4)}\Big)^k \\ &\le \frac{256\sqrt{2}}{\pi}\Big(\frac{8}{\epsilon}\Big)^k. \end{aligned} \tag{54}$$

It follows from (53) and (54) that, for all $k \in \{0, \dots, j\}$, $\nu \in \{1, 2, 3\}$,

$$\|\Phi E(\mathbf{p})^{-1} D_\nu D^{\beta_k}\chi_k\|_{\mathcal{B}_p} \le C_2\Big(\frac{8}{\epsilon}\Big)^k, \tag{55}$$

with C_2 as defined in (25).

It remains to estimate the second factor in (52). Recall the definition of the constant A in (24). It follows from (24) and (17) that, for all $\epsilon > 0$, $\ell \in \mathbb{N}_0$, and $\sigma \in \mathbb{N}_0^3$,

$$\epsilon^{|\sigma|} \sup_{\mathbf{x} \in \omega_{\epsilon\ell}} |D^\sigma V(\mathbf{x})| \leq A^{|\sigma|+1} |\sigma|!\, \ell^{-|\sigma|}\,, \tag{56}$$

with $\omega_{\epsilon\ell} \subseteq \omega$ as in defined in (16).

For $k = j$, since $\beta_j = \sigma$, we find, by (56) and the choice of C (see Remark 2.2), that

$$\|\theta_j V \varphi_i\|_p \leq \|V\|_{L^\infty(\omega)} \|\varphi_i\|_{L^p(\omega)} \leq CA\,. \tag{57}$$

The estimate for $k \in \{0, \dots, j-1\}$ is a bit more involved. We get, by Leibniz's rule, that

$$\begin{aligned} &\|\theta_k D^{\sigma-\beta_k}[V\varphi_i]\|_p \\ &\qquad \leq \sum_{\mu \leq \sigma-\beta_k} \binom{\sigma-\beta_k}{\mu} \|\theta_k D^\mu V\|_\infty \, \|\theta_k D^{\sigma-\beta_k-\mu}\varphi_i\|_p\,. \end{aligned} \tag{58}$$

Now, $\operatorname{supp}\theta_k = \operatorname{supp}\chi_k \subseteq \omega_{\epsilon(j-k+1/4)}$, so by (56), for all $\mu \leq \sigma - \beta_k$,

$$\|\theta_k D^\mu V\|_\infty \leq \sup_{\mathbf{x} \in \omega_{\epsilon(j-k+1/4)}} |D^\mu V(\mathbf{x})| \leq \epsilon^{-|\mu|} A^{|\mu|+1} |\mu|! (j-k)^{-|\mu|}\,. \tag{59}$$

By the induction hypothesis (in the form discussed in Remark 3.2),

$$\begin{aligned} \|\theta_k D^{\sigma-\beta_k-\mu}\varphi_i\|_p &\leq \|D^{\sigma-\beta_k-\mu}\varphi_i\|_{L^p(\omega_{\epsilon(j-k)})} \\ &\leq C\Big(\frac{|\sigma-\beta_k-\mu|}{j-k}\Big)^{|\sigma-\beta_k-\mu|}\Big(\frac{B}{\epsilon}\Big)^{|\sigma-\beta_k-\mu|}\,. \end{aligned} \tag{60}$$

It follows from (58), (59), and (60) that (using that $|\sigma| = j, |\beta_k| = k$, and (A.6), summing over $m = |\mu|$)

$$\begin{aligned} &\|\theta_k D^{\sigma-\beta_k}[V\varphi_i]\|_p \\ &\leq CA\Big(\frac{B}{\epsilon}\Big)^{j-k} \sum_{m=0}^{j-k} \binom{j-k}{m} \frac{m!(j-k-m)^{j-k-m}}{(j-k)^{j-k}} \Big(\frac{A}{B}\Big)^m\,. \end{aligned} \tag{61}$$

Note that, by (A.7), for $0 < m < j-k$,

$$\binom{j-k}{m} \frac{m!(j-k-m)^{j-k-m}}{(j-k)^{j-k}} \leq \frac{\mathrm{e}^{1/12}\sqrt{j-k}}{\sqrt{j-k-m}\,\mathrm{e}^m} \leq 1\,. \tag{62}$$

To see the last inequality, look at the cases $0 < m \leq (j-k)/2$ and $j-k > m \geq (j-k)/2$ separately.

Hence (since $B > 2A$, see Remark 2.2), for any $k \in \{0, \dots, j-1\}$,

$$\|\theta_k D^{\sigma-\beta_k}[V\varphi_i]\|_p \leq CA\Big(\frac{B}{\epsilon}\Big)^{j-k} \sum_{m=0}^{j-k} \Big(\frac{A}{B}\Big)^m \leq 2CA\Big(\frac{B}{\epsilon}\Big)^{j-k}\,. \tag{63}$$

Note that, by (57), the same estimate holds true if $k = j$.

So, from (52), (55), (63), the fact that $\epsilon \leq 1$ (since $\epsilon(j+1) \leq R/2 \leq 1/2$), and the choice of B (in particular, $B > 16$; see Remark 2.2), it follows that

$$\begin{aligned} &\Big\| \sum_{k=0}^{j} \Phi D_\nu E(\mathbf{p})^{-1} D^{\beta_k} \chi_k D^{\sigma-\beta_k}[V\varphi_i] \Big\|_p \\ &\leq 2CAC_2\Big(\frac{B}{\epsilon}\Big)^j \sum_{k=0}^{j} \Big(\frac{8}{B}\Big)^k \leq C(4AC_2)\Big(\frac{B}{\epsilon}\Big)^j \leq \frac{C}{12}\Big(\frac{B}{\epsilon}\Big)^{j+1}\,. \end{aligned} \tag{64}$$

The second sum in (51). Note first that $[\eta_k, D^{\mu_k}] = -(D^{\mu_k}\eta_k)$ (recall that $|\mu_k| = 1$; see Lemma B.1).

Comparing the second sum in (51) with the first sum in (51), one sees that the second sum is the first one with j replaced by $j-1$ and χ_k replaced by $-D^{\mu_k}\eta_k$. Having now a derivative on the localization functions we have one derivative less falling on the term $V\varphi_i$. More precisely, the operator $D^{\sigma-\beta_{k+1}}$ contains $|\sigma-\beta_{k+1}| = j-(k+1) = (j-1)-k$ derivatives instead of $|\sigma-\beta_k| = j-k$ in $D^{\sigma-\beta_k}$. Then, to control $D^{\sigma-\beta_{k+1}}[V\varphi_i]$ (with the same method used above for $D^{\sigma-\beta_k}[V\varphi_i]$) we need that $\operatorname{supp} D^{\mu_k}\eta_k$ is contained in $\omega_{\epsilon((j-1)-k+1/4)}$. Indeed we have much more: as for χ_k we have $\operatorname{supp} D^{\mu_k}\eta_k \subseteq \omega_{\epsilon(j-k+1/4)} \subseteq \omega_{\epsilon((j-1)-k+1/4)}$. Finally, $\|D^{\mu_k}\eta_k\|_\infty \le C_*/\epsilon$, with $C_* > 0$ the constant in (B.3) in Appendix B below.

It follows that the second sum in (51) can be estimated as the first one, up to *one* extra factor of C_*/ϵ *and* up to replacing j by $j-1$ in the estimate (64). Hence, using that $\epsilon \le 1$, and the choice of B (see Remark 2.2), we get that

$$\Big\| \sum_{k=0}^{j-1} \Phi D_\nu E(\mathbf{p})^{-1} D^{\beta_k}[\eta_k, D^{\mu_k}] D^{\sigma-\beta_{k+1}}[V\varphi_i] \Big\|_p \le \frac{C_*}{\epsilon} C(4AC_2)\Big(\frac{B}{\epsilon}\Big)^{j-1} \le C(4AC_2)\Big(\frac{B}{\epsilon}\Big)^{j} \le \frac{C}{12}\Big(\frac{B}{\epsilon}\Big)^{j+1}. \tag{65}$$

The last term in (51). It remains to study

$$\Phi D^\beta E(\mathbf{p})^{-1}[\eta_j V\varphi_i]. \tag{66}$$

We split V in two parts, one supported around $\mathbf{x} = 0$, and one supported away from $\mathbf{x} = 0$, and study the two terms separately. We will prove below that this way, $\eta_j V\varphi_i$ is actually a function in $L^1(\mathbb{R}^3) + L^3(\mathbb{R}^3)$. Upon using suitable operator bounds on $\Phi D^\beta E(\mathbf{p})^{-1}\chi$ (for some suitable smooth χ's), combined with bounds on the norms of the two parts of $\eta_j V\varphi_i$, we will finish the proof.

Let $\rho = |\mathbf{x}_0|/4$, and let θ_ρ and $\theta_{\rho/2}$ be the characteristic functions of the balls $B_\rho(0)$ and $B_{\rho/2}(0)$, respectively. Choose $\widetilde{\chi}_\rho \in C_0^\infty(\mathbb{R}^3)$ with $\operatorname{supp}\widetilde{\chi}_\rho \subseteq B_\rho(0)$, $0 \le \widetilde{\chi}_\rho \le 1$, and $\widetilde{\chi}_\rho = 1$ on $B_{\rho/2}(0)$. Note that then

$$\operatorname{dist}(\operatorname{supp}\Phi, \operatorname{supp}\widetilde{\chi}_\rho) \ge \frac{|\mathbf{x}_0|}{2} = 2\rho, \tag{67}$$

by the choice of $\omega = B_R(\mathbf{x}_0)$, $R = \min\{1, |\mathbf{x}_0|/4\}$, since $\operatorname{supp}\Phi \subseteq \omega_{\epsilon(j+1)} \subseteq \omega$.

Now,

$$\begin{aligned}\Phi D^\beta E(\mathbf{p})^{-1}[\eta_j V\varphi_i] &= \Phi D^\beta E(\mathbf{p})^{-1}[\eta_j V\widetilde{\chi}_\rho\varphi_i] \\ &\quad + \Phi D^\beta E(\mathbf{p})^{-1}[\eta_j V(1-\widetilde{\chi}_\rho)\varphi_i].\end{aligned} \tag{68}$$

For the first term in (68), we use Lemma C.2 , with $\mathfrak{p} = 1$, $\mathfrak{q} = p/(p-1)$, and $\mathfrak{r} = p$. Then $\mathfrak{p}, \mathfrak{r} \in [1,\infty)$ and $\mathfrak{q} > 1$, and $\mathfrak{q}^{-1} + p^{-1} = 1$. We get that (recall (67) and that $\widetilde{\chi}_\rho\theta_\rho = \widetilde{\chi}_\rho$),

$$\begin{aligned}\|\Phi D^\beta E(\mathbf{p})^{-1}[\eta_j V\widetilde{\chi}_\rho\varphi_i]\|_p &\le \|\Phi D^\beta E(\mathbf{p})^{-1}\widetilde{\chi}_\rho\|_{\mathcal{B}_{1,p}} \|\eta_j V\theta_\rho\varphi_i\|_1 \\ &\le \frac{4\sqrt{2}}{\pi}\beta!\Big(\frac{8}{2\rho}\Big)^{|\beta|}(2\rho)^{3/\mathfrak{r}-2}\big(\mathfrak{r}(|\beta|+2)-3\big)^{-1/\mathfrak{r}}\|V\theta_\rho\varphi_i\|_1.\end{aligned} \tag{69}$$

Here we used that $\|\Phi\|_\infty = \|\widetilde{\chi}_\rho\|_\infty = 1$ and that $\eta_j \equiv 1$ where $\theta_\rho \neq 0$. Note that $j+1 \leq \epsilon^{-1}$ (since, by assumption, $\epsilon(j+1) \leq R/2 \leq 1/2$). Therefore,

$$\beta! \leq |\beta|! = (j+1)! \leq (j+1)^{j+1} \leq \epsilon^{-(j+1)} = \epsilon^{-|\beta|}\,. \tag{70}$$

Note furthermore that since $|\beta| = j+1 \geq 2$ and $\mathfrak{r} \geq 1$,

$$\big(\mathfrak{r}(|\beta|+2)-3\big)^{-1/\mathfrak{r}} \leq 1\,, \tag{71}$$

independently of β. It follows that

$$\begin{aligned} &\|\Phi D^\beta E(\mathbf{p})^{-1}[\eta_j V \widetilde{\chi}_\rho \varphi_i]\|_p \\ &\qquad \leq \frac{4\sqrt{2}}{\pi}\Big(\frac{|\mathbf{x}_0|}{2}\Big)^{(3-2p)/p}\|V\theta_\rho\varphi_i\|_1\Big(\frac{16/|\mathbf{x}_0|}{\epsilon}\Big)^{|\beta|}\,. \end{aligned} \tag{72}$$

Using Schwarz's inequality and that $Z\alpha < 2/\pi$,

$$\|V\theta_\rho\varphi_i\|_1 \leq \|V\theta_\rho\|_2\|\varphi_i\|_2 = Z\alpha\sqrt{|\mathbf{x}_0|\pi}\|\varphi_i\|_2 \leq \frac{2}{\sqrt{\pi}}\sqrt{|\mathbf{x}_0|}\|\varphi_i\|_2\,. \tag{73}$$

(Note that $\|V\theta_\rho\|_t < \infty \Leftrightarrow t < 3$.) It follows from (72), (73), and the choice of B and C (see Remark 2.2) that

$$\begin{aligned} &\|\Phi D^\beta E(\mathbf{p})^{-1}[\eta_j V \widetilde{\chi}_\rho \varphi_i]\|_p \\ &\qquad \leq \frac{32}{\pi}|\mathbf{x}_0|^{3(2-p)/(2p)}\|\varphi_i\|_2\Big(\frac{16/|\mathbf{x}_0|}{\epsilon}\Big)^{|\beta|} \leq \frac{C}{24}\Big(\frac{B}{\epsilon}\Big)^{j+1}\,. \end{aligned} \tag{74}$$

We now consider the second term in (68). Recall that Φ is supported in $\omega_{\epsilon(j+1)}$ and

$$\mathrm{dist}(\operatorname{supp}\Phi, \operatorname{supp}\eta_j) \geq \epsilon(j+1/4)\,. \tag{75}$$

Again, we use Lemma C.2, this time with $\mathfrak{p} = 3$, $\mathfrak{q} = p/(p-1)$, and $\mathfrak{r} = 3p/(2p+3)$. Then $\mathfrak{p}^{-1} + \mathfrak{q}^{-1} + \mathfrak{r}^{-1} = 2$, $\mathfrak{p} \in [1,\infty)$, $\mathfrak{q} > 1$, $\mathfrak{r} \in [1, 3/2)$ (since $p > 3$), and $\mathfrak{q}^{-1} + p^{-1} = 1$. This gives that

$$\begin{aligned} \|\Phi D^\beta E(\mathbf{p})^{-1}[\eta_j V(1-\widetilde{\chi}_\rho)\varphi_i]\|_p &\leq \|\Phi D^\beta E(\mathbf{p})^{-1}\eta_j\|_{\mathcal{B}_{3,p}}\|V(1-\widetilde{\chi}_\rho)\varphi_i\|_3 \\ &\leq \frac{4\sqrt{2}}{\pi}\beta!\Big(\frac{8}{\epsilon(j+1/4)}\Big)^{|\beta|}\big(\epsilon(j+1/4)\big)^{3/\mathfrak{r}-2}\big(\mathfrak{r}(|\beta|+2)-3\big)^{-1/\mathfrak{r}} \\ &\qquad \times \|V(1-\widetilde{\chi}_\rho)\|_\infty\|\varphi_i\|_3\,. \end{aligned}$$

As before, we used that $\|\Phi\|_\infty = \|\eta_j\|_\infty = 1$. Note that

$$\beta!\Big(\frac{8}{j+1/4}\Big)^{|\beta|} \leq 32^{|\beta|}\frac{|\beta|!}{(j+1)^{|\beta|}} = 32^{|\beta|}\frac{(j+1)!}{(j+1)^{j+1}} \leq 32^{|\beta|}\,. \tag{76}$$

Since $\epsilon(j+1) \leq R/2 < 1$ and $\mathfrak{r} < 3/2$ it follows that $(\epsilon(j+1/4))^{3/\mathfrak{r}-2} \leq 1$. Also, by the choice of ρ, the definition of V, and since $Z\alpha < 2/\pi$,

$$\big|((1-\theta_{\rho/2})V)(\mathbf{x})\big| \leq \frac{8Z\alpha}{|\mathbf{x}_0|} \leq \frac{16}{\pi|\mathbf{x}_0|}\,, \quad \mathbf{x} \in \mathbb{R}^3\,. \tag{77}$$

It follows from (77) (and that $0 \le 1 - \widetilde{\chi}_\rho \le 1 - \theta_{\rho/2}$), (71), (76), and the choice of C and B (see Remark 2.2), that for all $i = 1, \dots, N$ (recall that $|\beta| = j+1$)

$$\|\Phi D^\beta E(\mathbf{p})^{-1}[\eta_j V(1-\widetilde{\chi}_\rho)\varphi_i]\|_p \le \frac{4\sqrt{2}}{\pi}\frac{16}{\pi|\mathbf{x}_0|}\|\varphi_i\|_3\Big(\frac{32}{\epsilon}\Big)^{|\beta|} \le \frac{C}{24}\Big(\frac{B}{\epsilon}\Big)^{j+1} . \tag{78}$$

It follows from (68), (74), and (78) that

$$\|\Phi D^\beta E(\mathbf{p})^{-1}[\eta_j V\varphi_i]\|_p \le \frac{C}{12}\Big(\frac{B}{\epsilon}\Big)^{j+1} . \tag{79}$$

The estimate (46) now follows from (51) and the estimates (64), (65), and (79). □

Proof of (47). Note that the constant functions $W_i(\mathbf{x}) = \alpha^{-1} + \varepsilon_i$ trivially satisfies the conditions on V $(= Z\alpha|\cdot|^{-1})$ needed in the proof above. In fact, having assumed $A \ge \alpha^{-1} + \max_{1\le i\le N}|\varepsilon_i|$ (See Remark 2.2), (24) (and therefore (56)) trivially holds for W_i. Also, for the term $\Phi D^\beta E(\mathbf{p})^{-1}[\eta_j W_i\varphi_i]$ we proceed directly as for the term $\Phi D^\beta E(\mathbf{p})^{-1}[\eta_j V(1-\widetilde{\chi}_\rho)\varphi_i]$ above (but without any splitting in $\widetilde{\chi}_\rho$ and $1-\widetilde{\chi}_\rho$), using that $|W_i(\mathbf{x})| \le A$, $\mathbf{x} \in \mathbb{R}^3$. The proof of (47) therefore follows from the proof of (46) above, by the choice of C and B (see Remark 2.2).

This finishes the proof of Lemma 3.3. □

Remark 4.1. *In fact, with a simple modification the arguments above (the local L^p-bound on the two terms in* (68)*) can be made to work just assuming that, for all $s > 0$,*

$$V\varphi_i \in L^1(B_s(0)) , \quad V\varphi_i \in L^3(\mathbb{R}^3 \setminus B_s(0)) . \tag{80}$$

5 Proof of Lemma 3.6

Proof of (50). Similarly to the case of the term with V in Lemma 3.3, we here use the localization functions introduced in Appendix B below. With the notation as in the previous section (in particular, $\beta = \sigma + e_\nu$ with $|\sigma| = j$), Lemma B.1 (with $\ell = j$) implies that

$$\begin{aligned}\Phi D^\beta E(\mathbf{p})^{-1}[U_{a,b}\varphi_i] &= \sum_{k=0}^{j} \Phi D_\nu E(\mathbf{p})^{-1} D^{\beta_k}\chi_k D^{\sigma-\beta_k}[U_{a,b}\varphi_i] \\ &\quad + \sum_{k=0}^{j-1} \Phi D_\nu E(\mathbf{p})^{-1} D^{\beta_k}[\eta_k, D^{\mu_k}] D^{\sigma-\beta_{k+1}}[U_{a,b}\varphi_i] \\ &\quad + \Phi D_\nu E(\mathbf{p})^{-1} D^\sigma[\eta_j U_{a,b}\varphi_i] ,\end{aligned} \tag{81}$$

as an identity in $H^{-|\beta|}(\mathbb{R}^3)$. As in the proof of Lemma 3.3, $[\,\cdot\,,\,\cdot\,]$ denotes the commutator, $|\beta_k| = k$, $|\mu_k| = 1$, and $0 \le \eta_k, \chi_k \le 1$. (For the support properties of η_k, χ_k, see the mentioned appendix.) As in the previous section, we will prove that each term on the right side of (81) belong to $L^p(\mathbb{R}^3)$, and bound their norms. The claim of the lemma will follow by summing these bounds.

The first sum in (81). We first proceed like for the similar sum in the proof of Lemma 3.3 (see (52), and after). Let θ_k be the characteristic function of the support of χ_k. It follows from the induction hypothesis, using that $-\Delta U_{a,b} = 4\pi\varphi_a\overline{\varphi_b}$, and Theorems D.5 and D.3, that the $D^{\sigma-\beta_k}[U_{a,b}\varphi_i]$'s belong to $L^p(\omega')$ for any $\omega' \subset\subset \omega$. As before, the operator $\Phi D_\nu E(\mathbf{p})^{-1} D^{\beta_k}\chi_k$ is bounded on $L^p(\mathbb{R}^3)$. Then, for $k \in \{0, \dots, j\}$

$$\begin{aligned}
&\|\Phi D_\nu E(\mathbf{p})^{-1} D^{\beta_k}\chi_k D^{\sigma-\beta_k}[U_{a,b}\varphi_i]\|_p \\
&\qquad = \|(\Phi E(\mathbf{p})^{-1} D_\nu D^{\beta_k}\chi_k)\theta_k D^{\sigma-\beta_k}[U_{a,b}\varphi_i]\|_p \\
&\qquad \leq \|\Phi E(\mathbf{p})^{-1} D_\nu D^{\beta_k}\chi_k\|_{\mathcal{B}_p}\|\theta_k D^{\sigma-\beta_k}[U_{a,b}\varphi_i]\|_p \,.
\end{aligned} \tag{82}$$

The first factor on the right side of (82) was estimated in the proof of Lemma 3.3 (see (55)): For all $k \in \{0, \dots, j\}$, $\nu \in \{1, 2, 3\}$,

$$\|\Phi E(\mathbf{p})^{-1} D_\nu D^{\beta_k}\chi_k\|_{\mathcal{B}_p} \leq C_2\Big(\frac{8}{\epsilon}\Big)^k, \tag{83}$$

with C_2 the constant in (25).

It remains to estimate the second factor in (82). For $k = j$, since $\beta_j = \sigma$, we find that, by (23) and the choice of C and B (see Remark 2.2),

$$\|\theta_j U_{a,b}\varphi_i\|_p \leq \|U_{a,b}\|_\infty \|\varphi_i\|_{L^p(\omega)} \leq C_1\, C \leq C\Big(\frac{B}{\epsilon}\Big)^{1/2}. \tag{84}$$

In the last inequality we also used that $\epsilon \leq 1$ (since $\epsilon(j+1) \leq R/2 < 1$).

The estimate for $k \in \{0, \dots, j-1\}$ is more involved. We get, by Leibniz's rule, that

$$\begin{aligned}
&\|\theta_k D^{\sigma-\beta_k}[U_{a,b}\varphi_i]\|_p \\
&\qquad \leq \sum_{\mu \leq \sigma-\beta_k} \binom{\sigma-\beta_k}{\mu} \|\theta_k (D^\mu U_{a,b})(D^{\sigma-\beta_k-\mu}\varphi_i)\|_p \,.
\end{aligned} \tag{85}$$

We estimate separately each term on the right side of (85).

We separate into two cases.

If $\mu = 0$ then, using the induction hypothesis (i.e., $\mathcal{P}(p, j-k)$; recall that $\operatorname{supp}\theta_k \subseteq \omega_{\epsilon(j-k)}$) and (23),

$$\|\theta_k U_{a,b} D^{\sigma-\beta_k}\varphi_i\|_p \leq C_1 C\Big(\frac{B}{\epsilon}\Big)^{j-k} \leq \frac{C}{2}\Big(\frac{B}{\epsilon}\Big)^{j-k+1/2}. \tag{86}$$

In the last inequality we used the choice of B (see Remark 2.2) and that $\epsilon \leq 1$.

If $0 < \mu \leq \sigma - \beta_k$, then (since $\operatorname{supp}\chi_k \subseteq \omega_{\epsilon(j-k+1/4)}$) Hölder's inequality (with $1/p = 1/(3p) + 2/(3p)$) and Corollary D.2 give that

$$\begin{aligned}
&\|\theta_k(D^\mu U_{a,b})(D^{\sigma-\beta_k-\mu}\varphi_i)\|_p \\
&\quad \leq \|\theta_k D^\mu U_{a,b}\|_{3p/2}\ \|\theta_k D^{\sigma-\beta_k-\mu}\varphi_i\|_{3p} \\
&\quad \leq K_2 \|D^\mu U_{a,b}\|_{L^{3p/2}(\omega_{\epsilon(j-k+1/4)})} \\
&\qquad \times \|D^{\sigma-\beta_k-\mu}\varphi_i\|^{\theta}_{W^{1,p}(\omega_{\epsilon(j-k+1/4)})} \|D^{\sigma-\beta_k-\mu}\varphi_i\|^{1-\theta}_{L^p(\omega_{\epsilon(j-k+1/4)})} \,.
\end{aligned} \tag{87}$$

Here, K_2 is the constant in Corollary D.2, and $\theta = 2/p < 1$. Note that $\omega_{\epsilon(j-k+1/4)} = B_r(\mathbf{x}_0)$ with $r \in [R/2, 1]$, since $\epsilon(j+1) \leq R/2$ and $R = \min\{1, |\mathbf{x}_0|/4\}$

We will use Lemma 5.3 below to bound the first factor in (87). The last two factors we now bound using the induction hypothesis.

If $\mu \in \mathbb{N}_0^3$ is such that $0 < \mu \leq \sigma - \beta_k$, then the induction hypothesis (in the form discussed in Remark 3.2) gives (recall here (18) and that $|\sigma| = j, |\beta_k| = k$) that for the last two factors in (87) we have

$$
\begin{aligned}
&\|D^{\sigma-\beta_k-\mu}\varphi_i\|^{1-\theta}_{L^p(\omega_{\epsilon(j-k+1/4)})} \\
&\qquad\leq \Big[C\Big(\frac{j-k-|\mu|}{j-k+1/4}\Big)^{j-k-|\mu|}\Big(\frac{B}{\epsilon}\Big)^{j-k-|\mu|}\Big]^{1-\theta}
\end{aligned}
\tag{88}
$$

and (using that $B > 1$ (see Remark 2.2) and $\epsilon(j-k+1/4) \leq \epsilon(j+1) \leq R/2 < 1$)

$$
\begin{aligned}
\|D^{\sigma-\beta_k-\mu}\varphi_i\|^{\theta}_{W^{1,p}(\omega_{\epsilon(j-k+1/4)})} &\leq \Big[C\Big(\frac{j-k-|\mu|}{j-k+1/4}\Big)^{j-k-|\mu|}\Big(\frac{B}{\epsilon}\Big)^{j-k-|\mu|} \\
&\qquad + 3C\Big(\frac{j-k-|\mu|+1}{j-k+1/4}\Big)^{j-k-|\mu|+1}\Big(\frac{B}{\epsilon}\Big)^{j-k-|\mu|+1}\Big]^{\theta} \\
&\leq \Big[4C\Big(\frac{j-k-|\mu|+1}{j-k+1/4}\Big)^{j-k-|\mu|+1}\Big(\frac{B}{\epsilon}\Big)^{j-k-|\mu|+1}\Big]^{\theta}.
\end{aligned}
\tag{89}
$$

It follows from (88) and (89) that for all $\mu \in \mathbb{N}_0^3$ with $0 < \mu \leq \sigma - \beta_k$,

$$
\begin{aligned}
&\|D^{\sigma-\beta_k-\mu}\varphi_i\|^{\theta}_{W^{1,p}(\omega_{\epsilon(j-k+1/4)})}\|D^{\sigma-\beta_k-\mu}\varphi_i\|^{1-\theta}_{L^p(\omega_{\epsilon(j-k+1/4)})} \\
&\qquad \leq C4^{\theta}\Big(\frac{B}{\epsilon}\Big)^{j-k-|\mu|+\theta}\Big(\frac{j-k-|\mu|+1}{j-k+1/4}\Big)^{j-k-|\mu|+\theta}.
\end{aligned}
\tag{90}
$$

From (87), Lemma 5.3, and (90) (using (A.6) in Appendix 5 below, summing over $m = |\mu|$), it follows that

$$
\begin{aligned}
\sum_{0<\mu\leq\sigma-\beta_k}\binom{\sigma-\beta_k}{\mu}\|\theta_k(D^{\mu}U_{a,b})(D^{\sigma-\beta_k-\mu}\varphi_i)\|_p &\leq C^3C_3K_2\Big(\frac{B}{\epsilon}\Big)^{j-k+\theta}\times \\
\times\sum_{m=1}^{j-k}4^{\theta}\binom{j-k}{m}&\frac{(j-k-m+1)^{j-k-m+\theta}(m+1/4)^m}{(j-k+1/4)^{j-k+\theta}}\times \\
&\times\Big[\Big(\frac{1}{\sqrt{B}}\Big)^m + \sqrt{m}\Big(\frac{B(m+1/4)}{\epsilon(j-k+1/4)}\Big)^{2\theta-2}\Big].
\end{aligned}
\tag{91}
$$

Here, C_3 is the constant from (26). Recall also that $\theta = 2/p$.

We prove that for $m \in \{1,\ldots,j-k\}$,

$$
4^{\theta}\binom{j-k}{m}\frac{(j-k-m+1)^{j-k-m+\theta}(m+1/4)^m}{(j-k+1/4)^{j-k+\theta}} \leq 10\epsilon^{-1/2+\theta}\frac{1}{\sqrt{m}}.
\tag{92}
$$

Note first that, since $\epsilon(j-k+1/4) \leq \epsilon(j+1) \leq 1$,

$$
(j-k+1/4)^{1/2-\theta} \leq \epsilon^{-1/2+\theta}.
\tag{93}
$$

This shows that the inequality in (92) is true for $m = j-k > 0$, since $\theta < 1$. For $m < j-k$, we use (A.8) in Appendix 5 below, and (93), to get that (since $(1+1/n)^n \leq \mathrm{e}$)

$$
\begin{aligned}
&\binom{j-k}{m}\frac{(j-k-m+1)^{j-k-m+\theta}(m+1/4)^m}{(j-k+1/4)^{j-k+\theta}} \\
&\qquad\leq \frac{\mathrm{e}^{25/12}}{\sqrt{2\pi}}\frac{(j-k-m+1)^{\theta}}{(j-k-m)^{1/2}}\epsilon^{-1/2+\theta}\frac{1}{\sqrt{m}}.
\end{aligned}
\tag{94}
$$

Since $\theta < 1/2$ and $m \leq j-k-1$, we have that

$$\frac{(j-k-m+1)^{\theta}}{(j-k-m)^{1/2}} \leq 2^{\theta} \leq \sqrt{2}\,. \tag{95}$$

The estimate (92) for $m \in \{1,\dots,j-k-1\}$ now follows from (94)–(95) (since $4^{\theta}\mathrm{e}^{25/12}/\sqrt{\pi} \leq 10$).

Inserting (92) in (91) (and using again $\epsilon(j-k+1/4) \leq 1$ and $2\theta-2<0$) we find that

$$\begin{aligned}
&\sum_{0<\mu\leq\sigma-\beta_k} \binom{\sigma-\beta_k}{\mu} \|\theta_k(D^{\mu}U_{a,b})(D^{\sigma-\beta_k-\mu}\varphi_i)\|_p \\
&\quad \leq 10C^3C_3K_2\Big(\frac{B}{\epsilon}\Big)^{j-k+\theta}\epsilon^{-1/2+\theta}\sum_{m=1}^{j-k}\Big[\Big(\frac{1}{\sqrt{B}}\Big)^m + \frac{1}{B^{2-2\theta}}\frac{1}{m^{2-2\theta}}\Big] \\
&\quad \leq 10C^3C_3K_2\Big(\frac{B}{\epsilon}\Big)^{j-k+1/2}\frac{1}{\sqrt{B}}\,(2+6)\,,
\end{aligned} \tag{96}$$

where we used that $\theta \leq 2/5$, $B \geq 4$ (see Remark 2.2), and $\sum_{m=1}^{\infty} m^{-6/5} \leq 1 + \int_1^{\infty} x^{-6/5}\,dx = 6$ to estimate

$$\sum_{m=1}^{\infty}\Big(\frac{1}{\sqrt{B}}\Big)^m \leq \frac{2}{\sqrt{B}}\,, \qquad \frac{1}{B^{2-2\theta}}\sum_{m=1}^{\infty}\frac{1}{m^{2-2\theta}} \leq \frac{6}{\sqrt{B}}\,. \tag{97}$$

This is the very essential reason for needing $p \geq 5$.

By the choice of B (see Remark 2.2) it follows that

$$\sum_{0<\mu\leq\sigma-\beta_k} \binom{\sigma-\beta_k}{\mu} \|\theta_k(D^{\mu}U_{a,b})(D^{\sigma-\beta_k-\mu}\varphi_i)\|_p \leq \frac{C}{2}\Big(\frac{B}{\epsilon}\Big)^{j-k+1/2}. \tag{98}$$

From , (85), (86), and (98) it follows that for all $k \in \{0,\dots,j-1\}$,

$$\|\theta_k D^{\sigma-\beta_k}[U_{a,b}\varphi_i]\|_p \leq C\Big(\frac{B}{\epsilon}\Big)^{j-k+1/2}. \tag{99}$$

Using (82), (83), (84), and (99) it follows for the first sum in (81) that

$$\begin{aligned}
&\Big\|\sum_{k=0}^{j}\Phi D_{\nu}E(\mathbf{p})^{-1}D^{\beta_k}\chi_k D^{\sigma-\beta_k}[U_{a,b}\varphi_i]\Big\|_p \\
&\quad \leq C_2\sum_{k=0}^{j}8^k\epsilon^{-k}\|\theta_k D^{\sigma-\beta_k}[U_{a,b}\varphi_i]\|_p \leq C_2C\Big(\frac{B}{\epsilon}\Big)^{j+1/2}\sum_{k=0}^{j}\Big(\frac{8}{B}\Big)^k.
\end{aligned} \tag{100}$$

Since $B > 16$ (see Remark 2.2) the last sum is less than 2 and so for the first term in (81) we finally get, by the choice of B (see Remark 2.2) that

$$\begin{aligned}
&\Big\|\sum_{k=0}^{j}\Phi D_{\nu}E(\mathbf{p})^{-1}D^{\beta_k}\chi_k D^{\sigma-\beta_k}[U_{a,b}\varphi_i]\Big\|_p \\
&\qquad\qquad \leq 2C_2C\Big(\frac{B}{\epsilon}\Big)^{j+1/2} \leq \frac{CZ}{12N}\Big(\frac{B}{\epsilon}\Big)^{j+1}.
\end{aligned} \tag{101}$$

The second sum in (81). By the same arguments as for the second sum in (51) (see after (64)), it follows that the second sum in (81) can be estimated as the first one, up to *one* extra factor of

C_*/ϵ (with $C_* > 0$ the constant in (B.3) in Appendix B below) *and* up to replacing j by $j-1$ in the estimate (101). Hence, by the choice of B (see Remark 2.2)

$$\Big\| \sum_{k=0}^{j-1} \Phi D_\nu E(\mathbf{p})^{-1} D^{\beta_k}[\eta_k, D^{\mu_k}] D^{\sigma-\beta_{k+1}}[U_{a,b}\varphi_i] \Big\|_p \leq \frac{C_*}{\epsilon}\frac{CZ}{12N}\Big(\frac{B}{\epsilon}\Big)^j \leq \frac{CZ}{12N}\Big(\frac{B}{\epsilon}\Big)^{j+1}. \tag{102}$$

The last term in (81). Since $\sigma + e_\nu = \beta$, the last term in (81) equals

$$\Phi D^\beta E(\mathbf{p})^{-1}[\eta_j U_{a,b}\varphi_i].$$

We proceed exactly as for the term $\Phi D^\beta E(\mathbf{p})^{-1}[\eta_j V(1-\widetilde{\chi}_\rho)\varphi_i]$ in (68) (but without any splitting in $\widetilde{\chi}_\rho$ and $1-\widetilde{\chi}_\rho$), except that the estimate in (77) is replaced by $\|U_{a,b}\|_\infty \leq C_1$ (see (23)). It follows, from the choice of B and C (see Remark 2.2) that (recall that $|\beta| = j+1$)

$$\begin{aligned}\|\Phi D^\beta E(\mathbf{p})^{-1}[\eta_j U_{a,b}\varphi_i]\|_p &\leq \|\Phi D^\beta E(\mathbf{p})^{-1}\eta_j\|_{\mathcal{B}_{3,p}}\|U_{a,b}\varphi_i\|_3 \\ &\leq \frac{4\sqrt{2}}{\pi}C_1\|\varphi_i\|_3\Big(\frac{32}{\epsilon}\Big)^{|\beta|} \leq \frac{CZ}{12N}\Big(\frac{B}{\epsilon}\Big)^{j+1}.\end{aligned} \tag{103}$$

The estimate (50) now follows from (81) and the estimates (101), (102), and (103).

This finishes the proof of Lemma 3.6. □

It remains to prove Lemma 5.3 below ($L^{3p/2}$-bound on derivatives of the Newton potential $U_{a,b}$ of products of orbitals, $\varphi_a\varphi_b$).

In the next lemma we first give an $L^{3p/2}$-estimate on the derivatives of the product of the orbitals φ_i, needed for the proof of the bound in Lemma 5.3 below.

Lemma 5.1. *Assume* (40) *(the induction hypothesis) holds. Then, for all $a, b \in \{1, \ldots, N\}$, all $\beta \in \mathbb{N}_0^3$ with $|\beta| \leq j-1$, and all $\epsilon > 0$ with $\epsilon(|\beta|+1) \leq R/2$,*

$$\|D^\beta(\varphi_a\overline{\varphi_b})\|_{L^{3p/2}(\omega_{\epsilon(|\beta|+1)})} \leq 10K_2^2C^2(1+\sqrt{|\beta|})\Big(\frac{B}{\epsilon}\Big)^{|\beta|+2\theta}, \tag{104}$$

with K_2 from Corollary D.2 , C from Remark 2.2, and $\theta = \theta(p) = 2/p$.

Proof. By Leibniz's rule and the Cauchy-Schwarz inequality we get that

$$\begin{aligned}&\|D^\beta(\varphi_a\overline{\varphi_b})\|_{L^{3p/2}(\omega_{\epsilon(|\beta|+1)})} \\ &\qquad\leq \sum_{\mu\leq\beta}\binom{\beta}{\mu}\|D^\mu\varphi_a\|_{L^{3p}(\omega_{\epsilon(|\beta|+1)})}\|D^{\beta-\mu}\varphi_b\|_{L^{3p}(\omega_{\epsilon(|\beta|+1)})}.\end{aligned}$$

We use Corollary D.2 (with $\omega_{\epsilon(|\beta|+1)} = B_r(\mathbf{x}_0)$, $r = R - \epsilon(|\beta|+1)$; note that $r \in [R/2, 1]$, since $\epsilon(|\beta|+1) \leq R/2$ and $R = \min\{1, |\mathbf{x}_0|/4\}$). This gives that, with K_2 from Corollary D.2, and $\theta = 2/p$,

$$\begin{aligned}&\|D^\beta(\varphi_a\overline{\varphi_b})\|_{L^{3p/2}(\omega_{\varepsilon(|\beta|+1)})} \\ &\qquad\leq K_2^2\sum_{\mu\leq\beta}\binom{\beta}{\mu}\|D^\mu\varphi_a\|^\theta_{W^{1,p}(\omega_{\epsilon(|\beta|+1)})}\|D^\mu\varphi_a\|^{1-\theta}_{L^p(\omega_{\epsilon(|\beta|+1)})} \\ &\qquad\qquad\times\|D^{\beta-\mu}\varphi_b\|^\theta_{W^{1,p}(\omega_{\epsilon(|\beta|+1)})}\|D^{\beta-\mu}\varphi_b\|^{1-\theta}_{L^p(\omega_{\epsilon(|\beta|+1)})}.\end{aligned} \tag{105}$$

We now use the induction hypothesis (in the form discussed in Remark 3.2) on each of the four factors in the sum on the right side of (105). Note that, by assumption, $\epsilon(|\beta|+1) \leq \epsilon j \leq R/2$ and $|\mu| < |\mu|+1 \leq |\beta|+1 \leq j$ (similarly, $|\beta-\mu| < |\beta-\mu|+1 \leq j$). Recalling (18), we therefore get that, for all $\mu \in \mathbb{N}_0^3$ such that $\mu \leq \beta$,

$$
\begin{aligned}
&\|D^\mu \varphi_a\|^\theta_{W^{1,p}(\omega_{\epsilon(|\beta|+1)})} \|D^\mu \varphi_a\|^{1-\theta}_{L^p(\omega_{\epsilon(|\beta|+1)})} \\
&\leq \Big[C\Big(\frac{|\mu|}{|\beta|+1}\Big)^{|\mu|}\Big(\frac{B}{\epsilon}\Big)^{|\mu|}\Big]^{1-\theta} \\
&\quad\times \Big[C\Big(\frac{|\mu|}{|\beta|+1}\Big)^{|\mu|}\Big(\frac{B}{\epsilon}\Big)^{|\mu|} + 3C\Big(\frac{|\mu|+1}{|\beta|+1}\Big)^{|\mu|+1}\Big(\frac{B}{\epsilon}\Big)^{|\mu|+1}\Big]^\theta \\
&\leq 4^\theta C\Big(\frac{B}{\epsilon}\Big)^{|\mu|+\theta} \frac{(|\mu|+1)^{\theta(|\mu|+1)}|\mu|^{|\mu|(1-\theta)}}{(|\beta|+1)^{|\mu|+\theta}}\,,
\end{aligned}
$$

since (recall that $\epsilon(|\beta|+1) \leq R/2 < 1$ and $B > 1$)

$$
\frac{|\mu|^{|\mu|}}{(|\mu|+1)^{|\mu|+1}}\,\epsilon(|\beta|+1)B^{-1} \leq 1\,.
$$

Proceeding similarly for the other two factors in (105), we get (using (A.6) in Appendix 5 and summing over $m = |\mu|$) that

$$
\begin{aligned}
&\sum_{\mu\leq\beta} \binom{\beta}{\mu} \|D^\mu \varphi_a\|_{L^{3p}(\omega_{\epsilon(|\beta|+1)})} \|D^{\beta-\mu}\varphi_b\|_{L^{3p}(\omega_{\epsilon(|\beta|+1)})} \\
&\leq 16^\theta (CK_2)^2 \Big(\frac{B}{\epsilon}\Big)^{|\beta|+2\theta} \times \\
&\sum_{m=0}^{|\beta|} \binom{|\beta|}{m} \frac{\big[(m+1)^{m+1}(|\beta|-m+1)^{|\beta|-m+1}\big]^\theta \big[m^m(|\beta|-m)^{|\beta|-m}\big]^{1-\theta}}{(|\beta|+1)^{|\beta|+2\theta}}\,.
\end{aligned}
\tag{106}
$$

We simplify the sum in m. Note that for $m = 0$ and $m = |\beta|$, the summand is bounded by 1. Therefore, for $|\beta| \leq 1$ the estimate (104) follows from (106), since $2\cdot 16^\theta \leq 7$. It remains to consider $|\beta| \geq 2$. For $m \geq 1$, $m < |\beta|$, we can use (A.8) in Appendix 5 to get (since $(1+1/n)^n \leq \mathrm{e}$) that

$$
\begin{aligned}
&\sum_{0<\mu<\beta} \binom{\beta}{\mu} \|D^\mu \varphi_a\|_{L^{3p}(\omega_{\epsilon(|\beta|+1)})} \|D^{\beta-\mu}\varphi_b\|_{L^{3p}(\omega_{\epsilon(|\beta|+1)})} \\
&\qquad\leq \frac{\mathrm{e}^{1/12}}{\sqrt{2\pi}} (CK_2)^2 (16\mathrm{e}^2)^\theta \Big(\frac{B}{\epsilon}\Big)^{|\beta|+2\theta} \frac{|\beta|^{|\beta|+1/2}}{(|\beta|+1)^{|\beta|+2\theta}} \\
&\qquad\quad\times \sum_{m=1}^{|\beta|-1} \frac{\big[(m+1)(|\beta|-m+1)\big]^\theta}{\sqrt{m}\sqrt{|\beta|-m}}\,.
\end{aligned}
$$

Since the function

$$
f(x) = (x+1)(|\beta|-x+1)\,, \quad x \in [1, |\beta|-1]\,,
$$

has its maximum (which is $(|\beta|/2+1)^2$) at $x = |\beta|/2$, and since

$$
\sum_{m=1}^{|\beta|-1} \frac{1}{\sqrt{m}\sqrt{|\beta|-m}} \leq \int_0^{|\beta|} \frac{1}{\sqrt{x}\sqrt{|\beta|-x}}\,dx = \pi\,,
$$

we get that

$$\sum_{0<\mu<\beta} \binom{\beta}{\mu} \|D^\mu \varphi_a\|_{L^{3p}(\omega_{\epsilon(|\beta|+1)})} \|D^{\beta-\mu}\varphi_b\|_{L^{3p}(\omega_{\epsilon(|\beta|+1)})} \\ \leq \mathrm{e}^{1/12}(16\mathrm{e}^2)^\theta \sqrt{\frac{\pi}{2}} (CK_2)^2 \sqrt{|\beta|} \Big(\frac{B}{\epsilon}\Big)^{|\beta|+2\theta} . \tag{107}$$

The estimate (104) now follows from (105), (106), and (107), since (as $p \geq 5$),

$$\mathrm{e}^{1/12}(16\mathrm{e}^2)^\theta \sqrt{\frac{\pi}{2}} \leq 10 , \qquad 2\cdot 16^\theta \leq 7 .$$

This finishes the proof of Lemma 5.1. □

The next two lemmas, used in the proof above of Lemma 3.6, control the $L^{3p/2}$-norm of derivatives of $U_{a,b}$.

Lemma 5.2. *Define $U_{a,b}$ by* (48). *Then for all $a, b \in \{1, \dots, N\}$, and all $\mu \in \mathbb{N}_0^3$ with $|\mu| \leq 2$,*

$$\|D^\mu U_{a,b}\|_{L^{3p/2}(\omega)} \leq 4\pi K_3 (C^2 + 2C_1/R^2) , \tag{108}$$

with K_3 from Corollary D.4 , C from Remark 2.2, C_1 from (23), *and $R = \min\{1, |\mathbf{x}_0|/4\}$.*

Proof. Recall that $\omega = B_R(\mathbf{x}_0)$, $R = \min\{1, |\mathbf{x}_0|/4\}$. Using (18), and Corollary D.4 , we get that, for all $\mu \in \mathbb{N}_0^3$ with $|\mu| \leq 2$,

$$\|D^\mu U_{a,b}\|_{L^{3p/2}(\omega)} \leq \|U_{a,b}\|_{W^{2,3p/2}(B_R(\mathbf{x}_0))} \\ \leq K_3 \big\{ \|\Delta U_{a,b}\|_{L^{3p/2}(B_{2R}(\mathbf{x}_0))} + \frac{1}{R^2} \|U_{a,b}\|_{L^{3p/2}(B_{2R}(\mathbf{x}_0))} \big\} . \tag{109}$$

By the definition of $U_{a,b}$ (see (48)) we have

$$-\Delta U_{a,b}(\mathbf{x}) = 4\pi\, \varphi_a(\mathbf{x}) \overline{\varphi_b}(\mathbf{x}) \quad \text{for} \quad \mathbf{x} \in \mathbb{R}^3 , \tag{110}$$

and $\|U_{a,b}\|_\infty \leq C_1$ (see (23)). Hence, from (109), Hölder's inequality, and the choice of C (see Remark 2.2; recall also that $p \geq 5$)

$$\|D^\mu U_{a,b}\|_{L^{3p/2}(\omega)} \leq 4\pi K_3 \big\{ \|\varphi_a\|_{L^{3p}(B_{2R}(\mathbf{x}_0))} \|\varphi_b\|_{L^{3p}(B_{2R}(\mathbf{x}_0))} \\ + \frac{1}{R^2} \|U_{a,b}\|_\infty |B_{2R}(\mathbf{x}_0)|^{2/3p} \big\} \\ \leq 4\pi K_3 (C^2 + 2C_1/R^2) .$$

This finishes the proof of the lemma. □

Lemma 5.3. *Assume* (40) *(the induction hypothesis) holds, and define $U_{a,b}$ by* (48). *Then for all $a, b \in \{1, \dots, N\}$, all $k \in \{0, \dots, j-1\}$, all $\mu \in \mathbb{N}_0^3$ with $|\mu| \leq j-k$, and all $\epsilon > 0$ with $\epsilon(j+1) \leq R/2$,*

$$\|D^\mu U_{a,b}\|_{L^{3p/2}(\omega_{\epsilon(j-k+1/4)})} \leq C_3 C^2 \Big(\frac{\sqrt{B}}{\epsilon}\Big)^{|\mu|} \Big(\frac{|\mu|+1/4}{j-k+1/4}\Big)^{|\mu|} \\ + C_3 C^2 \sqrt{|\mu|} \Big(\frac{B}{\epsilon}\Big)^{|\mu|+2\theta-2} \Big(\frac{|\mu|+1/4}{j-k+1/4}\Big)^{|\mu|+2\theta-2} , \tag{111}$$

with $\theta = \theta(p) = 2/p$, C and B from Remark 2.2, and C_3 the constant in (26).

Proof. If $m := |\mu| \leq 2$, (111) follows from Lemma 5.2 and the definition of C_3 in (26), since $\epsilon(j-k+1/4) \leq \epsilon(j+1) \leq R/2 < 1$, and $C, B > 1$ (see Remark 2.2).

If $m := |\mu| \geq 3$ then we write $\mu = \mu_{m-2} + e_{\nu_1} + e_{\nu_2}$ with $\nu_i \in \{1,2,3\}, i = 1,2$, $|\mu_{m-2}| = m-2$. Then by the definition of the $W^{2,3p/2}$-norm (recall (18)) we find that

$$\begin{aligned}\|D^{\mu}U_{a,b}\|_{L^{3p/2}(\omega_{\epsilon(j-k+1/4)})} &\leq \|D^{\mu_{m-2}}U_{a,b}\|_{W^{2,3p/2}(\omega_{\epsilon(j-k+1/4)})} \\ &= \|D^{\mu_{m-2}}U_{a,b}\|_{W^{2,3p/2}(\omega_{\tilde{\epsilon}_1(m-1+1/4)})}, \end{aligned}\tag{112}$$

with $\tilde{\epsilon}_1$ such that

$$\tilde{\epsilon}_1(m-1+1/4) = \epsilon(j-k+1/4)\,. \tag{113}$$

To estimate the norm in (112) we will again use that $U_{a,b}$ satisfies (110). Applying $D^{\mu_{m-2}}$ to (110) and using the elliptic *a priori* estimate in Corollary D.4 (with $r = r_1 = R - \tilde{\epsilon}_1(m-1+1/4)$ and $\delta = \delta_1 = \tilde{\epsilon}_1/4$; recall that $\omega_\rho = B_{R-\rho}(\mathbf{x}_0)$) we get that

$$\begin{aligned}\|D^{\mu}U_{a,b}\|_{L^{3p/2}(\omega_{\epsilon(j-k+1/4)})} &\leq 4\pi K_3 \|D^{\mu_{m-2}}(\varphi_a\overline{\varphi_b})\|_{L^{3p/2}(\omega_{\tilde{\epsilon}_1(m-1)})} \\ &\quad + \frac{16K_3}{\tilde{\epsilon}_1^2}\|D^{\mu_{m-2}}U_{a,b}\|_{L^{3p/2}(\omega_{\tilde{\epsilon}_1(m-1)})}\,, \end{aligned}\tag{114}$$

with $K_3 = K_3(p)$ the constant in (D.9). Notice that for this estimate we needed to enlarge the domain, taking the ball with a radius $\tilde{\epsilon}_1/4$ larger.

We now iterate the procedure (on the second term on the right side of (114)), with $\tilde{\epsilon}_i$ ($i = 2, \ldots, \lfloor\frac{m}{2}\rfloor$) such that

$$\tilde{\epsilon}_i(m-2i+1+1/4) = \tilde{\epsilon}_{i-1}(m-2(i-1)+1)\,, \tag{115}$$

and with $r = r_i = R - \tilde{\epsilon}_i(m-2i+1+1/4)$ and $\delta = \delta_i = \tilde{\epsilon}_i/4$. Note that (113) and (115) imply that, for $i = 2, \ldots, \lfloor\frac{m}{2}\rfloor$,

$$\tilde{\epsilon}_i \geq \tilde{\epsilon}_{i-1} \geq \ldots \geq \tilde{\epsilon}_1 = \epsilon\,\frac{j-k+1/4}{m-1+1/4}\,, \tag{116}$$

and

$$\begin{aligned}\tilde{\epsilon}_i(m-2i+1) &\leq \tilde{\epsilon}_{i-1}(m-2(i-1)+1) \\ &\leq \ldots \leq \tilde{\epsilon}_1(m-1) \leq \epsilon(j-k+1/4)\,. \end{aligned}\tag{117}$$

We get that (with $\prod_{\ell=1}^{0} \equiv 1$ and $|\mu_{m-2i}| = m-2i$),

$$\begin{aligned}&\|D^{\mu}U_{a,b}\|_{L^{3p/2}(\omega_{\epsilon(j-k+1/4)})} \\ &\quad\leq 4\pi K_3 \sum_{i=1}^{\lfloor\frac{m}{2}\rfloor}\Big[\|D^{\mu_{m-2i}}(\varphi_a\overline{\varphi_b})\|_{L^{3p/2}(\omega_{\tilde{\epsilon}_i(m-2i+1)})}\prod_{\ell=1}^{i-1}\Big(\frac{16K_3}{\tilde{\epsilon}_\ell^2}\Big)\Big] \\ &\qquad + \Big[\prod_{\ell=1}^{\lfloor\frac{m}{2}\rfloor}\frac{16K_3}{\tilde{\epsilon}_\ell^2}\Big]\|D^{\mu_{m-2\lfloor\frac{m}{2}\rfloor}}\,U_{a,b}\|_{L^{3p/2}(\omega_{\tilde{\epsilon}_{\lfloor\frac{m}{2}\rfloor}(m-2\lfloor\frac{m}{2}\rfloor+1)})}\,. \end{aligned}\tag{118}$$

Using (116), and Lemma 5.1 for each $i = 1, \ldots, \lfloor\frac{m}{2}\rfloor$ fixed (note that $\tilde{\epsilon}_i(m-2i+1) \leq R/2$ by (117) since $\epsilon(j+1) \leq R/2$) we get that

$$\begin{aligned}&\|D^{\mu_{m-2i}}(\varphi_a\overline{\varphi_b})\|_{L^{3p/2}(\omega_{\tilde{\epsilon}_i(m-2i+1)})}\prod_{\ell=1}^{i-1}\Big(\frac{16K_3}{\tilde{\epsilon}_\ell^2}\Big) \\ &\quad\leq 20K_2^2C^2\sqrt{m}\Big(\frac{B}{\epsilon}\Big)^{m+2\theta-2}\Big(\frac{m-1+1/4}{j-k+1/4}\Big)^{m+2\theta-2}\Big(\frac{16K_3}{B^2}\Big)^{i-1}, \end{aligned}\tag{119}$$

with K_2 from Corollary D.2, and $\theta = \theta(p) = 2/p$. Here we also used that $1 + \sqrt{m-2i} \le 2\sqrt{m}$. Note that $\sum_{i=1}^{\lfloor \frac{m}{2} \rfloor} (16K_3/B^2)^{i-1} < 2$ since $B^2 > 32K_3$ (see Remark 2.2). It follows that

$$4\pi K_3 \sum_{i=1}^{\lfloor \frac{m}{2} \rfloor} \Big[\| D^{\mu_{m-2i}}(\varphi_a \overline{\varphi_b}) \|_{L^{3p/2}(\omega_{\tilde{\epsilon}_i(m-2i+1)})} \prod_{\ell=1}^{i-1} \Big(\frac{16K_3}{\tilde{\epsilon}_\ell^2} \Big) \Big]$$
$$\le 160\pi K_2^2 K_3 C^2 \sqrt{m} \Big(\frac{B}{\epsilon} \Big)^{m+2\theta-2} \Big(\frac{m+1/4}{j-k+1/4} \Big)^{m+2\theta-2} . \tag{120}$$

We now estimate the last term in (118). Let $\delta = m - 2\lfloor \frac{m}{2} \rfloor \in \{0,1\}$ (depending on whether m is even or odd). Then, using (116) and Lemma 5.2, we get that

$$\Big[\prod_{\ell=1}^{\lfloor \frac{m}{2} \rfloor} \frac{16K_3}{\tilde{\epsilon}_\ell^2} \Big] \| D^{\mu_{m-2\lfloor \frac{m}{2} \rfloor}} U_{a,b} \|_{L^{3p/2}(\omega_{\tilde{\epsilon}_{\lfloor \frac{m}{2} \rfloor}(m-2\lfloor \frac{m}{2} \rfloor+1)})}$$
$$\le 4\pi K_3 (C^2 + 2C_1/R^2) \Big(\frac{\sqrt{16K_3}}{\epsilon} \Big)^m \Big(\frac{m-1+1/4}{j-k+1/4} \Big)^m$$
$$\times \Big(\frac{\epsilon(j-k+1/4)}{m-1+1/4} \Big)^\delta$$
$$\le 4\pi K_3 (1 + 2C_1/R^2) C^2 \Big(\frac{\sqrt{B}}{\epsilon} \Big)^m \Big(\frac{m+1/4}{j-k+1/4} \Big)^m . \tag{121}$$

Here we also used that $m \ge 3$ and $K_3 \ge 1$ (See Corollary D.4), that $C > 1$ and $B > 16K_3$ (see Remark 2.2), and that $\epsilon(j-k+1/4) \le 1$.

Combining (118), (120), and (121) finishes the proof of (111) in the case $m = |\mu| \ge 3$.

This finishes the proof of Lemma 5.3. $\square$

A Multiindices and Stirling's Formula

We denote $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$. For $\sigma = (\sigma_1, \sigma_2, \sigma_3) \in \mathbb{N}_0^3$ we let $|\sigma| := \sigma_1 + \sigma_2 + \sigma_3$, and

$$D^\sigma := D_1^{\sigma_1} D_2^{\sigma_2} D_3^{\sigma_3} , \quad D_\nu := -\,\mathrm{i} \frac{\partial}{\partial x_\nu} =: -\,\mathrm{i}\,\partial_\nu , \quad \nu = 1,2,3 . \tag{A.1}$$

This way,

$$\partial^\sigma := \frac{\partial^{|\sigma|}}{\partial \mathbf{x}^\sigma} := \frac{\partial^{|\sigma|}}{\partial x_1^{\sigma_1} x_2^{\sigma_2} x_3^{\sigma_3}} = (-\mathrm{i})^{|\sigma|} D^\sigma .$$

We let $\sigma! := \sigma_1! \sigma_2! \sigma_3!$, and, for $n \in \mathbb{N}_0$,

$$\binom{n}{\sigma} := \frac{n!}{\sigma!} = \frac{n!}{\sigma_1! \sigma_2! \sigma_3!} . \tag{A.2}$$

With this notation we have the multinomial formula, for $\mathbf{x} = (x_1, x_2, x_3) \in \mathbb{R}^3$ and $n \in \mathbb{N}_0$,

$$(x_1 + x_2 + x_3)^n = \sum_{\mu \in \mathbb{N}_0^3, |\mu| = n} \binom{n}{\mu} \mathbf{x}^\mu . \tag{A.3}$$

Here, $\mathbf{x}^\mu := x_1^{\mu_1} x_2^{\mu_2} x_3^{\mu_3}$. It follows that

$$|\sigma|! \le 3^{|\sigma|} \sigma! \ \text{ for all } \sigma \in \mathbb{N}_0^3 , \tag{A.4}$$

since, using (A.2), that $(1,1,1)^\mu = 1$ for all $\mu \in \mathbb{N}_0^3$, and (A.3),

$$\frac{|\sigma|!}{\sigma!} = \binom{|\sigma|}{\sigma} \leq \sum_{\mu\in\mathbb{N}_0^3, |\mu|=|\sigma|} \binom{|\sigma|}{\mu}(1,1,1)^\mu = (1+1+1)^{|\sigma|} = 3^{|\sigma|}\,.$$

We also define

$$\binom{\sigma}{\mu} := \frac{\sigma!}{\mu!(\sigma-\mu)!} \tag{A.5}$$

for $\sigma, \mu \in \mathbb{N}_0^3$ with $\mu \leq \sigma$, that is, $\mu_\nu \leq \sigma_\nu$, $\nu = 1,2,3$. Note that for all $\sigma \in \mathbb{N}_0^3$ and $k \in \mathbb{N}_0$ (see [19, Proposition 2.1]),

$$\sum_{\mu\leq\sigma, |\mu|=k} \binom{\sigma}{\mu} = \binom{|\sigma|}{k}\,. \tag{A.6}$$

Finally, by [1, 6.1.38], we have the following generalization of Stirling's Formula: For $m \in \mathbb{N}$,

$$m! = \sqrt{2\pi}m^{m+\frac{1}{2}}\exp(-m + \frac{\vartheta}{12m}) \text{ for some } \vartheta = \vartheta(m) \in (0,1)\,, \tag{A.7}$$

and so for $n, m \in \mathbb{N}$, $m < n$,

$$\begin{aligned}\binom{n}{m} &= \frac{1}{\sqrt{2\pi}}\frac{n^{n+1/2}}{m^{m+1/2}(n-m)^{n-m+1/2}}\exp(\frac{\vartheta(n)}{12n} - \frac{\vartheta(m)}{12m} - \frac{\vartheta(n-m)}{12(n-m)}) \\ &\leq \frac{\mathrm{e}^{1/12}}{\sqrt{2\pi}}\,\frac{n^{n+1/2}}{m^{m+1/2}(n-m)^{n-m+1/2}}\,. \end{aligned}\tag{A.8}$$

B Choice of the localization

Recall that, for $\mathbf{x}_0 \in \mathbb{R}^3\backslash\{0\}$ and $R = \min\{1, |\mathbf{x}_0|/4\}$, we have defined $\omega = B_R(\mathbf{x}_0)$, $\omega_\delta = B_{R-\delta}(\mathbf{x}_0)$, and that $\epsilon > 0$ is such that $\epsilon(j+1) \leq R/2$. Also, recall (see (44)) that we have chosen a function Φ (depending on j) satisfying

$$\Phi \in C_0^\infty(\omega_{\epsilon(j+3/4)})\,, \quad 0 \leq \Phi \leq 1\,, \quad \text{with } \Phi \equiv 1 \text{ on } \omega_{\epsilon(j+1)}\,. \tag{B.1}$$

For $j \in \mathbb{N}$ we choose functions $\{\chi_k\}_{k=0}^j$, and $\{\eta_k\}_{k=0}^j$ (all depending on j) with the following properties (for an illustration, see figures 1 and 2). The functions $\{\chi_k\}_{k=0}^j$ are such that

$$\chi_0 \in C_0^\infty(\omega_{\epsilon(j+1/4)}) \quad \text{with} \quad \chi_0 \equiv 1 \quad \text{on } \omega_{\epsilon(j+1/2)}\,,$$

and, for $k = 1, \ldots, j$,

$$\begin{aligned}&\chi_k \in C_0^\infty(\omega_{\epsilon(j-k+1/4)}) \\ &\quad\text{with} \begin{cases}\chi_k \equiv 1 & \text{on } \omega_{\epsilon(j-k+1/2)} \setminus \omega_{\epsilon(j-k+1+1/4)}\,, \\ \chi_k \equiv 0 & \text{on } \mathbb{R}^3 \setminus (\omega_{\epsilon(j-k+1/4)} \setminus \omega_{\epsilon(j-k+1+1/2)})\,,\end{cases}\end{aligned}$$

Finally, the functions $\{\eta_k\}_{k=0}^j$ are such that for $k = 0, \ldots, j$,

$$\eta_k \in C^\infty(\mathbb{R}^3) \quad \text{with} \quad \begin{cases}\eta_k \equiv 1 & \text{on } \mathbb{R}^3 \setminus \omega_{\epsilon(j-k+1/4)}\,, \\ \eta_k \equiv 0 & \text{on } \omega_{\epsilon(j-k+1/2)}\,.\end{cases}$$

Moreover we ask that

$$
\begin{array}{lll}
\chi_0 + \eta_0 \equiv 1 & \text{on} & \mathbb{R}^3, \\
\chi_k + \eta_k \equiv 1 & \text{on} & \mathbb{R}^3 \setminus \omega_{\epsilon(j-k+1+1/4)} \ \text{ for } \ k = 1, \dots, j\,, \\
\eta_k \equiv \chi_{k+1} + \eta_{k+1} & \text{on} & \mathbb{R}^3 \ \text{ for } \ k = 0, \dots, j-1\,.
\end{array}
\tag{B.2}
$$

Furthermore, we choose these localization functions such that, for a constant $C_* > 0$ (independent of ϵ, k, j, β) and for all $\beta \in \mathbb{N}_0^3$ with $|\beta| = 1$, we have that

$$
|D^\beta \chi_k(\mathbf{x})| \le \frac{C_*}{\epsilon} \quad \text{and} \quad |D^\beta \eta_k(\mathbf{x})| \le \frac{C_*}{\epsilon}\,, \tag{B.3}
$$

for $k = 0, \dots, j$, and all $\mathbf{x} \in \mathbb{R}^3$.

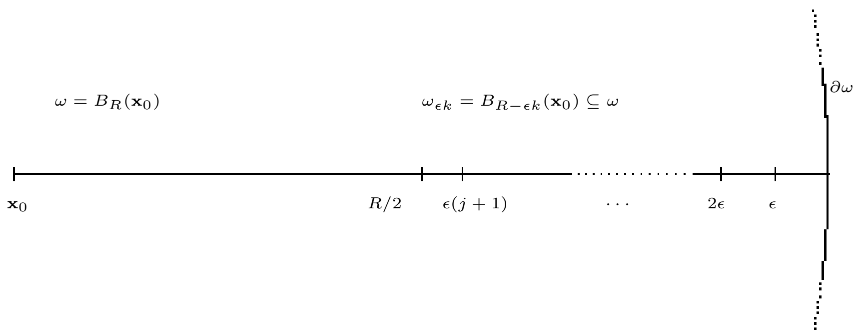

Figure 19: The geometry of $\omega = B_R(\mathbf{x}_0)$ and the $\omega_{\epsilon k} = B_{R-\epsilon k}(\mathbf{x}_0)$'s.

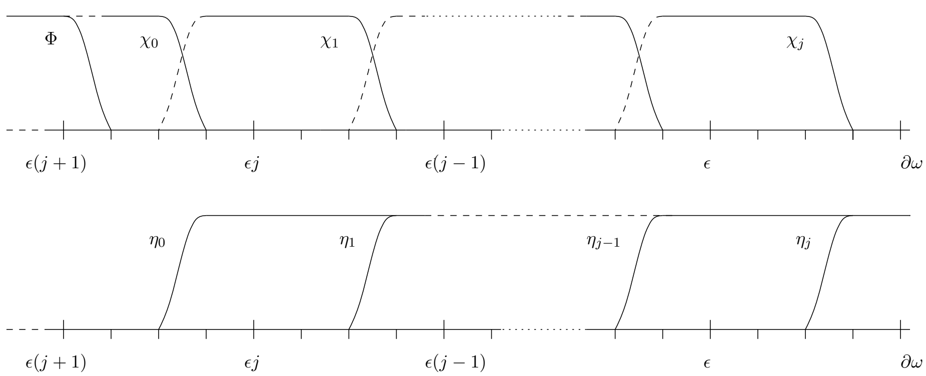

Figure 20: The localization functions.

The next lemma shows how to use these localization functions.

Lemma B.1. *For $j \in \mathbb{N}$ fixed, choose functions $\{\chi_k\}_{k=0}^j$, and $\{\eta_k\}_{k=0}^j$ as above, and let $\sigma \in \mathbb{N}_0^3$ with $|\sigma| = j$. For $\ell \in \mathbb{N}$ with $\ell \le j$, choose multiindices $\{\beta_k\}_{k=0}^\ell$ such that:*

$$
|\beta_k| = k \text{ for } k = 0, \dots, \ell\,,\ \beta_{k-1} < \beta_k \ \text{ for } \ k = 1, \dots, \ell, \ \text{ and } \ \beta_\ell \le \sigma\,.
$$

Then for all $g \in \mathcal{S}'(\mathbb{R}^3)$,

$$
\begin{aligned}
D^\sigma g = & \sum_{k=0}^{\ell} D^{\beta_k} \chi_k D^{\sigma - \beta_k} g \\
& + \sum_{k=0}^{\ell-1} D^{\beta_k} [\eta_k, D^{\mu_k}] D^{\sigma - \beta_{k+1}} g + D^{\beta_\ell} \eta_\ell D^{\sigma - \beta_\ell} g\,,
\end{aligned}
\tag{B.4}
$$

with $\mu_k = \beta_{k+1} - \beta_k$ for $k = 0, \dots, \ell - 1$ (hence, $|\mu_k| = 1$).

Proof. We prove the lemma by induction on ℓ from $\ell = 1$ to $\ell = j$. We start by proving the claim for $\ell = 1$. By using property (B.2) of the localization functions and that $\beta_1 = \beta_0 + \mu_0 = \mu_0$ (since $\beta_0 = 0$) we find that

$$D^\sigma g = \chi_0 D^\sigma g + \eta_0 D^\sigma g = \chi_0 D^\sigma g + \eta_0 D^{\sigma-\beta_1+\mu_0} g\,. \tag{B.5}$$

The first term on the right side of (B.5) is the term corresponding to $k = 0$ in the first sum in (B.4). In the second term in (B.5), commuting the derivative through η_0, we find that

$$\eta_0 D^{\sigma-\beta_1+\mu_0} g = D^{\mu_0}\eta_0 D^{\sigma-\beta_1} g + [\eta_0, D^{\mu_0}] D^{\sigma-\beta_1} g\,.$$

Since $\eta_0 = \chi_1 + \eta_1$ by property (B.2), this implies that

$$\begin{aligned}&\eta_0 D^{\sigma-\beta_1+\mu_0} g\\ &\quad = D^{\beta_1}\chi_1 D^{\sigma-\beta_1} g + D^{\beta_1}\eta_1 D^{\sigma-\beta_1} g + [\eta_0, D^{\mu_0}] D^{\sigma-\beta_1} g\,.\end{aligned} \tag{B.6}$$

The identity (B.4) for $\ell = 1$ follows from (B.5) and (B.6).

We now assume that (B.4) holds for $\ell - 1$ for some $\ell \geq 2$, i.e.,

$$\begin{aligned}D^\sigma g = &\sum_{k=0}^{\ell-1} D^{\beta_k}\chi_k D^{\sigma-\beta_k} g\\ &+ \sum_{k=0}^{\ell-2} D^{\beta_k}[\eta_k, D^{\mu_k}] D^{\sigma-\beta_{k+1}} g + D^{\beta_{\ell-1}}\eta_{\ell-1} D^{\sigma-\beta_{\ell-1}} g\,,\end{aligned} \tag{B.7}$$

and prove it then holds for ℓ. Since $\beta_{\ell-1} = \beta_\ell - \mu_{\ell-1}$ we can rewrite the last term on the right side of (B.7) as

$$D^{\beta_{\ell-1}}\eta_{\ell-1} D^{\sigma-\beta_{\ell-1}} g = D^{\beta_{\ell-1}}\eta_{\ell-1} D^{\sigma-\beta_\ell+\mu_{\ell-1}} g\,.$$

Again, commuting the $\mu_{\ell-1}$-derivative through $\eta_{\ell-1}$ this implies that

$$\begin{aligned}&D^{\beta_{\ell-1}}\eta_{\ell-1} D^{\sigma-\beta_{\ell-1}} g\\ &\quad = D^{\beta_{\ell-1}+\mu_{\ell-1}}\eta_{\ell-1} D^{\sigma-\beta_\ell} g + D^{\beta_{\ell-1}}[\eta_{\ell-1}, D^{\mu_{\ell-1}}] D^{\sigma-\beta_\ell} g\\ &\quad = D^{\beta_\ell}(\eta_\ell + \chi_\ell) D^{\sigma-\beta_\ell} g + D^{\beta_{\ell-1}}[\eta_{\ell-1}, D^{\mu_{\ell-1}}] D^{\sigma-\beta_\ell} g\,,\end{aligned} \tag{B.8}$$

using (B.2). Collecting together (B.7) and (B.8) proves that (B.4) holds for ℓ.

The claim of the lemma then follows by induction. □

C Norms of some operators on $L^p(\mathbb{R}^3)$

In this section we prove two lemmas on bounds on certain operators involving the operator $E(\mathbf{p}) = \sqrt{-\Delta + \alpha^{-2}}$.

Lemma C.1. *Let the operators $S_\nu = E(\mathbf{p})^{-1} D_\nu$, $\nu \in \{1, 2, 3\}$, be defined for $f \in \mathcal{S}(\mathbb{R}^3)$ by*

$$(S_\nu f)(\mathbf{x}) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} \mathrm{e}^{\mathrm{i}\mathbf{x}\cdot\mathbf{p}} E(\mathbf{p})^{-1} p_\nu \hat{f}(\mathbf{p})\, d\mathbf{p}\,,$$

with $\hat{f}(\mathbf{p}) = (2\pi)^{-3/2}\int_{\mathbb{R}^3} \mathrm{e}^{-\mathrm{i}\mathbf{x}\cdot\mathbf{p}} f(\mathbf{x})\, d\mathbf{x}$ the Fourier transform of f. (Here, $\mathbf{p} = (p_1, p_2, p_3)$.)

Then, for all $\mathfrak{p} \in (1, \infty)$, S_ν extend to bounded operators, $S_\nu : L^{\mathfrak{p}}(\mathbb{R}^3) \to L^{\mathfrak{p}}(\mathbb{R}^3)$, $\nu \in \{1, 2, 3\}$. Clearly, $\|S_\nu\|_{\mathcal{B}_{\mathfrak{p}}} = \|S_\mu\|_{\mathcal{B}_{\mathfrak{p}}}$, $\nu \neq \mu$. We let

$$K_1 \equiv K_1(\mathfrak{p}) := \|S_1\|_{\mathcal{B}_{\mathfrak{p}}} \,. \tag{C.1}$$

Proof. This follows from [30, Theorem 0.2.6] and the *Remarks* right after it. In fact, since (by induction),

$$D^\gamma_{\mathbf{p}}\big(p_\nu E(\mathbf{p})^{-1}\big) = P_{\gamma,\nu}(\mathbf{p}) E(\mathbf{p})^{-1-2|\gamma|}\,, \quad \gamma \in \mathbb{N}_0^3\,,$$

for some polynomials $P_{\gamma,\nu}$ of degree $|\gamma| + 1$, the functions $m_\nu(\mathbf{p}) = p_\nu E(\mathbf{p})^{-1}$ are smooth and satisfy the estimates

$$|D^\gamma_{\mathbf{p}} m_\nu(\mathbf{p})| \le C_{\gamma,\nu} |\mathbf{p}|^{-|\gamma|}\,, \quad \gamma \in \mathbb{N}_0^3\,,$$

for some constants $C_{\gamma,\nu} > 0$, which is what is needed in the reference above. □

For $\mathfrak{p}, \mathfrak{q} \in [1, \infty]$, denote by $\|\cdot\|_{\mathcal{B}_{\mathfrak{p},\mathfrak{q}}}$ the operator norm on bounded operators from $L^{\mathfrak{p}}(\mathbb{R}^3)$ to $L^{\mathfrak{q}}(\mathbb{R}^3)$.

Lemma C.2. *For all $\mathfrak{p}, \mathfrak{r} \in [1, \infty)$, $\mathfrak{q} \in (1, \infty)$, with $\mathfrak{p}^{-1} + \mathfrak{q}^{-1} + \mathfrak{r}^{-1} = 2$, all $\alpha > 0$, all $\beta \in \mathbb{N}_0^3$ (with $|\beta| > 1$ if $\mathfrak{r} = 1$), and all $\Phi, \chi \in C^\infty(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ with*

$$\mathrm{dist}(\mathrm{supp}(\chi), \mathrm{supp}(\Phi)) \ge d\,, \tag{C.2}$$

the operator $\Phi E(\mathbf{p})^{-1} D^\beta \chi$ is bounded from $L^{\mathfrak{p}}(\mathbb{R}^3)$ to $(L^{\mathfrak{q}}(\mathbb{R}^3))' = L^{\mathfrak{q}^*}(\mathbb{R}^3)$ (with $\mathfrak{q}^{-1} + \mathfrak{q}^{*-1} = 1$), and

$$\begin{aligned} &\|\Phi E(\mathbf{p})^{-1} D^\beta \chi\|_{\mathcal{B}_{\mathfrak{p},\mathfrak{q}^*}} \\ &\qquad \le \frac{4\sqrt{2}}{\pi} \beta! \Big(\frac{8}{d}\Big)^{|\beta|} d^{3/\mathfrak{r}-2} \big(\mathfrak{r}(|\beta| + 2) - 3\big)^{-1/\mathfrak{r}} \|\Phi\|_\infty \|\chi\|_\infty\,. \end{aligned} \tag{C.3}$$

In particular, (when $\mathfrak{r} = 1$, i.e., $\mathfrak{q}^* = \mathfrak{p}$),

$$\|\Phi E(\mathbf{p})^{-1} D^\beta \chi\|_{\mathcal{B}_{\mathfrak{p}}} \le \frac{32\sqrt{2}}{\pi} \frac{\beta!}{|\beta| - 1} \Big(\frac{8}{d}\Big)^{|\beta|-1} \|\Phi\|_\infty \|\chi\|_\infty\,, \tag{C.4}$$

for all $\beta \in \mathbb{N}_0^3$ with $|\beta| > 1$.

Proof. We use duality. Let $f, g \in \mathcal{S}(\mathbb{R}^3)$. Note that, since $\Phi f, D^\beta(\chi g) \in L^2(\mathbb{R}^3)$, the spectral theorem, and the formula

$$\frac{1}{\sqrt{x}} = \frac{1}{\pi} \int_0^\infty \frac{1}{x + t} \frac{dt}{\sqrt{t}}\,, \ x > 0\,, \tag{C.5}$$

imply that

$$(f, \Phi E(\mathbf{p})^{-1} D^\beta \chi g) = \frac{1}{\pi} \int_0^\infty \frac{dt}{\sqrt{t}} \, (f, \Phi(-\Delta + \alpha^{-2} + t)^{-1} D^\beta \chi g)\,.$$

By using the formula for the kernel of the operator $(-\Delta + \alpha^{-2} + t)^{-1}$ [29, (IX.30)], and integrating by parts, we get that

$$\begin{aligned} &(f, \Phi E(\mathbf{p})^{-1} D^\beta \chi g) \\ &= \frac{1}{\pi} \int_0^\infty \frac{dt}{\sqrt{t}} \int_{\mathbb{R}^3} \overline{f(\mathbf{x})} \Phi(\mathbf{x}) \int_{\mathbb{R}^3} \frac{\mathrm{e}^{-\sqrt{\alpha^{-2}+t}\,|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x} - \mathbf{y}|} \, [D^\beta(\chi g)](\mathbf{y}) \, d\mathbf{x} d\mathbf{y} \\ &= \frac{(-1)^{|\beta|}}{\pi} \int_0^\infty \frac{dt}{\sqrt{t}} \int_{\mathbb{R}^3} \overline{f(\mathbf{x})} \Phi(\mathbf{x}) \int_{\mathbb{R}^3} \Big(D^\beta_{\mathbf{y}} \frac{\mathrm{e}^{-\sqrt{\alpha^{-2}+t}\,|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x} - \mathbf{y}|}\Big) \chi(\mathbf{y}) g(\mathbf{y}) \, d\mathbf{x} d\mathbf{y}\,. \end{aligned}$$

Notice that the integrand is different from zero only for $|\mathbf{x}-\mathbf{y}|\geq d$, due to the assumption (C.2). Hence, by Fubini's theorem,

$$(f,\Phi E(\mathbf{p})^{-1}D^{\beta}\chi g)=\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}F(\mathbf{x})H(\mathbf{x}-\mathbf{y})G(\mathbf{y})\,d\mathbf{x}d\mathbf{y}\,, \tag{C.6}$$

with $F(\mathbf{x})=\overline{f(\mathbf{x})}\Phi(\mathbf{x})$, $G(\mathbf{y})=\chi(\mathbf{y})g(\mathbf{y})$, and

$$\begin{aligned} H(\mathbf{z}) &\equiv H_{\alpha,\beta,d}(\mathbf{z}) \\ &= \mathbb{1}_{\{|\cdot|\geq d\}}(\mathbf{z})\frac{(-1)^{|\beta|}}{\pi}\int_0^\infty\Big(D_{\mathbf{z}}^{\beta}\,\frac{\mathrm{e}^{-\sqrt{\alpha^{-2}+t}\,|\mathbf{z}|}}{4\pi|\mathbf{z}|}\Big)\frac{dt}{\sqrt{t}}\,. \end{aligned} \tag{C.7}$$

Now, by (C.9) in Lemma C.3 below, uniformly for $\alpha>0$,

$$\begin{aligned} |H(\mathbf{z})| &\leq \mathbb{1}_{\{|\cdot|\geq d\}}(\mathbf{z})\frac{\sqrt{2}}{4\pi^2}\frac{\beta!}{|\mathbf{z}|}\Big(\frac{8}{|\mathbf{z}|}\Big)^{|\beta|}\int_0^\infty \mathrm{e}^{-\sqrt{t}|\mathbf{z}|/2}\frac{dt}{\sqrt{t}} \\ &= \mathbb{1}_{\{|\cdot|\geq d\}}(\mathbf{z})\frac{\sqrt{2}}{\pi^2}\frac{\beta!}{|\mathbf{z}|^2}\Big(\frac{8}{|\mathbf{z}|}\Big)^{|\beta|}, \end{aligned}$$

and so, for all $\alpha>0$, $\mathfrak{r}\in[1,\infty)$, and all $\beta\in\mathbb{N}_0^3$ (with $|\beta|>1$ if $\mathfrak{r}=1$),

$$\begin{aligned} \|H\|_{\mathfrak{r}} &\leq (4\pi)^{1/\mathfrak{r}}\frac{\sqrt{2}}{\pi^2}\beta!\,8^{|\beta|}\Big(\int_d^\infty\big(|\mathbf{z}|^{-|\beta|-2}\big)^{r}|\mathbf{z}|^2\,d|\mathbf{z}|\Big)^{1/\mathfrak{r}} \\ &= (4\pi)^{1/\mathfrak{r}}\frac{\sqrt{2}}{\pi^2}\beta!\Big(\frac{8}{d}\Big)^{|\beta|}d^{3/\mathfrak{r}-2}\big(\mathfrak{r}(|\beta|+2)-3\big)^{-1/\mathfrak{r}}. \end{aligned}$$

From this, (C.6), and Young's inequality [24, Theorem 4.2] (notice that $C_Y\leq 1$), follows that, with $\mathfrak{p},\mathfrak{q},\mathfrak{r}\in[1,\infty)$, $\mathfrak{p}^{-1}+\mathfrak{q}^{-1}+\mathfrak{r}^{-1}=2$,

$$\begin{aligned} |(f,\Phi E(\mathbf{p})^{-1}D^{\beta}\chi g)| &\leq \|F\|_{\mathfrak{q}}\|H\|_{\mathfrak{r}}\|G\|_{\mathfrak{p}} \\ &\leq (4\pi)^{1/\mathfrak{r}}\frac{\sqrt{2}}{\pi^2}\beta!\Big(\frac{8}{d}\Big)^{|\beta|}d^{3/\mathfrak{r}-2}\big(\mathfrak{r}(|\beta|+2)-3\big)^{-1/\mathfrak{r}}\|F\|_{\mathfrak{q}}\|G\|_{\mathfrak{p}} \\ &\leq \frac{4\sqrt{2}}{\pi}\beta!\Big(\frac{8}{d}\Big)^{|\beta|}d^{3/\mathfrak{r}-2}\big(\mathfrak{r}(|\beta|+2)-3\big)^{-1/\mathfrak{r}}\|\Phi\|_\infty\|\chi\|_\infty\|f\|_{\mathfrak{q}}\|g\|_{\mathfrak{p}}\,. \end{aligned}$$

Since $\mathcal{S}(\mathbb{R}^3)$ is dense in both $L^{\mathfrak{p}}(\mathbb{R}^3)$ and $L^{\mathfrak{q}^*}(\mathbb{R}^3)$, this finishes the proof of the lemma. □

Lemma C.3. *For all $s>0$, $\mathbf{x}\in\mathbb{R}^3\setminus\{0\}$, and $\beta\in\mathbb{N}_0^3$,*

$$\Big|\partial_{\mathbf{x}}^{\beta}\frac{1}{|\mathbf{x}|}\Big|\leq\frac{\sqrt{2}\beta!}{|\mathbf{x}|}\Big(\frac{8}{|\mathbf{x}|}\Big)^{|\beta|}, \tag{C.8}$$

$$\Big|\partial_{\mathbf{x}}^{\beta}\frac{\mathrm{e}^{-s|\mathbf{x}|}}{|\mathbf{x}|}\Big|\leq\frac{\sqrt{2}\beta!}{|\mathbf{x}|}\Big(\frac{8}{|\mathbf{x}|}\Big)^{|\beta|}\mathrm{e}^{-s|\mathbf{x}|/2}. \tag{C.9}$$

Proof. We will use the Cauchy inequalities [18, Theorem 2.2.7]. To avoid confusion with the Euclidean norm $|\cdot|$ (in $\mathbb{R}^3$ or in $\mathbb{C}^3$), we denote by $|\cdot|_{\mathbb{C}}$ the absolut value in $\mathbb{C}$.

Let, for $\mathbf{w}=(w_1,w_2,w_3)\in\mathbb{C}^3$ and $r>0$,

$$P_r^3(\mathbf{w})=\{\mathbf{z}\in\mathbb{C}^3\mid|z_\nu-w_\nu|_{\mathbb{C}}<r\,,\ \nu=1,2,3\} \tag{C.10}$$

be the *poly-disc* with *poly-radius* $\mathbf{r} = (r,r,r)$. The Cauchy inequalities then state that if u is analytic in $P_r^3(\mathbf{w})$ and if $\sup_{\mathbf{z}\in P_r^3(\mathbf{w})} |u(\mathbf{z})|_{\mathbb{C}} \le M$, then

$$|\partial_{\mathbf{z}}^{\beta} u(\mathbf{w})|_{\mathbb{C}} \le M\beta!\, r^{-|\beta|} \quad \text{for all } \beta \in \mathbb{N}_0^3\,. \tag{C.11}$$

We take $\mathbf{w} = \mathbf{x} \in \mathbb{R}^3 \setminus \{0\} \subseteq \mathbb{C}^3$ and choose $r = |\mathbf{x}|/8$. We prove below that then we have (with $\mathbf{z}^2 := \sum_{\nu=1}^{3} z_\nu^2 \in \mathbb{C}$)

$$\mathrm{Re}(\mathbf{z}^2) \ge \frac{1}{2}|\mathbf{x}|^2 \;\text{ for } \mathbf{z} \in P_r^3(\mathbf{x})\,. \tag{C.12}$$

It follows that $\sqrt{\mathbf{z}^2} := \exp(\frac{1}{2}\mathrm{Log}\,\mathbf{z^2})$ is well-defined and analytic on $P_r^3(\mathbf{x})$ with Log being the principal branch of the logarithm.

We will also argue below that

$$\mathrm{Re}(\sqrt{\mathbf{z}^2}) \ge \frac{1}{2}|\mathbf{x}| \;\text{ for } \mathbf{z} \in P_r^3(\mathbf{x})\,. \tag{C.13}$$

Then (by (C.12)) for all $\mathbf{z} \in P_r^3(\mathbf{x})$,

$$|\sqrt{\mathbf{z}^2}|_{\mathbb{C}} = \sqrt{|\mathbf{z}^2|_{\mathbb{C}}} \ge \sqrt{|\mathrm{Re}\,\mathbf{z}^2|} \ge |\mathbf{x}|/\sqrt{2}\,, \tag{C.14}$$

and (by (C.13)), for all $s \ge 0$ and all $\mathbf{z} \in P_r^3(\mathbf{x})$,

$$|\exp(-s\sqrt{\mathbf{z}^2})|_{\mathbb{C}} = \exp(-s\mathrm{Re}(\sqrt{\mathbf{z}^2})) \le \exp(-s|\mathbf{x}|/2)\,. \tag{C.15}$$

Therefore, (C.8) and (C.9) follow from (C.11), (C.14), and (C.15).

It remains to prove (C.12) and (C.13).

For $\mathbf{z} \in P_r^3(\mathbf{x})$, write $\mathbf{z} = \mathbf{x} + \alpha + \mathrm{i}\mathbf{b}$ with $\alpha, \mathbf{b} \in \mathbb{R}^3$ satisfying $|z_\nu - x_\nu|_{\mathbb{C}}^2 = a_\nu^2 + b_\nu^2 \le (|\mathbf{x}|/8)^2$. Then

$$\mathbf{z}^2 = |\mathbf{x}+\alpha|^2 - |\mathbf{b}|^2 + 2\mathrm{i}(\mathbf{x}+\alpha)\cdot\mathbf{b}\,,$$

so, with $\epsilon = 1/8$,

$$\begin{aligned}\mathrm{Re}(\mathbf{z}^2) &= |\mathbf{x}|^2 + |\alpha|^2 + 2\,\mathbf{x}\cdot\alpha - |\mathbf{b}|^2 \\ &\ge (1-\epsilon)|\mathbf{x}|^2 + (2-\epsilon^{-1})|\alpha|^2 - (|\alpha|^2 + |\mathbf{b}|^2) \\ &\ge \frac{35}{64}|\mathbf{x}|^2 > \frac{1}{2}|\mathbf{x}|^2\,.\end{aligned}$$

This establishes (C.12) .

It follows from (C.12) that, with Arg the principal branch of the argument,

$$-\frac{\pi}{4} \le \frac{1}{2}\mathrm{Arg}(\mathbf{z}^2) \le \frac{\pi}{4} \;\text{ for } \mathbf{z} \in P_r^3(\mathbf{x})\,. \tag{C.16}$$

Furthermore (still for $\mathbf{z} \in P_r^3(\mathbf{x})$), because of (C.16),

$$\mathrm{Re}(\sqrt{\mathbf{z}^2}) = |\mathbf{z}^2|_{\mathbb{C}}^{1/2}\cos(\tfrac{1}{2}\mathrm{Arg}(\mathbf{z}^2)) \ge |\mathbf{z}^2|_{\mathbb{C}}^{1/2}/\sqrt{2}\,. \tag{C.17}$$

Combining with (C.12) we get (C.13).

This finishes the proof of the lemma. □

D Needed results

In this section we gather some results from the literature which are needed in our proofs.

Theorem D.1. *[2, Theorem 5.8] Let Ω be a domain in $\mathbb{R}^n$ satisfying the cone condition. Let $m \in \mathbb{N}, \mathfrak{p} \in (1,\infty)$. If $m\mathfrak{p} > n$, let $\mathfrak{p} \le \mathfrak{q} \le \infty$; if $m\mathfrak{p} = n$, let $\mathfrak{p} \le \mathfrak{q} < \infty$; if $m\mathfrak{p} < n$, let $\mathfrak{p} \le \mathfrak{q} \le \mathfrak{p}^* = n\mathfrak{p}/(n - m\mathfrak{p})$. Then there exists a constant K depending on $m, n, \mathfrak{p}, \mathfrak{q}$ and the dimensions of the cone C providing the cone condition for Ω, such that for all $u \in W^{m,\mathfrak{p}}(\Omega)$,*

$$\|u\|_{L^{\mathfrak{q}}(\Omega)} \le K \|u\|_{W^{m,\mathfrak{p}}(\Omega)}^{\theta} \|u\|_{L^{\mathfrak{p}}(\Omega)}^{1-\theta}, \tag{D.1}$$

where $\theta = (n/m\mathfrak{p}) - (n/m\mathfrak{q})$.

We write $K = K(m,n,\mathfrak{p},\mathfrak{q},\Omega)$. We always use Theorem D.1 with $n = 3$, $m = 1$, and $\mathfrak{p} = p, \mathfrak{q} = 3p$ for some $p > 3$. Hence $m\mathfrak{p} > n$, $\mathfrak{p} \le \mathfrak{q} \le \infty$, and $\theta = \theta(p) = 2/p < 1$. Moreover, we always use it with Ω being a ball, whose radius in all cases is bounded from above by 1 and from below by $R/2$ for some $R > 0$ fixed.

Let $K_0 \equiv K_0(p) \equiv K(1,3,p,3p,B_1(0))$ with $B_1(0) \subseteq \mathbb{R}^3$ the unit ball (which does satisfy the cone condition). Note that then, by scaling, (D.1) implies that for all $r \le 1$ and all $\mathbf{x}_0 \in \mathbb{R}^3$,

$$\|u\|_{L^{3p}(B_r(\mathbf{x}_0))} \le K_0 r^{-\theta} \|u\|_{W^{1,p}(B_r(\mathbf{x}_0))}^{\theta} \|u\|_{L^p(B_r(\mathbf{x}_0))}^{1-\theta}, \tag{D.2}$$

with $\theta = 2/p$.

To summarize, we therefore have the following corollary.

Corollary D.2. *Let $p > 3$ and $R \in (0,1]$. Then there exists a constant K_2, depending only on p and R, such that for all $r \in [R/2, 1]$, $\mathbf{x}_0 \in \mathbb{R}^3$, and all $u \in W^{1,p}(B_r(\mathbf{x}_0))$,*

$$\|u\|_{L^{3p}(B_r(\mathbf{x}_0))} \le K_2 \|u\|_{W^{1,p}(B_r(\mathbf{x}_0))}^{\theta} \|u\|_{L^p(B_r(\mathbf{x}_0))}^{1-\theta}, \tag{D.3}$$

with $\theta = 2/p$.

Here,

$$K_2 \equiv K_2(p,R) = (2/R)^{2/p} K_0(p), \tag{D.4}$$

where $K_0(p) = K(1,3,p,3p,B_1(0))$ in Theorem D.1 above.

Theorem D.3. *[4, Theorem 4.2] Let Ω be a bounded domain in $\mathbb{R}^n$ and let $a^{ij} \in C(\overline{\Omega})$, $b^i, c \in L^\infty(\Omega)$ $i,j \in \{1,\dots,n\}$, with $\lambda, \Lambda > 0$ such that*

$$\sum_{i,j=1}^{n} a^{ij}\xi_i\xi_j \ge \lambda|\xi|^2, \quad \text{for all} \quad x \in \Omega,\, \xi \in \mathbb{R}^n, \tag{D.5}$$

$$\sum_{i,j=1}^{n} \|a^{ij}\|_{L^\infty(\Omega)} + \sum_{i=1}^{n} \|b^i\|_{L^\infty(\Omega)} + \|c\|_{L^\infty(\Omega)} \le \Lambda. \tag{D.6}$$

Suppose $u \in W^{2,\mathfrak{p}}_{\mathrm{loc}}(\Omega)$ satisfies

$$Lu = \sum_{i,j=1}^{n} -a^{ij}D_iD_ju + \sum_{i=1}^{n} b^iD_iu + cu = f. \tag{D.7}$$

Then for any $\Omega' \subset\subset \Omega$,

$$\|u\|_{W^{2,\mathfrak{p}}(\Omega')} \le C\Big\{\frac{1}{\lambda}\|f\|_{L^{\mathfrak{p}}(\Omega)} + \|u\|_{L^{\mathfrak{p}}(\Omega)}\Big\}, \tag{D.8}$$

where C depends only on $n, \mathfrak{p}, \Lambda/\lambda, \operatorname{dist}\{\Omega', \partial\Omega\}$, and the modulus of continuity of the a^{ij}'s.

We use Theorem D.3 in the case where Ω' and Ω are concentric balls (and with $n = 3$, $\mathfrak{p} = 3p/2$, $a^{ij} = \delta_{ij}, b^i = c = 0$; hence $\Lambda = \lambda = 1$). Reading the proof of the theorem above with this case in mind (see [4, Lemma 4.1] in particular), one can make the dependence on $\operatorname{dist}\{\Omega', \partial\Omega\}$ explicit. More precisely, we have the following corollary.

Corollary D.4. *For all $p > 1$ there exists a constant $K_3 = K_3(p) \geq 1$ such that for all $u \in W^{2,3p/2}(B_{r+\delta}(\mathbf{x}_0))$ (with $\mathbf{x}_0 \in \mathbb{R}^3, r, \delta > 0$)*

$$\begin{aligned} &\|u\|_{W^{2,3p/2}(B_r(\mathbf{x}_0))} \\ &\qquad \leq K_3\big\{\|\Delta u\|_{L^{3p/2}(B_{r+\delta}(\mathbf{x}_0))} + \delta^{-2}\|u\|_{L^{3p/2}(B_{r+\delta}(\mathbf{x}_0))}\big\}\,. \end{aligned} \tag{D.9}$$

Theorem D.5. *[8, Theorem 5, Section 5.6.2 (Morrey's inequality)] Let Ω be a bounded, open subset in $\mathbb{R}^n$, $n \geq 2$, and suppose $\partial\Omega$ is C^1. Assume $n < \mathfrak{p} < \infty$, and $u \in W^{1,\mathfrak{p}}(\Omega)$. Then u has a version $u^* \in C^{0,\gamma}(\overline{\Omega})$, for $\gamma = 1 - n/\mathfrak{p}$, with the estimate*

$$\|u^*\|_{C^{0,\gamma}(\overline{\Omega})} \leq K_4\|u\|_{W^{1,\mathfrak{p}}(\Omega)}\,. \tag{D.10}$$

The constant K_4 depends only on $\mathfrak{p}, n$, and Ω.

Here, u^* is a version of the given u if $u = u^*$ a.e.. Above,

$$\|u\|_{C^{0,\gamma}(\overline{\Omega})} := \sup_{\mathbf{x}\in\Omega}|u(\mathbf{x})| + \sup_{\mathbf{x},\mathbf{y}\in\Omega,\,\mathbf{x}\neq\mathbf{y}} \frac{|u(\mathbf{x}) - u(\mathbf{y})|}{|\mathbf{x}-\mathbf{y}|^\gamma}\,. \tag{D.11}$$

Of course, $\sup_{\mathbf{x}\in\Omega}|u(\mathbf{x})| \leq \|u\|_{C^{0,\gamma}(\overline{\Omega})}$.

Remark D.6. *Note that [8, p. 245] uses a definition of the $W^{m,\mathfrak{p}}$-norm which is slightly different from ours (see* (18)*), but which is an equivalent norm by equivalence of norms in finite dimensional vectorspaces. Therefore,* (D.10) *holds with our definition of the norm (but the constant K_4 is not the same as the one in [8, Theorem 5, Section 5.6.2]).*

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Excess charge for pseudo-relativistic atoms in Hartree-Fock theory[1]

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Abstract

We prove within the Hartree-Fock theory of pseudo-relativistic atoms that the maximal negative ionization charge and the ionization energy of an atom remain bounded independently of the nuclear charge Z and the fine structure constant α as long as $Z\alpha$ is bounded.

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Contents

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1 Introduction

A long standing open problem in the mathematical physics literature is the Ionization conjecture. It can be formulated as follows. Consider atoms with arbitrarily large nuclear charge Z, is it true that the radius (see Definition 1.8) and the maximal negative ionization remain bounded? A positive answer to this question in the non-relativistic Hartree-Fock model has been given by the second author in [23]. One of the aims of the present paper is to extend the result taking into account some relativistic effects. The ionization conjecture for the full Schrödinger theory is still open both in the non-relativistic and relativistic case. See [13], [16], [17], [6], [7] and [22] for some Z-dependent bounds on the maximal negative ionization. The best result is that $N(Z) = Z + O(Z^a)$ with $a = 47/56$ where $N(Z)$ denotes the maximal number of electrons a nucleus of charge Z binds (see [6], [7] and [22]).

As a model for an atom with nuclear charge Z and N electrons we consider (in units where $\hbar = m = e = 1$) the operator

$$H = \sum_{i=1}^{N} \alpha^{-1}\big(\sqrt{-\Delta_i + \alpha^{-2}} - \alpha^{-1} - \frac{Z\alpha}{|\mathbf{x}_i|}\big) + \sum_{1\le i<j\le N} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|}, \tag{1}$$

where α is Sommerfeld's fine structure constant. The operator H acts on a dense subset of the N body Hilbert space $\mathcal{H}_F := \wedge_{i=1}^{N} L^2(\mathbb{R}^3;\mathbb{C}^q)$ of antisymmetric wave functions, where q is the number of spin states. The operator H is bounded from below on this subspace if $Z\alpha \le 2/\pi$ (see [9] for $N = 1$, [5] and [19] for $N \ge 1$). In this paper we will consider the sub-critical case $Z\alpha < 2/\pi$. Let us notice here that to define the operator H there is an issue. Indeed for $Z\alpha < 2/\pi$ the nuclear potential is only a small form perturbation of the kinetic energy and hence one needs to work with forms to define the operator H. This has been done in detail in [2].

The quantum ground state energy is the infimum of the spectrum of H considered as an operator acting on $\mathcal{H}_F$. In the Hartree-Fock approximation one restricts to wave-functions ψ which are pure wedge products, also called Slater determinants:

$$\psi(\mathbf{x}_1,\sigma_1,\mathbf{x}_2,\sigma_2,\dots,\mathbf{x}_N,\sigma_N) = \tfrac{1}{\sqrt{N!}}\det(u_i(\mathbf{x}_j,\sigma_j))_{i,j=1}^{N}, \tag{2}$$

with $\{u_i\}_{i=1}^{N}$ orthonormal in $L^2(\mathbb{R}^3;\mathbb{C}^q)$. The u_i's are also called orbitals. Notice that $\|\psi\|_{L^2(\mathbb{R}^{3N},\mathbb{C}^{qN})} = 1$. The Hartree-Fock ground state energy is

$$E^{\mathrm{HF}}(N,Z,\alpha) := \inf\{\mathrm{q}(\psi,\psi)|\psi \in \mathcal{Q}(H) \text{ and } \psi \text{ a Slater determinant}\},$$

with q the quadratic form defined by H and $\mathcal{Q}(H)$ the corresponding form domain.

One of the main result of the paper is the following.

Theorem 1.1. *Let $Z \ge 1$ and $\alpha > 0$. Let $Z\alpha = \kappa$ and assume that $0 \le \kappa < 2/\pi$. There is a constant $Q > 0$ depending only on κ such that if N is such that a Hartree-Fock minimizer exists then $N \le Z + Q$.*

The idea of the proof is the same as in [23]. One shows that the Thomas-Fermi model is a good approximation of the Hartree-Fock model except in the region far away from the nucleus. We first introduce some notation in order to introduce the Hartree-Fock and Thomas-Fermi models.

1.1 Notation

Let e be the quadratic form with domain $H^{\frac{1}{2}}(\mathbb{R}^3, \mathbb{C}^q)$ such that

$$\mathrm{e}(u, v) = (E(\mathbf{p})^{\frac{1}{2}} u, E(\mathbf{p})^{\frac{1}{2}} v) \text{ for all } u, v \in H^{\frac{1}{2}}(\mathbb{R}^3, \mathbb{C}^q), \tag{3}$$

where $E(\mathbf{p})$ denotes the operator $E(i\nabla) = \sqrt{-\Delta + \alpha^{-2}}$. As usual (u, v) denotes the scalar product of u and v in $L^2(\mathbb{R}^3, \mathbb{C}^q)$. Let $V(\mathbf{x}) := Z\alpha/|\mathbf{x}|$ and v be the quadratic form with domain $H^{\frac{1}{2}}(\mathbb{R}^3, \mathbb{C}^q)$ defined by

$$\mathrm{v}(u, v) = (V^{\frac{1}{2}} u, V^{\frac{1}{2}} v) \text{ for all } u, v \in H^{\frac{1}{2}}(\mathbb{R}^3, \mathbb{C}^q). \tag{4}$$

From [10, 5.33 p.307] we have

$$\int_{\mathbb{R}^3} \frac{|f(\mathbf{x})|^2}{|\mathbf{x}|} \, d\mathbf{x} \leq \frac{2}{\pi} \int_{\mathbb{R}^3} |\mathbf{p}| |\hat{f}(\mathbf{p})|^2 \, d\mathbf{p} \text{ for } f \in H^{\frac{1}{2}}(\mathbb{R}^3, \mathbb{C}) \tag{5}$$

with $\hat{f}$ the Fourier transform of f. Thus since $Z\alpha \leq 2/\pi$ and $E(\mathbf{p}) \geq |\mathbf{p}|$ it follows that $\mathrm{v}(u, u) \leq \mathrm{e}(u, u)$ for all $u \in H^{\frac{1}{2}}(\mathbb{R}^3, \mathbb{C}^q)$.

In the following t denotes the quadratic form associated to the kinetic energy; i.e. for all $u, v \in H^{\frac{1}{2}}(\mathbb{R}^3, \mathbb{C}^q)$

$$\mathrm{t}(u, v) := \alpha^{-1} \mathrm{e}(u, v) - \alpha^{-2}(u, v) = \alpha^{-1}(T(\mathbf{p})^{\frac{1}{2}} u, T(\mathbf{p})^{\frac{1}{2}} v), \tag{6}$$

with $T(\mathbf{p}) := E(\mathbf{p}) - \alpha^{-1}$.

A *density matrix* γ is a self-adjoint trace class operator that satisfies the operator inequality $0 \leq \gamma \leq Id$. A density matrix $\gamma : L^2(\mathbb{R}^3; \mathbb{C}^q) \to L^2(\mathbb{R}^3; \mathbb{C}^q)$ has an integral kernel

$$\gamma(\mathbf{x}, \sigma, \mathbf{y}, \tau) = \sum_j \lambda_j u_j(\mathbf{x}, \sigma) u_j(\mathbf{y}, \tau)^*, \tag{7}$$

where λ_j, u_j are the eigenvalues and corresponding eigenfunctions of γ. We choose the u_j's to be orthonormal in $L^2(\mathbb{R}^3, \mathbb{C}^q)$. Let $\rho_\gamma \in L^1(\mathbb{R}^3)$ denote the 1-particle density associated to γ given by

$$\rho_\gamma(\mathbf{x}) = \sum_{\sigma=1}^{q} \sum_j \lambda_j |u_j(\mathbf{x}, \sigma)|^2.$$

We define

$$\mathcal{A} := \{\gamma \text{ density matrix: } \operatorname{Tr}[T(\mathbf{p})\gamma] < +\infty\}, \tag{8}$$

where for $\gamma \in \mathcal{A}$ written as in (7) $\operatorname{Tr}[T(\mathbf{p})\gamma] := \operatorname{Tr}[E(\mathbf{p})\gamma] - \alpha^{-1} \operatorname{Tr}[\gamma]$ and

$$\operatorname{Tr}[E(\mathbf{p})\gamma] := \sum_j \lambda_j \mathrm{e}(u_j, u_j). \tag{9}$$

Similarly we use the following notation $\operatorname{Tr}[V\gamma] := \sum_j \lambda_j \mathrm{v}(u_j, u_j)$.

Remark 1.2. *If $\gamma \in \mathcal{A}$ then $\rho_\gamma \in L^1(\mathbb{R}^3)$ since γ is trace class and $\rho_\gamma \in L^{4/3}(\mathbb{R}^3)$. The second inclusion follows from Daubechies' inequality, a generalization of the Lieb-Thirring inequality (see Theorem 2.3).*

1.2 Hartree-Fock theory

In Hartree-Fock theory one considers wave functions that are pure wedge products and that satisfy the right statistics: determinantal wave functions as in (2). To define the HF-energy functional it is convenient to use the one to one correspondence between Slater determinants and projections onto finite dimensional subspaces of $L^2(\mathbb{R}^3, \mathbb{C}^q)$. Indeed if ψ is given by (2) and γ is the projection onto the space spanned by $u_1, \ldots, u_N$ the energy expectation depends only on γ: $(\psi, H\psi) = \mathcal{E}^{\mathrm{HF}}(\gamma)$. Here $\mathcal{E}^{\mathrm{HF}}$ defines the HF-energy functional

$$\mathcal{E}^{\mathrm{HF}}(\gamma) = \alpha^{-1}\,\mathrm{Tr}[(T(\mathbf{p}) - V)\gamma] + \mathcal{D}(\gamma) - \mathcal{E}x\,(\gamma)\,, \tag{10}$$

where $\mathcal{D}(\gamma)$ is the direct Coulomb energy

$$\mathcal{D}(\gamma) = \tfrac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\rho_\gamma(\mathbf{x})\rho_\gamma(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{x}d\mathbf{y},$$

and $\mathcal{E}x(\gamma)$ is the exchange Coulomb energy

$$\mathcal{E}x(\gamma) = \tfrac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\mathrm{Tr}_{\mathbb{C}^q}\left[|\gamma(\mathbf{x},\mathbf{y})|^2\right]}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{x}d\mathbf{y},$$

where we think of the integral kernel $\gamma(x, y)$ as a $q \times q$ matrix.

Using projections we can define as follows the HF-ground state.

Definition 1.3 (The HF-ground state)**.** *Let $Z > 0$ be a real number and $N \geq 0$ be an integer. The HF-ground state energy is*

$$E^{\mathrm{HF}}(N, Z, \alpha) := \inf\left\{\mathcal{E}^{\mathrm{HF}}(\gamma) : \gamma^2 = \gamma,\ \gamma \in \mathcal{A},\ \ \mathrm{Tr}[\gamma] = N\right\}.$$

If a minimizer exists we say that the atom has a HF ground state described by γ^{HF}.

We may extend the definition of the HF-functional from projections to density matrices in $\mathcal{A}$. We first notice that if $\gamma \in \mathcal{A}$, then all the terms in $\mathcal{E}^{\mathrm{HF}}(\gamma)$ are finite. From (5) it follows that

$$\mathrm{Tr}[V\gamma] = \sum_j \lambda_j \mathrm{v}(u_j, u_j) \leq \sum_j \lambda_j \mathrm{e}(u_j, u_j) = \mathrm{Tr}[E(\mathbf{p})\gamma].$$

On the other hand if $\gamma \in \mathcal{A}$ then $\rho_\gamma \in L^1(\mathbb{R}^3) \cap L^{\frac{4}{3}}(\mathbb{R}^3)$ (see Remark 1.2). By Hölder's inequality $\rho_\gamma \in L^{\frac{6}{5}}(\mathbb{R}^3)$ and hence $\mathcal{D}(\gamma)$ is bounded by Hardy-Littlewood-Sobolev's inequality. The boundness of the exchange term follows from $0 \leq \mathcal{E}x(\gamma) \leq \mathcal{D}(\gamma)$. On the other hand if γ is a density matrix with $\gamma \notin \mathcal{A}$ then $\mathcal{E}^{\mathrm{HF}}(\gamma) = \infty$. Here we use also that $Z\alpha < 2/\pi$.

Extending the set where we minimize, we could have lowered the ground state energy and/or changed the minimizer. That this is not the case follows from Lieb's variational principle.

Theorem 1.4 (Lieb's variational principle, [12])**.** *For all N non-negative integers it holds that*

$$\inf\{\mathcal{E}^{\mathrm{HF}}(\gamma) : \gamma \in \mathcal{A},\ \gamma^2 = \gamma,\ \ \mathrm{Tr}[\gamma] = N\} = \inf\{\mathcal{E}^{\mathrm{HF}}(\gamma) : \gamma \in \mathcal{A},\ \ \mathrm{Tr}[\gamma] = N\},$$

and if the infimum over all density matrices is attained so is the infimum over projections.

The following existence theorem for the HF-minimizer in the pseudo-relativistic case has been recently proved in [2].

Theorem 1.5. *Let $Z\alpha < 2/\pi$ and let $N \geq 2$ be a positive integer such that $N < Z + 1$.*

Then there exists an N-dimensional projection $\gamma^{\mathrm{HF}} = \gamma^{\mathrm{HF}}(N, Z, \alpha)$ minimizing the HF-energy functional $\mathcal{E}^{\mathrm{HF}}$ given by (10), that is, $E^{\mathrm{HF}}(N, Z, \alpha)$ is attained. Moreover, one can write

$$\gamma^{\mathrm{HF}}(\mathbf{x}, \sigma, \mathbf{y}, \tau) = \sum_{i=1}^{N} u_i(\mathbf{x}, \sigma) u_i(\mathbf{y}, \tau)^*,$$

with $u_i \in L^2(\mathbb{R}^3, \mathbb{C}^q)$, $i = 1, \ldots, N$, orthonormal, such that the HF-orbitals $\{u_i\}_{i=1}^N$ satisfy:

1. *$h_{\gamma^{\mathrm{HF}}} u_i = \varepsilon_i u_i$, with $0 > \varepsilon_N \geq \varepsilon_{N-1} \geq \cdots \geq \varepsilon_1 > -\alpha^{-1}$ and*

$$h_{\gamma^{\mathrm{HF}}} := T(\mathbf{p}) - \frac{Z\alpha}{|\mathbf{x}|} + \rho^{\mathrm{HF}} * |\mathbf{x}|^{-1} - \mathcal{K}_{\gamma^{\mathrm{HF}}}, \tag{11}$$

where ρ^{HF} denotes the density of the HF-minimizer and for $f \in H^{\frac{1}{2}}(\mathbb{R}^3)$

$$(\mathcal{K}_{\gamma^{\mathrm{HF}}} f)(\mathbf{x}, \sigma) = \sum_{i=1}^{N} u_i(\mathbf{x}, \sigma) \sum_{\tau=1}^{q} \int_{\mathbb{R}^3} u_i(\mathbf{y}, \tau)^* f(\mathbf{y}, \tau) |\mathbf{x} - \mathbf{y}|^{-1} d\mathbf{y}.$$

2. *$u_i \in C^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^q)$ for $i = 1, \ldots, N$;*

3. *$u_i \in H^1(\mathbb{R}^3 \setminus B_R(0))$ for all $R > 0$ and $i = 1, \ldots, N$.*

In the opposite direction the following result gives an upper bound on the excess charge.

Theorem 1.6. *Let $\alpha Z < \frac{2}{\pi}$. If N is a positive integer such that $N > 2Z + 1$ there are no minimizers for the HF-energy functional.*

This theorem for $Z\alpha < 1/2$ was proved by Lieb in [13]. With an improved approximation argument the proof can be extended to $Z\alpha < 2/\pi$ (see [3]). Notice that both proofs work not only in the Hartree-Fock approximation but for the minimization problem on $\wedge^N L^2(\mathbb{R}^3)$.

Definition 1.7. *Let γ^{HF} be the HF-minimizer. The function*

$$\varphi^{\mathrm{HF}}(\mathbf{x}) := \frac{Z}{|\mathbf{x}|} - \int_{\mathbb{R}^3} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|} d\mathbf{y} \text{ for } \mathbf{x} \in \mathbb{R}^3,$$

is called the HF-mean field potential and

$$\Phi_R^{\mathrm{HF}}(\mathbf{x}) := \frac{Z}{|\mathbf{x}|} - \int_{|\mathbf{y}|<R} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|} d\mathbf{y} \text{ for } \mathbf{x} \in \mathbb{R}^3,$$

is the HF-screened nuclear potential.

Definition 1.8. *We define the HF-radius $R_{Z,N}^{\mathrm{HF}}(\nu)$ to the ν last electrons by*

$$\int_{|\mathbf{x}| \geq R_{Z,N}^{\mathrm{HF}}(\nu)} \rho^{\mathrm{HF}}(\mathbf{x})\, d\mathbf{x} = \nu.$$

1.3 A bit of Thomas-Fermi theory

In this subsection we present briefly the Thomas-Fermi theory and especially the result that will be used in the rest of the paper. We refer the interested reader to [11].

Let U be a potential in $L^{5/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ with

$$\inf\{\|W\|_\infty : U - W \in L^{\frac{5}{2}}(\mathbb{R}^3)\} = 0.$$

Then the TF-energy functional is defined by

$$\mathcal{E}_U^{\mathrm{TF}}(\rho) = \tfrac{3}{10}(\tfrac{6\pi^2}{q})^{\frac{2}{3}} \int_{\mathbb{R}^3} \rho(\mathbf{x})^{\frac{5}{3}} d\mathbf{x} - \int_{\mathbb{R}^3} U(\mathbf{x})\rho(\mathbf{x}) d\mathbf{x} + \tfrac{1}{2} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\rho(\mathbf{x})\rho(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{x}d\mathbf{y},$$

on non-negative functions $\rho \in L^{5/3}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$. As before, q denotes the number of spin states.

We recall some properties of the TF-model, see [18].

Theorem 1.9. *Let U be as above. For all $N' \geq 0$ there exists a unique non-negative $\rho_U^{\mathrm{TF}} \in L^{5/3}(\mathbb{R}^3)$ such that $\int \rho_U^{\mathrm{TF}} \leq N'$ and*

$$\mathcal{E}_U^{\mathrm{TF}}(\rho_V^{\mathrm{TF}}) = \inf\{\mathcal{E}_U^{\mathrm{TF}}(\rho) : \rho \in L^{5/3}(\mathbb{R}^3),\ \int_{\mathbb{R}^3} \rho(\mathbf{x})\, d\mathbf{x} \leq N'\}.$$

There exists a unique chemical potential $\mu_U^{\mathrm{TF}}(N')$, with $0 \leq \mu_U^{\mathrm{TF}}(N') \leq \sup U$, such that ρ_U^{TF} is uniquely characterized by

$$\begin{aligned} &\mathcal{E}_U^{\mathrm{TF}}(\rho_U^{\mathrm{TF}}) + \mu_U^{\mathrm{TF}}(N') \int_{\mathbb{R}^3} \rho_U^{\mathrm{TF}}(\mathbf{x})\, d\mathbf{x} \\ = \;& \inf\{\mathcal{E}_U^{\mathrm{TF}}(\rho) + \mu_U^{\mathrm{TF}}(N') \int_{\mathbb{R}^3} \rho(\mathbf{x})\, d\mathbf{x} : 0 \leq \rho \in L^{5/3}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)\}. \end{aligned}$$

Moreover ρ_U^{TF} is the unique solution in $L^{5/3}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$ to the TF-equation

$$\tfrac{1}{2}(\tfrac{6\pi^2}{q})^{\frac{2}{3}}(\rho_U^{\mathrm{TF}}(\mathbf{x}))^{\frac{2}{3}} = \left[U(\mathbf{x}) - \rho_U^{\mathrm{TF}} * |\mathbf{x}|^{-1} - \mu_U^{\mathrm{TF}}(N')\right]_+ .$$

If $\mu_U^{\mathrm{TF}}(N') > 0$ then $\int \rho_U^{\mathrm{TF}} = N'$. For all $\mu > 0$ there is a unique minimizer $0 \leq \rho \in L^{5/3}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$ to $\mathcal{E}_U^{\mathrm{TF}}(\rho) + \mu \int \rho$.

One defines the *TF-mean field potential* φ_U^{TF}, the *TF-screened nuclear potential* $\Phi_{U,R}^{\mathrm{TF}}$ and the TF-radius $R_{N,Z}^{\mathrm{TF}}(\nu)$ to the ν last-electron similarly as in Definitions 1.7 and 1.8 replacing the HF-density with the TF-density.

Theorem 1.10. *If $U(\mathbf{x}) = Z/|\mathbf{x}|$ (the Coulomb potential), then the minimizer of $\mathcal{E}_U^{\mathrm{TF}}$, under the condition $\int \rho \leq N$, exists for every N. Moreover, $\mu_U^{\mathrm{TF}}(N) = 0$ if and only if $N \geq Z$.*

When $U(\mathbf{x}) = Z/|\mathbf{x}|$ we denote the minimizer of the TF-functional, under the condition $\int \rho \leq Z$, simply by ρ^{TF} and $\int \rho^{\mathrm{TF}} = Z$. Correspondingly φ^{TF} and Φ_R^{TF} denote, respectively, its mean field and screened nuclear potential. With this notation

$$\mathcal{E}^{\mathrm{TF}}(\rho^{\mathrm{TF}}) = -e_0 Z^{\frac{7}{3}}, \tag{12}$$

where e_0 is the total binding energy of a neutral TF-atom of unit nuclear charge.

We recall here a result due to Sommerfeld on the asymptotic behavior of the TF-mean field potential, see [23, Th. 4.6].

Theorem 1.11 (Sommerfeld asymptotics)**.** *Assume that the potential U is continuous and harmonic for $|\mathbf{x}| > R$ and that it satisfies $\lim_{|\mathbf{x}|\to\infty} U(\mathbf{x}) = 0$.*

Consider the corresponding TF-mean field potential φ_U^{TF} and assume that $\mu_U^{\mathrm{TF}} < \liminf_{r\searrow R} \inf_{|\mathbf{x}|=r} \varphi_U^{\mathrm{TF}}(\mathbf{x})$. With $\zeta = (-7+\sqrt{73})/2$ define

$$\begin{aligned} a(R) &:= \liminf_{r\searrow R} \sup_{|\mathbf{x}|=r} \Big[\Big(\frac{\varphi_U^{\mathrm{TF}}(\mathbf{x})}{3^4 2^{-1} q^{-2}\pi^2 r^{-4}}\Big)^{-\frac{1}{2}} - 1\Big] r^{\zeta} \\ A(R, \mu_U^{\mathrm{TF}}) &:= \liminf_{r\searrow R} \sup_{|\mathbf{x}|=r} \Big[\frac{\varphi_U^{\mathrm{TF}}(\mathbf{x}) - \mu_U^{\mathrm{TF}}}{3^4 2^{-1} q^{-2}\pi^2 r^{-4}} - 1\Big] r^{\zeta}. \end{aligned}$$

Then we find for all $|\mathbf{x}| > R$

$$\begin{aligned} \varphi_U^{\mathrm{TF}}(\mathbf{x}) &\leq \tfrac{3^4\pi^2}{2q^2}(1 + A(R,\mu_U^{\mathrm{TF}})|\mathbf{x}|^{-\zeta})|\mathbf{x}|^{-4} + \mu_U^{\mathrm{TF}} \quad \textit{and} \\ \varphi_U^{\mathrm{TF}}(\mathbf{x}) &\geq \max\Big\{\tfrac{3^4\pi^2}{2q^2}(1 + a(R)|\mathbf{x}|^{-\zeta})^{-2}|\mathbf{x}|^{-4}, \nu(\mu_U^{\mathrm{TF}})|\mathbf{x}|^{-1}\Big\}, \end{aligned}$$

where

$$\nu(\mu_U^{\mathrm{TF}}) := \inf_{|\mathbf{x}|\geq R} \max\big\{\tfrac{3^4\pi^2}{2q^2}(1 + a(R)|\mathbf{x}|^{-\zeta})^{-2}|\mathbf{x}|^{-3}, \mu_U^{\mathrm{TF}}|\mathbf{x}|\big\}.$$

For easy reference we give here the estimate on the TF-mean field potential corresponding to the Coulomb potential.

Theorem 1.12 (Atomic Sommerfeld estimate, [23, Thm 5.2-5.4])**.** *The atomic TF-mean field potential satisfies the bound*

$$\frac{Z}{|\mathbf{x}|} - \min\Big\{\frac{Z}{|\mathbf{x}|}, \frac{Z^{\frac{4}{3}}}{2\beta_0}\Big\} \leq \varphi^{\mathrm{TF}}(\mathbf{x}) \leq \min\Big\{\tfrac{3^4\pi^2}{2q^2}\frac{1}{|\mathbf{x}|^4}, \frac{Z}{|\mathbf{x}|}\Big\}, \tag{13}$$

with $2\beta_0 = \pi^{\frac{2}{3}}3^{-\frac{5}{3}}2^{-\frac{1}{3}}q^{-\frac{2}{3}}$, and for $|\mathbf{x}| \geq R > 0$

$$\varphi^{\mathrm{TF}}(\mathbf{x}) \geq \tfrac{3^4\pi^2}{2q^2}(1 + a(R)|\mathbf{x}|^{-\zeta})^{-2}|\mathbf{x}|^{-4},$$

where ζ and $a(R)$ are defined in Theorem 1.11.

Corollary 1.13. *Let ζ and β_0 be defined as in Theorem 1.11 and 1.12 respectively. Then the TF-mean field potential satisfies the bound*

$$\varphi^{\mathrm{TF}}(\mathbf{x}) \geq \begin{cases} \dfrac{Z}{|\mathbf{x}|} - \dfrac{Z^{\frac{4}{3}}}{2\beta_0} & \textit{if } |\mathbf{x}| \leq \beta_0 Z^{-\frac{1}{3}} \\ \dfrac{3^4\pi^2}{2q^2}(1 + aZ^{-\frac{\zeta}{3}}|\mathbf{x}|^{-\zeta})^{-2}|\mathbf{x}|^{-4} & \textit{if } |\mathbf{x}| > \beta_0 Z^{-\frac{1}{3}}, \end{cases}$$

with $a = \beta_0^{\zeta}(3^2\pi/(q\beta_0^{\frac{3}{2}}) - 1)$.

Corollary 1.14. *The TF-screened nuclear potential satisfies*

$$\Phi_{|\mathbf{x}|}^{\mathrm{TF}}(\mathbf{x}) \leq \tfrac{3^4 2\pi^2}{q^2}|\mathbf{x}|^{-4} \quad \textit{for all } \mathbf{x} \in \mathbb{R}^3.$$

Corollary 1.15. *The following estimate holds*

$$\int_{\mathbb{R}^3} (\rho^{\mathrm{TF}}(\mathbf{x}))^{\frac{5}{3}} d\mathbf{x} \leq 4\tfrac{2^{\frac{2}{3}}}{\pi^2}\tfrac{5}{7}q^{\frac{4}{3}}Z^{\frac{7}{3}}.$$

Proof. By the TF-equation and since $\mu^{\mathrm{TF}} = 0$ we find

$$\int_{\mathbb{R}^3} (\rho^{\mathrm{TF}}(\mathbf{x}))^{\frac{5}{3}} d\mathbf{x} = 2^{\frac{5}{2}}(\tfrac{q}{6\pi^2})^{\frac{5}{3}} \int_{\mathbb{R}^3} (\varphi^{\mathrm{TF}}(\mathbf{x}))^{\frac{5}{2}} d\mathbf{x}.$$

The estimate follows from the atomic Sommerfeld upper bound. □

1.4 Construction and main results

We present the basic idea for the proof of Theorem 1.1. Let us consider an atomic system with $N \geq 2$ fermionic particles and a nucleus of charge $Z \geq 1$ with $Z\alpha = \kappa$ and $0 \leq \kappa < 2/\pi$. We assume that $N \geq Z$ and that N is such that a HF-minimizer exists. That is: there exists a density matrix $\gamma^{\mathrm{HF}} \in \mathcal{A}$ such that $\mathrm{Tr}[\gamma^{\mathrm{HF}}] = N$ and

$$\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) = \inf\left\{\mathcal{E}^{\mathrm{HF}}(\gamma) : \gamma = \gamma^*, 0 \leq \gamma \leq I, \mathrm{Tr}[\gamma] = N\right\}.$$

Let ρ^{TF} be the TF-minimizer with potential $U(\mathbf{x}) = Z/|\mathbf{x}|$ and under the condition $\int \rho^{\mathrm{TF}} = Z$. We know that such a minimizer exists and that the corresponding chemical potential is zero (see Theorem 1.10).

Denoting by ρ^{HF} the density of the minimizer γ^{HF}, we find for all $r > 0$

$$\begin{aligned} N &= \int_{\mathbb{R}^3} \rho^{\mathrm{HF}}(\mathbf{x}) d\mathbf{x} \\ &= \int_{|\mathbf{x}|<r} \left[\rho^{\mathrm{HF}}(\mathbf{x}) - \rho^{\mathrm{TF}}(\mathbf{x})\right] d\mathbf{x} + \int_{|\mathbf{x}|<r} \rho^{\mathrm{TF}}(\mathbf{x})\, d\mathbf{x} + \int_{|\mathbf{x}|>r} \rho^{\mathrm{HF}}(\mathbf{x})\, d\mathbf{x}. \end{aligned}$$

By the equalities above and since $\int_{|\mathbf{x}|<r} \rho^{\mathrm{TF}}(\mathbf{x})d\mathbf{x} \leq Z$, Theorem 1.1 follows from the following result.

Theorem 1.16. *There exist $r > 0$ and positive constants c_1 and c_2 independent of N and Z but possibly depending on κ such that*

$$\int_{|\mathbf{x}|<r} \left[\rho^{\mathrm{HF}}(\mathbf{x}) - \rho^{\mathrm{TF}}(\mathbf{x})\right] d\mathbf{x} \leq c_1 \text{ and } \int_{|\mathbf{x}|>r} \rho^{\mathrm{HF}}(\mathbf{x}) d\mathbf{x} \leq c_2.$$

The following theorem is the principal ingredient in the proof of the previous one and is the main technical estimate in the paper.

Theorem 1.17. *Let $Z\alpha = \kappa$, $0 \leq \kappa < 2/\pi$. Assume $N \geq Z \geq 1$.*

Then there exist universal constants $\alpha_0 > 0$, $0 < \varepsilon < 4$ and C_M and C_Φ depending on κ such that for all $\alpha \leq \alpha_0$

$$\left|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})\right| \leq C_\Phi |\mathbf{x}|^{-4+\varepsilon} + C_M.$$

This main estimate is proven by an iterative procedure. We first prove the estimate for small $\mathbf{x}$ (i.e. $|\mathbf{x}| \leq \beta_0 Z^{-\frac{1}{3}}$), then for intermediate $\mathbf{x}$ (i.e. up to a fixed distance independent of Z) and finally for big $\mathbf{x}$.

By proving Theorem 1.17 we also get the following interesting results. The proofs of those are given in Section 5.

Theorem 1.18 (Asymptotic formula for the radius)**.** *Let $Z\alpha = \kappa$, $0 \leq \kappa < 2/\pi$. Both* $\liminf_{Z\to\infty} R^{\mathrm{HF}}_{Z,Z}(\nu)$ *and* $\limsup_{Z\to\infty} R^{\mathrm{HF}}_{Z,Z}(\nu)$ *are bounded and behave asymptotically as*

$$3^{\frac{4}{3}} \frac{2^{\frac{1}{2}} \pi^{\frac{2}{3}}}{q^{\frac{2}{3}}} \nu^{-\frac{1}{3}} + o(\nu^{-\frac{1}{3}}) \text{ as } \nu \to \infty.$$

Theorem 1.19 (Bound on the ionization energy of a neutral atom)**.** *Let $Z\alpha = \kappa$, $0 \leq \kappa < 2/\pi$ and $Z \geq 1$. The ionization energy of a neutral atom $E^{\mathrm{HF}}(Z-1, Z) - E^{\mathrm{HF}}(Z, Z)$ is bounded by a universal constant.*

Theorem 1.20 (Potential estimate)**.** *Let $Z\alpha = \kappa$, $0 \leq \kappa < 2/\pi$. For all $Z \geq 1$ and N with $N \geq Z$ for which a HF minimizer exists with $\int \rho^{\mathrm{HF}} = N$, we have*

$$|\varphi^{\mathrm{TF}}(\mathbf{x}) - \varphi^{\mathrm{HF}}(\mathbf{x})| \leq A_\varphi |\mathbf{x}|^{-4+\varepsilon_0} + A_1,$$

with A_0, A_1 and ε_0 universal constants.

2 Prerequisites

In this section we recall some results that will be used in the rest of the paper.

Localization of the kinetic energy. The following is the IMS formula corresponding to the operator $T(\mathbf{p})$.

Theorem 2.1 ([19]). *Let χ_i, $i = 0, \dots, K$, be real valued Lipschitz continuous functions on $\mathbb{R}^3$ such that $\sum_{i=0}^{K} \chi_i^2(\mathbf{x}) = 1$ for all $\mathbf{x} \in \mathbb{R}^3$. Then for every $f \in H^{1/2}(\mathbb{R}^3)$*

$$\mathrm{t}(f,f) = \sum_{i=0}^{K} \mathrm{t}(\chi_i f, \chi_i f) - \alpha^{-1} \sum_{i=0}^{K} (f, L_i f),$$

where L_i is a bounded operator with kernel

$$L_i(\mathbf{x},\mathbf{y}) = \tfrac{\alpha^{-2}}{4\pi^2} \frac{|\chi_i(\mathbf{x}) - \chi_i(\mathbf{y})|^2}{|\mathbf{x}-\mathbf{y}|^2} K_2(\alpha^{-1}|\mathbf{x}-\mathbf{y}|), \tag{14}$$

where K_2 is a modified Bessel function of the second kind.

Remark 2.2. *As in [24, App.A, pages 94–98] we use the following integral formula for the modified Bessel function*

$$K_2(t) = t \int_0^\infty e^{-t\sqrt{s^2+1}} s^2 \, ds \,, \quad t > 0.$$

We recall that this function is decreasing and smooth in $\mathbb{R}^+$. Moreover,

$$\int_0^{+\infty} t^2 K_2(t)\, dt = \tfrac{3\pi}{2} \ \text{ and } \ K_2(t) \le 16\, t^{-2} e^{-\frac{1}{2}t} \text{ for } t > 0. \tag{15}$$

The integral is computed in [21, (A6)] while the estimate follows directly from the integral formula for K_2 by estimating $\sqrt{s^2+1} \ge \frac{1}{2} + \frac{1}{2}s$.

Generalization of the Lieb-Thirring inequality. This result due to Daubechies generalizes the Lieb-Thirring inequality to the pseudo-relativistic case.

Theorem 2.3 (Daubechies' inequality, [4]). *For $\gamma \in \mathcal{A}$*

$$\mathrm{Tr}[T(\mathbf{p})\gamma] \ge \int_{\mathbb{R}^3} G_\alpha(\rho_\gamma(\mathbf{x})) d\mathbf{x},$$

where $G_\alpha(\rho) = \frac{3}{8}\alpha^{-4} C g(\alpha(\rho/C)^{\frac{1}{3}}) - \alpha^{-1}\rho$ with $C = .163q$, q the number of spin states and $g(t) = t(1+t^2)^{\frac{1}{2}}(1+2t^2) - \ln(t + (1+t^2)^{\frac{1}{2}})$.

Remark 2.4. *The function G_α defined in the previous theorem is convex and it has the following behavior:*

$$\tfrac{9}{20} \min\left\{ \tfrac{1}{5}\alpha C^{-\frac{2}{3}} \rho^{\frac{5}{3}}, \tfrac{1}{2} C^{-\frac{1}{3}} \rho^{\frac{4}{3}} \right\} \le G_\alpha(\rho) \le \tfrac{3}{2} \min\left\{ \tfrac{1}{5}\alpha C^{-\frac{2}{3}} \rho^{\frac{5}{3}}, \tfrac{1}{2} C^{-\frac{1}{3}} \rho^{\frac{4}{3}} \right\}. \tag{16}$$

(The proof of the estimate above is in Appendix A.) Notice that when $\alpha \searrow 0$ then $\alpha^{-1}G_\alpha(\rho)$ tends to a constant times $\rho^{5/3}$.

Theorem 2.5 (Generalization of the Lieb-Thirring inequality, [4]). *Let f^{-1} be the inverse of the function $f(t) := \sqrt{t^2 + \alpha^{-2}} - \alpha^{-1}$, $t \ge 0$, and define $F(s) = \int_0^s dt\, [f^{-1}(t)]^3$. Then for any density matrix γ it holds*

$$\mathrm{Tr}[(T(\mathbf{p}) - U)\gamma] \ge -Cq \int_{\mathbb{R}^3} F(|U(\mathbf{x})|) d\mathbf{x},$$

with $C \le 0.163$.

Remark 2.6. *Since $f^{-1}(t) = (t^2 + 2\alpha^{-1}t)^{1/2}$ we find for F*

$$F(s) = 2^{\frac{3}{2}}\alpha^{-3/2}\int_0^s t^{3/2}\big(1 + \tfrac{1}{2}\alpha t\big)^{3/2}\,dt \quad \textit{for } s \geq 0, \tag{17}$$

and since by convexity $(1 + \frac{1}{2}\alpha t)^{\frac{3}{2}} \leq \sqrt{2} + \frac{1}{2}(\alpha t)^{\frac{3}{2}}$ we have

$$F(s) \leq \tfrac{2^3}{5}\alpha^{-\frac{3}{2}}s^{\frac{5}{2}} + \tfrac{1}{2\sqrt{2}}s^4 \textit{ for } s \geq 0.$$

Hence for any density matrix γ and potential $U \in L^{\frac{5}{2}}(\mathbb{R}^3) \cap L^4(\mathbb{R}^3)$

$$\mathrm{Tr}[(T(\mathbf{p}) - U)\gamma] \geq -Cq\int_{\mathbb{R}^3}\Big(\tfrac{2^3}{5}\alpha^{-\frac{3}{2}}|U(\mathbf{x})|^{\frac{5}{2}} + \tfrac{1}{2\sqrt{2}}|U(\mathbf{x})|^4\Big)d\mathbf{x}. \tag{18}$$

Coulomb norm estimate. We present here only the definition of Coulomb norm and the result we need. For a more complete presentation we refer to [23, Sec.9].

Definition 2.7. *For $f, g \in L^{\frac{6}{5}}(\mathbb{R}^3)$ we define the Coulomb inner product*

$$D(f,g) := \tfrac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{f(\mathbf{x})\overline{g(\mathbf{y})}}{|\mathbf{x}-\mathbf{y}|}d\mathbf{x}d\mathbf{y},$$

and the corresponding norm $\|g\|_C := D(g,g)^{\frac{1}{2}}$.

In the following we write the direct term in the HF-energy functional using the Coulomb scalar product: i.e. $\mathcal{D}(\gamma) = D(\rho_\gamma, \rho_\gamma) = D(\rho_\gamma)$. Similarly, for $\rho \in L^1(\mathbb{R}^3) \cap L^{\frac{5}{3}}(\mathbb{R}^3)$ the term $D(\rho)$ denotes $D(\rho,\rho)$.

The next proposition follows as Corollary 9.3 in [23].

Proposition 2.8. *For $s > 0$, $\mathbf{x} \in \mathbb{R}^3$ and $f \in L^{\frac{6}{5}}(\mathbb{R}^3)$ it holds*

$$f * |\mathbf{x}|^{-1} \leq \int_{|\mathbf{x}-\mathbf{y}|<s}[f(\mathbf{y})]_+\Big(\frac{1}{|\mathbf{x}-\mathbf{y}|} - \frac{1}{s}\Big)d\mathbf{y} + \sqrt{2}\,s^{-\frac{1}{2}}\|f\|_C.$$

Moreover, for $k > 0$

$$\int_{|\mathbf{y}|<|\mathbf{x}|}\frac{f(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} \leq \int_{A(|\mathbf{x}|,k)}\frac{[f(\mathbf{y})]_+}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} + 2^{\frac{3}{2}}k^{-1}|\mathbf{x}|^{-\frac{1}{2}}\|f\|_C,$$

where $A(|\mathbf{x}|,k)$ denotes the annulus

$$A(|\mathbf{x}|,k) := \big\{\mathbf{y} \in \mathbb{R}^3 : (1-2k)|\mathbf{x}| \leq |\mathbf{y}| \leq |\mathbf{x}|\big\}.$$

2.1 Improved relativistic Lieb-Thirring inequalities

A major difference between the pseudo-relativistic HF-model and the non-relativistic one studied in [23] is that the boundness of the functional does not yield a bound on the $L^{\frac{5}{3}}$ norm of the HF-density ρ^{HF} in the pseudorelativistic case. By Theorem 2.3 and Remark 2.4 we see that we can control only the $L^{\frac{4}{3}}$-norm of ρ^{HF}. Therefore one cannot estimate the term $\rho^{\mathrm{HF}} * |\mathbf{x}|^{-1}$ in L^1-norm simply by Hölder's inequality with $p = 5/2$ and $q = 5/3$. To estimate it we are going to use a combined Daubechies-Lieb-Yau inequality.

The following lemma can be found in [24, pages 98–99][1].

[1] The result of the lemma and the proof given in [24] are actually due to us, but we communicated the result to the authors of [24], where it is referred to as a a private communication.

Lemma 2.9. *For $f \in \mathcal{S}(\mathbb{R}^3)$,*

$$\int_{\mathbb{R}^3} \frac{e^{-\mu|\mathbf{x}|^2}}{|\mathbf{x}|}|f(\mathbf{x})|^2 d\mathbf{x} \leq \frac{\pi}{2}\frac{1}{\sqrt{2}-1}\,(f, T(\mathbf{p})f),$$

with $\mu = \pi^{-1}\alpha^{-2}$.

The following is a slight generalization of the Daubechies-Lieb-Yau inequality formulated in Theorem 2.8 in [24].

Theorem 2.10 (Daubechies-Lieb-Yau inequality)**.** *Assume that the potential $U \in L^1_{loc}(\mathbb{R}^3)$ satisfies*

$$0 \geq -U(\mathbf{x}) \geq -\kappa|\mathbf{x}|^{-1} \quad \textit{for } |\mathbf{x}| < \max\{\alpha, R\}\,, \tag{19}$$

for $\alpha, R > 0$ and $0 \leq \kappa \leq 2/\pi$. Then we have

$$\mathrm{Tr}[T(\mathbf{p}) - U]_- \geq -C\kappa^{5/2}\alpha^{-3/2}R^{1/2} - C\kappa^4\alpha^{-1} - C\int_{|\mathbf{x}|>R}\left(\alpha^{-\frac{3}{2}}|U(\mathbf{x})|^{\frac{5}{2}} + |U(\mathbf{x})|^4\right)d\mathbf{x}.$$

Proof. If $(\sqrt{2}-1)/\pi \leq \kappa \leq 2/\pi$ then $\kappa^{5/2}\alpha^{-3/2}R^{1/2} + \kappa^4\alpha^{-1} \geq C\kappa^{5/2}\alpha^{-1}$ and the result follows immediately from Theorem 2.8 in [24] observing that for $R > \alpha$ the two integrals of the potential on $\{\alpha < |\mathbf{x}| < R\}$ are bounded by the constants.

If $0 \leq \kappa < (\sqrt{2}-1)/\pi$ we write

$$U(x) = e^{-\mu|x|^2}U(x)\chi_{|\mathbf{x}|<R} + (1 - e^{-\mu|x|^2})U(x)\chi_{|\mathbf{x}|<R} + U(x)\chi_{|\mathbf{x}|>R}$$

with $\mu = \alpha^{-2}\pi^{-1}$. Using (19) and Lemma 2.9 we find that

$$T(\mathbf{p}) - U(\mathbf{x}) \geq \frac{1}{2}T(\mathbf{p}) - \kappa(1 - e^{-\mu|\mathbf{x}|^2})|\mathbf{x}|^{-1}\chi_{|\mathbf{x}|<R} - U(\mathbf{x})\chi_{|\mathbf{x}|>R}.$$

Hence from the generalization of the Lieb-Thirring inquality Theorem 2.5 (see (18)) we obtain

$$\begin{aligned} \mathrm{Tr}[T(\mathbf{p}) - U]_- \quad \geq \quad & -C\int_{|\mathbf{x}|<R}\alpha^{-\frac{3}{2}}\left(\kappa(1 - e^{-\mu|\mathbf{x}|^2})|\mathbf{x}|^{-1}\right)\right)^{\frac{5}{2}}d\mathbf{x} \\ & -C\int_{|\mathbf{x}|<R}\left(\kappa(1 - e^{-\mu|\mathbf{x}|^2})|\mathbf{x}|^{-1}\right)^4 d\mathbf{x} \\ & -C\int_{|\mathbf{x}|>R}\left(\alpha^{-\frac{3}{2}}|U(\mathbf{x})|^{\frac{5}{2}} + |U(\mathbf{x})|^4\right)d\mathbf{x}. \end{aligned}$$

Since the two first integrals above are estimated below by $-C\kappa^{5/2}\alpha^{-3/2}R^{1/2} - C\kappa^4\alpha^{-1}$ we get the result in the theorem. □

By Theorem 2.10 we find

$$\kappa\int_{|\mathbf{x}-\mathbf{y}|<R}\frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} \leq \mathrm{Tr}[T(\mathbf{p})\gamma^{\mathrm{HF}}] + C_1\kappa Z^{\frac{3}{2}}R^{\frac{1}{2}} + C_2\kappa^3 Z, \tag{20}$$

with $\kappa \in [0, 2/\pi]$, $\kappa = Z\alpha$ and $R > 0$ parameters to be chosen. This is the inequality that we use to estimate $\rho^{\mathrm{HF}} * |\mathbf{x}|^{-1}$ (see proof of Lemma 3.2 below).

2.1.1 Bound on the Hartree-Fock energy

As a first application of Theorem 2.10 we can give a lower bound to the HF-energy.

Theorem 2.11 (Bound on the HF-energy)**.** *Let $N > 0$, $Z > 0$ and such that $Z\alpha = \kappa$ with $0 \le \kappa \le 2/\pi$. Then*

$$E^{\mathrm{HF}}(N, Z) \ge -2C^{\frac{2}{3}} Z^2 N^{\frac{1}{3}} - C\kappa^2 Z^2,$$

with C the constant in Theorem 2.10.

Proof. Let γ be a N-dimensional projection. Since the electron-electron iteraction is positive we see that

$$\begin{aligned}\mathcal{E}^{\mathrm{HF}}(\gamma) &\ge \alpha^{-1} \operatorname{Tr}[(T(\mathbf{p}) - \frac{Z\alpha}{|\cdot|})\gamma] \\ &= \alpha^{-1} \operatorname{Tr}[(T(\mathbf{p}) - \frac{\kappa}{|\cdot|}\chi_{|\mathbf{x}|<R})\gamma] - \alpha^{-1} \operatorname{Tr}[\frac{\kappa}{|\cdot|}(1 - \chi_{|\mathbf{x}|<R})\gamma]\end{aligned}$$

with $R > 0$ a parameter to be choosen. By Theorem 2.10 we find

$$\mathcal{E}^{\mathrm{HF}}(\gamma) \ge -2C^{\frac{2}{3}} Z^2 N^{\frac{1}{3}} - C\kappa^2 Z^2,$$

using that $\kappa = Z\alpha$ and by choosing $R = C^{-\frac{2}{3}} Z^{-1} N^{\frac{2}{3}}$. □

3 Near the nucleus

In this section we prove the estimate in Theorem 1.17 in the region near the nucleus (i.e. at distance of $Z^{-\frac{1}{3}}$).

We again assume that $N \ge Z$ and that an HF-minimizer γ^{HF} exists for this N and Z. We denote the density of γ^{HF} by ρ^{HF}. We assume throughout that $\alpha Z = \kappa$ is fixed with $0 \le \kappa < 2/\pi$ and $Z \ge 1$.

Lemma 3.1. *Let $Z\alpha = \kappa$ be fixed with $0 \le \kappa < 2/\pi$ and $Z \ge 1$. Let G_α be the function defined in Theorem 2.3. Then, there exists $\alpha_0 > 0$ such that for all $\alpha \le \alpha_0$*

$$\begin{aligned}\alpha^{-1} \int_{\mathbb{R}^3} G_\alpha(\rho^{\mathrm{HF}}(\mathbf{x})) d\mathbf{x} \le CZ^{7/3}, \quad \alpha^{-1} \operatorname{Tr}[T(\mathbf{p})\gamma^{\mathrm{HF}}] \le CZ^{7/3} \\ \textit{and} \quad \|\rho^{\mathrm{TF}} - \rho^{\mathrm{HF}}\|_C^2 \le CZ^{2+\frac{3}{11}},\end{aligned} \tag{21}$$

with C a universal constant depending only on κ.

Proof. Let $\mu \in (0, 1)$ be such that $\mu^{-1}\kappa < 2/\pi$. Notice that here we need $\kappa < 2/\pi$. Splitting the kinetic energy into two parts we find

$$\begin{aligned}\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) &= (1 - \mu)\alpha^{-1} \operatorname{Tr}[T(\mathbf{p})\gamma^{\mathrm{HF}}] + \mathcal{D}(\gamma^{\mathrm{HF}}) - \mathcal{E}x(\gamma^{\mathrm{HF}}) \\ &\quad + \mu \operatorname{Tr}[(\alpha^{-1}T(\mathbf{p}) - \frac{Z}{\mu|\mathbf{x}|})\gamma^{\mathrm{HF}}] = \dots,\end{aligned}$$

and introducing $\rho \in L^{\frac{5}{3}}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$, $\rho \ge 0$, to be chosen

$$\begin{aligned}\dots &= (1 - \mu)\alpha^{-1} \operatorname{Tr}[T(\mathbf{p})\gamma^{\mathrm{HF}}] + \mu\|\rho - \rho^{\mathrm{HF}}\|_C^2 + (1 - \mu)\mathcal{D}(\gamma^{\mathrm{HF}}) \\ &\quad - \mathcal{E}x(\gamma^{\mathrm{HF}}) - \mu D(\rho) + \mu \operatorname{Tr}[(\alpha^{-1}T(\mathbf{p}) - (\frac{Z}{\mu|\mathbf{x}|} - \rho * \frac{1}{|\mathbf{x}|}))\gamma^{\mathrm{HF}}].\end{aligned} \tag{22}$$

Here $\|\cdot\|_C$ denotes the Coulomb norm defined in Definition 2.7 and we used that

$$\|\rho-\rho^{\mathrm{HF}}\|_C^2 = D(\rho) - \iint \frac{\rho^{\mathrm{HF}}(\mathbf{x})\rho(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}d\mathbf{y} + \mathcal{D}(\gamma^{\mathrm{HF}}).$$

The estimates in the claim will follow from (22) with different choices of μ and ρ. The main idea is to relate, up to lower order term, the last term on the right hand side of (22) to the TF-energy of a neutral atom of nuclear charge $Z\mu^{-1}$. This has been done in [21]. For completeness and easy reference we repeat the reasoning in Propositions B.1 and B.2 in Appendix B.

To prove the first inequality in (21) we choose ρ as the minimizer of the TF-energy functional of a neutral atom with charge $\mu^{-1}Z$. Since the corresponding TF-mean field potential is $Z/(\mu|\mathbf{x}|) - \rho * 1/|\mathbf{x}|$ by Proposition B.2 in Appendix B we find

$$\mathrm{Tr}[(\alpha^{-1}T(\mathbf{p}) - (\frac{Z}{\mu|\mathbf{x}|} - \rho * \frac{1}{|\mathbf{x}|}))\gamma^{\mathrm{HF}}] \geq -C_1 Z^{\frac{7}{3}} + D(\rho). \tag{23}$$

Here we use (12). Since $\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) \leq 0$ from (22) and (23) leaving out the positive terms we find

$$0 \;\geq\; (1-\mu)\alpha^{-1}\,\mathrm{Tr}[T(\mathbf{p})\gamma^{\mathrm{HF}}] - \mathcal{E}x(\gamma^{\mathrm{HF}}) - C_1 Z^{\frac{7}{3}}. \tag{24}$$

From (24) and Theorem 2.3 we get

$$(1-\mu)\alpha^{-1}\int_{\mathbb{R}^3} G_\alpha(\rho^{\mathrm{HF}}(\mathbf{x}))\,d\mathbf{x} \leq (1-\mu)\alpha^{-1}\,\mathrm{Tr}[T(\mathbf{p})\gamma^{\mathrm{HF}}] \leq \mathcal{E}x(\gamma^{\mathrm{HF}}) + C_1 Z^{\frac{7}{3}}. \tag{25}$$

It remains to estimate the exchange term. By the exchange inequality (see [15])

$$\mathcal{E}x(\gamma^{\mathrm{HF}}) \;\leq\; 1.68\int_{\mathbb{R}^3}\big(\rho^{\mathrm{HF}}(\mathbf{x})\big)^{\frac{4}{3}}\,d\mathbf{x}.$$

To proceed we separate $\mathbb{R}^3$ into two regions. Let us define

$$\Sigma = \big\{\mathbf{x}\in\mathbb{R}^3 : \alpha\big(C^{-1}\rho^{\mathrm{HF}}(\mathbf{x})\big)^{\frac{1}{3}} \geq \tfrac{5}{2}\big\}, \tag{26}$$

with the same notation as in (16). By Remark 2.4, $G_\alpha(\rho^{\mathrm{HF}}(\mathbf{x})) \geq C_2(\rho^{\mathrm{HF}}(\mathbf{x}))^{\frac{4}{3}}$ in Σ and $\alpha^{-1}G_\alpha(\rho^{\mathrm{HF}}(\mathbf{x})) \geq C_3(\rho^{\mathrm{HF}}(\mathbf{x}))^{\frac{5}{3}}$ in $\mathbb{R}^3\setminus\Sigma$. Hence by Hölder's inequality we find

$$\begin{aligned}
\mathcal{E}x(\gamma^{\mathrm{HF}}) \;&\leq\; 1.68\int_\Sigma(\rho^{\mathrm{HF}}(\mathbf{x}))^{\frac{4}{3}}\,d\mathbf{x} \\
&\quad +1.68\Big(\int_{\mathbb{R}^3\setminus\Sigma}(\rho^{\mathrm{HF}}(\mathbf{x}))^{\frac{5}{3}}\,d\mathbf{x}\Big)^{\frac{1}{2}}\Big(\int_{\mathbb{R}^3\setminus\Sigma}\rho^{\mathrm{HF}}(\mathbf{x})\,d\mathbf{x}\Big)^{\frac{1}{2}} \\
&\leq\; C_4\int_{\mathbb{R}^3} G_\alpha(\rho^{\mathrm{HF}}(\mathbf{x}))\,d\mathbf{x} + C_5\Big(\int_{\mathbb{R}^3}\alpha^{-1}G_\alpha(\rho^{\mathrm{HF}}(\mathbf{x}))\,d\mathbf{x}\Big)^{\frac{1}{2}} N^{\frac{1}{2}}.
\end{aligned} \tag{27}$$

Choosing α_0 such that $1-\mu > 2C_4\alpha$ for $\alpha \leq \alpha_0$, from (25) and (27) we find

$$\tfrac{1-\mu}{2}\alpha^{-1}\int_{\mathbb{R}^3} G_\alpha(\rho^{\mathrm{HF}}(\mathbf{x}))\,d\mathbf{x} \leq C_1 Z^{\frac{7}{3}} + C_5\Big(\int_{\mathbb{R}^3}\alpha^{-1}G_\alpha(\rho^{\mathrm{HF}}(\mathbf{x}))\,d\mathbf{x}\Big)^{\frac{1}{2}} N^{\frac{1}{2}}.$$

The first estimate in (21) follows from the estimate above using that $x^2 - bx - c \leq 0$ implies $x^2 \leq b^2 + 2c$ and that $N \leq 2Z+1$ (Theorem 1.6). The second inequality in (21) follows then from (25) and the bound on the exchange term.

To prove the third inequality in (21) we estimate from above and from below $\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}})$. For the one from below we choose in (22) $\mu = 1$ and $\rho = \rho^{\mathrm{TF}}$ the TF-minimizer of a neutral atom with nucleus of charge Z. We find

$$\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) = \sum_{i=1}^{N}(u_i, (\alpha^{-1}T(\mathbf{p}) - \varphi^{\mathrm{TF}})u_i) + \|\rho^{\mathrm{HF}} - \rho^{\mathrm{TF}}\|_C^2 - D(\rho^{\mathrm{TF}}) - \mathcal{E}x(\gamma^{\mathrm{HF}}). \tag{28}$$

From (28) and the proof of Proposition B.2 (see (B37)), we find

$$\begin{aligned}\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) \quad &\geq \quad -\tfrac{2^{\frac{3}{2}}}{15\pi^2}q\int d\mathbf{q}(\varphi^{\mathrm{TF}}(\mathbf{q}))^{\frac{5}{2}} - CZ^{2+1/5} \\ &\quad\quad -D(\rho^{\mathrm{TF}}) + \|\rho^{\mathrm{HF}} - \rho^{\mathrm{TF}}\|_C^2 - \mathcal{E}x(\gamma^{\mathrm{HF}}).\end{aligned} \tag{29}$$

To estimate from above $\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}})$ we may proceed exactly as in [23, page 543] using that $\alpha^{-1}T(\mathbf{p}) \leq \frac{1}{2}|\mathbf{p}|^2$. For completeness we repeat the main ideas. We consider γ the density matrix that acts identically on each of the spin components as

$$\gamma^j = \tfrac{1}{(2\pi)^3}\iint_{\frac{1}{2}|\mathbf{p}|^2 \leq \varphi^{\mathrm{TF}}(\mathbf{q})} \Pi_{\mathbf{p},\mathbf{q}}\, d\mathbf{q}d\mathbf{p} \text{ for } j = 1, \ldots, q.$$

Here $\Pi_{\mathbf{p},\mathbf{q}}$ is the projection onto the space spanned by $h_s^{\mathbf{p},\mathbf{q}}(\mathbf{x}) := h_s(\mathbf{x} - \mathbf{q})e^{i\mathbf{p}.\mathbf{x}}$ where h_s is the ground state (normalized in $L^2(\mathbb{R}^3)$) for the Dirichlet Laplacian on the ball of radius Z^{-s} with $s \in (1/3, 2/3)$ to be chosen. One sees that $\mathrm{Tr}[\gamma] = Z \leq N$ since

$$\rho_\gamma(\mathbf{x}) = \tfrac{2^{3/2}q}{6\pi^2}(\varphi^{\mathrm{TF}})^{3/2} * h_s^2(\mathbf{x}) = \rho^{\mathrm{TF}} * h_s^2(\mathbf{x}),$$

where we have used the TF-equation. Hence $\mathcal{E}^{\mathrm{HF}}(\gamma) \geq \mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}})$. Now we estimate from above $\mathcal{E}^{\mathrm{HF}}(\gamma)$. Since $\alpha^{-1}T(\mathbf{p}) \leq \frac{1}{2}|\mathbf{p}|^2$ and $\mathcal{E}x(\gamma) \geq 0$ we find

$$\mathcal{E}^{\mathrm{HF}}(\gamma) \leq \mathrm{Tr}[(-\tfrac{1}{2}\Delta - \frac{Z}{|\cdot|})\gamma] + D(\rho_\gamma) = \ldots,$$

and proceeding as in [23, page 543])

$$\cdots = \tfrac{q}{(2\pi)^3}\iint_{\frac{1}{2}|\mathbf{p}|^2 \leq \varphi^{\mathrm{TF}}(\mathbf{q})} \tfrac{1}{2}|\mathbf{p}|^2\, d\mathbf{p}d\mathbf{q} - \tfrac{\pi^2}{2}Z^{2s}N - \int_{\mathbb{R}^3}\frac{Z}{|\mathbf{x}|}\rho_\gamma(\mathbf{x})\, d\mathbf{x} + D(\rho_\gamma).$$

Computing the integral and summing and subtracting the term $\int \rho^{\mathrm{TF}}\varphi^{\mathrm{TF}}$ we get

$$\begin{aligned}\mathcal{E}^{\mathrm{HF}}(\gamma) \quad &\leq \quad \tfrac{q2^{\frac{1}{2}}}{5\pi^2}\int_{\mathbb{R}^3}(\varphi^{\mathrm{TF}}(\mathbf{q}))^{\frac{5}{2}}\, d\mathbf{q} - \tfrac{\pi^2}{2}Z^{2s}N - \int_{\mathbb{R}^3}\varphi^{\mathrm{TF}}(\mathbf{x})\rho^{\mathrm{TF}}(\mathbf{x})\, d\mathbf{x} \\ &\quad\quad - \int_{\mathbb{R}^3}\frac{Z}{|\mathbf{x}|}(\rho_\gamma(\mathbf{x}) - \rho^{\mathrm{TF}}(\mathbf{x}))d\mathbf{x} - 2D(\rho^{\mathrm{TF}}) + D(\rho_\gamma).\end{aligned} \tag{30}$$

By Newton's theorem one sees that $D(\rho_\gamma) \leq D(\rho^{\mathrm{TF}})$ and that

$$Z\int_{\mathbb{R}^3}\frac{\rho^{\mathrm{TF}}(\mathbf{x}) - \rho_\gamma(\mathbf{x})}{|\mathbf{x}|}\, d\mathbf{x} \leq Z\int_{|\mathbf{x}| \leq Z^{-s}}\frac{\rho^{\mathrm{TF}}(\mathbf{x})}{|\mathbf{x}|}\, d\mathbf{x} \leq CZ^{\frac{1}{5}(12-s)}.$$

In the last step we use Hölder's inequality and Corollary 1.15. From (30) using the TF-equation, that $N \leq 2Z + 1$ (Theorem 1.6) and optimizing in s we find

$$\mathcal{E}^{\mathrm{HF}}(\gamma) \leq -\tfrac{2^{\frac{3}{2}}}{15\pi^2}q\int_{\mathbb{R}^3}(\varphi^{\mathrm{TF}}(\mathbf{q}))^{\frac{5}{2}}\, d\mathbf{q} + CZ^{\frac{1}{5}(12-\frac{7}{11})} - D(\rho^{\mathrm{TF}}). \tag{31}$$

Hence from (29) and (31) we obtain

$$\left\|\rho^{\mathrm{HF}} - \rho^{\mathrm{TF}}\right\|_C^2 \leq CZ^{2+\frac{3}{11}} + \mathcal{E}x(\gamma^{\mathrm{HF}}).$$

The last estimate in (21) follows from the estimate above since $\mathcal{E}x(\gamma^{\mathrm{HF}}) \leq CZ^{\frac{5}{3}}$ using (27) and the estimate just proved on $\alpha^{-1}\int G_\alpha(\rho^{\mathrm{HF}}(\mathbf{x}))\,d\mathbf{x}$. □

Lemma 3.2. *Let $Z\alpha = \kappa$ be fixed with $0 \leq \kappa < 2/\pi$ and $Z \geq 1$. Then, there exists an $\alpha_0 > 0$ such that for all $\alpha \leq \alpha_0$, $\mu > 0$ and $\mathbf{x} \in \mathbb{R}^3$ with $|\mathbf{x}| \leq \beta Z^{-\frac{1+\mu}{3}}$ we have*

$$|\Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x})| \leq C\beta^{\frac{4}{1+\mu}}(1 + \beta^{\frac{9}{22(1+\mu)}}|\mathbf{x}|^{\frac{2+11\mu}{22(1+\mu)}})|\mathbf{x}|^{-4+\frac{4\mu}{1+\mu}}.$$

Proof. By the definition of screened nuclear potential we have

$$\left|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})\right| \leq \int_{|\mathbf{y}|<|\mathbf{x}|} \frac{|\rho^{\mathrm{HF}}(\mathbf{y}) - \rho^{\mathrm{TF}}(\mathbf{y})|}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} = \dots$$

and for all $k > 0$ by Proposition 2.8

$$\dots \quad \leq \quad 2^{\frac{3}{2}}k^{-1}|\mathbf{x}|^{-\frac{1}{2}}\left\|\rho^{\mathrm{HF}} - \rho^{\mathrm{TF}}\right\|_C + \int_{A(|\mathbf{x}|,k)} \frac{\rho^{\mathrm{HF}}(\mathbf{y}) + \rho^{\mathrm{TF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y}. \tag{32}$$

Since $\|\rho^{\mathrm{TF}}\|_{L^{\frac{5}{3}}(\mathbb{R}^3)} \leq CZ^{\frac{7}{5}}$ (Corollary 1.15) and

$$\int_{A(|\mathbf{x}|,k)} \frac{1}{|\mathbf{x}-\mathbf{y}|^{\frac{5}{2}}}d\mathbf{y} \leq 8\pi|\mathbf{x}|^{\frac{1}{2}}(2k)^{\frac{1}{2}}. \tag{33}$$

(see [23] page 549) one finds

$$\int_{A(|\mathbf{x}|,k)} \frac{\rho^{\mathrm{TF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} \quad \leq \quad CZ^{\frac{7}{5}}|\mathbf{x}|^{\frac{1}{5}}k^{\frac{1}{5}}. \tag{34}$$

The term with the HF-density has to be treated differently since we do not have a bound for the $L^{\frac{5}{3}}$-norm of ρ^{HF}. For a $R \in \mathbb{R}^+$ to be chosen later we consider the splitting

$$\int_{A(|\mathbf{x}|,k)} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} = \int_{\substack{A(|\mathbf{x}|,k)\\ |\mathbf{x}-\mathbf{y}|>R}} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} + \int_{\substack{A(|\mathbf{x}|,k)\\ |\mathbf{x}-\mathbf{y}|<R}} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y}. \tag{35}$$

We consider these two terms separately. Let Σ be defined as in (26); i.e. the region where $G_\alpha(\rho^{\mathrm{HF}})$ behaves like $(\rho^{\mathrm{HF}})^{\frac{4}{3}}$ (Remark 2.4). By Hölder's inequality we find

$$\begin{aligned}\int_{\substack{A(|\mathbf{x}|,k)\\ |\mathbf{x}-\mathbf{y}|>R}} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} \quad &\leq \quad \Big(\int_{\substack{A(|\mathbf{x}|,k)\\ |\mathbf{x}-\mathbf{y}|>R}} \frac{1}{|\mathbf{x}-\mathbf{y}|^4}d\mathbf{y}\Big)^{\frac{1}{4}}\Big(\int_{\mathbf{y}\in\Sigma}(\rho^{\mathrm{HF}}(\mathbf{y}))^{\frac{4}{3}}d\mathbf{y}\Big)^{\frac{3}{4}}\\ &\quad + \Big(\int_{A(|\mathbf{x}|,k)} \frac{1}{|\mathbf{x}-\mathbf{y}|^{\frac{5}{2}}}d\mathbf{y}\Big)^{\frac{2}{5}}\Big(\int_{\mathbf{y}\in\mathbb{R}^3\setminus\Sigma}(\rho^{\mathrm{HF}}(\mathbf{y}))^{\frac{5}{3}}d\mathbf{y}\Big)^{\frac{3}{5}}.\end{aligned}$$

From the inequality above, Remark 2.4 and estimate (21) we get

$$\int_{\substack{A(|\mathbf{x}|,k)\\ |\mathbf{x}-\mathbf{y}|>R}} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} \quad \leq \quad CR^{-\frac{3}{8}}|\mathbf{x}|^{\frac{1}{8}}k^{\frac{1}{8}}Z + C|\mathbf{x}|^{\frac{1}{5}}k^{\frac{1}{5}}Z^{\frac{7}{5}}. \tag{36}$$

On the other hand for the second term on the right hand side of (35) by (20) and Lemma 3.1 we find

$$\int_{|\mathbf{x}-\mathbf{y}|<R} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y} \leq C(Z^{\frac{4}{3}} + R^{\frac{1}{2}} Z^{\frac{3}{2}}). \tag{37}$$

Hence from (32), Lemma 3.1, (34), (36) and (37), we get

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq C\big(\frac{Z^{1+\frac{3}{22}}}{|\mathbf{x}|^{1/2}k} + Z^{\frac{7}{5}}|\mathbf{x}|^{\frac{1}{5}}k^{\frac{1}{5}} + R^{-\frac{3}{8}}|\mathbf{x}|^{\frac{1}{8}}k^{\frac{1}{8}}Z + R^{\frac{1}{2}}Z^{\frac{3}{2}} + Z^{\frac{4}{3}}\big). \tag{38}$$

Choosing k such that $Z^{\frac{4}{3}} = Z^{\frac{7}{5}}|\mathbf{x}|^{\frac{1}{5}}k^{\frac{1}{5}}$, i.e. $k = |\mathbf{x}|^{-1}Z^{-\frac{1}{3}}$ and R such that $R^{-\frac{3}{8}}Z^{1-\frac{1}{24}} = Z^{\frac{4}{3}}$, i.e. $R = Z^{-1}$ we find

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq C(|\mathbf{x}|^{\frac{1}{2}}Z^{\frac{4}{3}+\frac{3}{22}} + Z^{\frac{4}{3}}).$$

The claim follows using that $|\mathbf{x}| \leq \beta Z^{-\frac{1+\mu}{3}}$. □

Theorem 3.3. *Let $Z\alpha = \kappa$ be fixed with $0 \leq \kappa < 2/\pi$ and $Z \geq 1$. Then there exists an $\alpha_0 > 0$ such that for all $\alpha \leq \alpha_0$ and $\mathbf{x} \in \mathbb{R}^3$ with $|\mathbf{x}| \leq \beta Z^{-\frac{1}{3}}$ we have*

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq C\beta^{2-\frac{1}{66}}(1 + \beta^2 + \beta^{\frac{5}{2}} + \beta^{2+\frac{789}{1936}}|\mathbf{x}|^{\frac{179}{1936}})|\mathbf{x}|^{-4+\frac{1}{66}}. \tag{39}$$

Moreover if $|\mathbf{x}| \leq \beta Z^{-\frac{1-\mu}{3}}$ for $\mu < \frac{2}{11}\frac{1}{49}$, then

$$|\Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x})| \leq C\beta^{2-a(\mu)}(1 + \beta^2 + \beta^{\frac{5}{2}} + \beta^{b(\mu)}|\mathbf{x}|^{c(\mu)})|\mathbf{x}|^{-4+a(\mu)}, \tag{40}$$

with $a(\mu) = \frac{1}{66(1-\mu)} - \frac{49\mu}{12(1-\mu)}$, $b(\mu) = 2 + \frac{3}{176}\frac{24-24\mu-\frac{1}{11}+\frac{49}{2}\mu}{1-\mu}$ and $c(\mu) = \frac{1}{11} - \frac{\frac{3}{11}-\frac{3}{2}49\mu}{22(8-8\mu)}$ strictly positive constants.

Proof. Proceeding as in the proof of Lemma 3.2 up to (36) we get

$$\begin{aligned} |\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| &\leq C(k^{-1}|\mathbf{x}|^{-\frac{1}{2}}Z^{1+\frac{3}{22}} + Z^{\frac{7}{5}}|\mathbf{x}|^{\frac{1}{5}}k^{\frac{1}{5}} + R^{-\frac{3}{8}}|\mathbf{x}|^{\frac{1}{8}}k^{\frac{1}{8}}Z) \\ &+ \int_{|\mathbf{x}-\mathbf{y}|\leq R} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y}, \end{aligned} \tag{41}$$

for $R \in \mathbb{R}^+$ to be chosen. It remains to estimate the last term on the right hand side of (41). For 'small' R which is relevant for small $\mathbf{x}$ we already did it in Lemma 3.2, for 'big' R which is relevant for big $\mathbf{x}$ we use Proposition B.1 in Appendix B.

Take $\gamma \leq 1/263$ to be chosen. If $|\mathbf{x}| \leq \beta Z^{-\frac{1+\gamma}{3}}$ then by Lemma 3.2

$$|\Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x})| \leq C\beta^{\frac{4}{1+\gamma}}(1 + \beta^{\frac{9}{22(1+\gamma)}}|\mathbf{x}|^{\frac{2+11\gamma}{22(1+\gamma)}})|\mathbf{x}|^{-4+\frac{4\gamma}{1+\gamma}}. \tag{42}$$

If instead $|\mathbf{x}| > \beta Z^{-\frac{1+\gamma}{3}}$, let $H_{\mathbf{x}}$ be the Hamiltonian defined in (B2) with $\mathbf{P} = \mathbf{x}$ and $\nu = Z$. Then by the definition of $H_{\mathbf{x}}$ and taking the HF-minimizer as a trial wave function we have

$$\begin{aligned} \inf_{\substack{\psi\in\wedge_{i=1}^N L^2(\mathbb{R}^3)\\ \|\psi\|_2=1}} \langle\psi, H_{\mathbf{x}}\psi\rangle &\leq \mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) - Z\int_{|\mathbf{x}-\mathbf{y}|<R} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} \\ &= \inf_{\gamma\in\mathcal{A}} \mathcal{E}^{\mathrm{HF}}(\gamma) - Z\int_{|\mathbf{x}-\mathbf{y}|<R} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} = \ldots . \end{aligned}$$

Since $\frac{1}{2}|\mathbf{p}|^2 \geq \alpha^{-1}T(\mathbf{p})$, $\inf_{\gamma\in\mathcal{A}}\mathcal{E}^{\rm HF}(\gamma)$ is estimated from above by the HF-ground state energy of the non-relativistic model (i.e. when the kinetic energy is given by $-\frac{1}{2}\Delta$). Moreover, this last one can be estimated from above by $\mathcal{E}^{\rm TF}(\rho^{\rm TF}) + CN^{\frac{1}{5}}Z^2$ (see [18] and [11]). Hence we find

$$\cdots \leq \mathcal{E}^{\rm TF}(\rho^{\rm TF}) + CN^{\frac{1}{5}}Z^2 - Z\int_{|\mathbf{x}-\mathbf{y}|\leq R}\frac{\rho^{\rm HF}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y}.$$

On the other hand since $|\mathbf{x}| > \beta Z^{-\frac{1+\gamma}{3}}$ choosing for some $l > \frac{1+\gamma}{3}$, $R < \beta Z^{-l}/4$ from Proposition B.1 it follows that there exists a constant depending only on κ such that for $t \in ((1+\gamma)/3, \min\{l, 3/5\})$, and for every $\psi \in \wedge_{i=1}^N L^2(\mathbb{R}^3)$ with $\|\psi\|_2 = 1$ we have

$$\langle\psi, H_{\mathbf{x}}\psi\rangle \quad\geq\quad \mathcal{E}^{\rm TF}(\rho^{\rm TF}) - C(\beta^{1/2}+\beta^{-2})Z^{\frac{5}{2}-\frac{t}{2}},$$

Hence combining the two inequalities above we find

$$\int_{|\mathbf{x}-\mathbf{y}|\leq R}\frac{\rho^{\rm HF}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} \leq C(\beta^{1/2}+\beta^{-2})Z^{\frac{1}{2}(3-t)}. \tag{43}$$

From (41) and the inequality above we get

$$\begin{aligned}|\Phi^{\rm HF}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\rm TF}_{|\mathbf{x}|}(\mathbf{x})| \quad&\leq\quad Ck^{-1}|\mathbf{x}|^{-\frac{1}{2}}Z^{1+\frac{3}{22}} + CZ^{\frac{7}{5}}|\mathbf{x}|^{\frac{1}{5}}k^{\frac{1}{5}}\\ &\qquad +CR^{-\frac{3}{8}}|\mathbf{x}|^{\frac{1}{8}}k^{\frac{1}{8}}Z + C(\beta^{1/2}+\beta^{-2})Z^{\frac{1}{2}(3-t)}.\end{aligned}$$

Choosing k such that $Z^{\frac{1}{2}(3-t)} = Z^{\frac{7}{5}}|\mathbf{x}|^{\frac{1}{5}}k^{\frac{1}{5}}$, i.e $k = |\mathbf{x}|^{-1}Z^{\frac{1}{2}(1-5t)}$ and R such that $Z^{\frac{1}{2}(3-t)} \sim R^{-\frac{3}{8}}Z^{1+\frac{1}{16}(1-5t)}$, i.e $R = \beta Z^{-\frac{7}{6}+\frac{1}{2}t}/4$ we find

$$|\Phi^{\rm HF}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\rm TF}_{|\mathbf{x}|}(\mathbf{x})| \leq C(|\mathbf{x}|^{\frac{1}{2}}Z^{\frac{7}{11}+\frac{5}{2}t} + (\beta^{1/2}+\beta^{-2})Z^{\frac{1}{2}(3-t)}). \tag{44}$$

Notice that $R < \beta Z^{-l}/4$ is satisfied choosing $l = 4t/3$. Then for $\mathbf{x}$ such that $\beta Z^{-\frac{1+\gamma}{3}} \leq |\mathbf{x}| \leq \beta Z^{-\frac{1}{3}}$ we find

$$|\Phi^{\rm HF}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\rm TF}_{|\mathbf{x}|}(\mathbf{x})| \leq C(|\mathbf{x}|^{-\frac{31}{22}-\frac{15}{2}t}\beta^{\frac{21}{11}+\frac{15}{2}t} + (\beta^{1/2}+\beta^{-2})\beta^{\frac{3}{2}(3-t)}|\mathbf{x}|^{-\frac{3}{2}(3-t)}).$$

Optimizing in t gives $t = 1/3 + 1/99$. For this value of t we get

$$|\Phi^{\rm HF}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\rm TF}_{|\mathbf{x}|}(\mathbf{x})| \leq C(1+\beta^{\frac{5}{2}})\beta^{2-\frac{1}{66}}|\mathbf{x}|^{-4+\frac{1}{66}}. \tag{45}$$

Inequality (39) follows from (42) and (45) choosing γ such that $4\gamma/(1+\gamma) = 1/66$, i.e. $\gamma = 1/263$.

On the other hand from (44) for $\mathbf{x}$ such that $\beta Z^{-\frac{1+\gamma}{3}} \leq |\mathbf{x}| \leq \beta Z^{-\frac{1-\mu}{3}}$ we find

$$\begin{aligned}|\Phi^{\rm HF}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\rm TF}_{|\mathbf{x}|}(\mathbf{x})| \quad&\leq\quad C|\mathbf{x}|^{\frac{1}{2}-\frac{3}{1-\mu}(\frac{7}{11}+\frac{5}{2}t)}\beta^{\frac{3}{1-\mu}(\frac{7}{11}+\frac{5}{2}t)}\\ &\qquad +C(\beta^{1/2}+\beta^{-2})\beta^{\frac{3}{2(1-\mu)}(3-t)}|\mathbf{x}|^{-\frac{3}{2(1-\mu)}(3-t)}.\end{aligned}$$

Optimizing in t gives $t = 1/3 + 1/99 - \frac{1}{18}\mu$. For this value of t we get

$$|\Phi^{\rm HF}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\rm TF}_{|\mathbf{x}|}(\mathbf{x})| \leq C(1+\beta^{\frac{5}{2}})\beta^{2-\frac{1}{66(1-\mu)}+\frac{49\mu}{12(1-\mu)}}|\mathbf{x}|^{-4+\frac{1}{66(1-\mu)}-\frac{49\mu}{12(1-\mu)}}.$$

Inequality (40) follows from the one above and (42) choosing γ such that $4\gamma/(1+\gamma) = \frac{1}{66(1-\mu)} - \frac{49\mu}{12(1-\mu)}$. $\square$

4 The exterior part

In this section we complete the proof of Theorem 1.17. We first estimate the exterior integral of the density and study the minimization problem that the exterior part of the minimizer satisfies. Then we prove the main estimate in Theorem 1.17 in an intermediate zone, i.e. far from the nucleus but not further than a fixed distance independent of Z. To study this area we need first to construct a TF-model that gives a good approximation of the HF-density in this intermediate zone. By the estimate on the exterior integral of the density we can then also prove Theorem 1.17 in the region far away from the nucleus.

4.1 The exterior integral of the density

The main result of this section is the following lemma.

Lemma 4.1 (The exterior integral of the density)**.** *Assume that for some $R, \sigma, \varepsilon' > 0$*

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq \sigma |\mathbf{x}|^{-4+\varepsilon'}, \tag{46}$$

holds for $|\mathbf{x}| \leq R$. Then for $0 < r \leq R$

$$\Big| \int_{|\mathbf{x}|<r} (\rho^{\mathrm{HF}}(\mathbf{x}) - \rho^{\mathrm{TF}}(\mathbf{x}))\, d\mathbf{x} \Big| \leq \sigma r^{-3+\varepsilon'} \tag{47}$$

and

$$\int_{|\mathbf{x}|>r} \rho^{\mathrm{HF}}(\mathbf{x}) d\mathbf{x} \leq C(1+\sigma r^{\varepsilon'})(1+r^{-3}), \tag{48}$$

with C a universal constant.

We proceed similarly as in the proof of Lemma 10.5 in [23]. Since we need to localize we first present some technical lemmas that will take care of the error terms due to the localization. The localization error that will appear in the argument below (see (58)) will be in the form of an operator L similar to the error (14) in the IMS formula. We estimate this error in Lemma 4.3.

Remark 4.2. *Let $0 \leq \beta_1 < .. < \beta_4$ be real numbers with possibly $\beta_4 = \infty$. Let us denote $\Sigma_r(\beta_i, \beta_j) = \{\mathbf{x} \in \mathbb{R}^3 : \beta_i r \leq |\mathbf{x}| \leq \beta_j r\}$. Then we have*

$$\iint_{\substack{\mathbf{x} \in \Sigma_r(\beta_1,\beta_2) \\ \mathbf{y} \in \Sigma_r(\beta_3,\beta_4)}} K_2(\alpha^{-1}|\mathbf{x}-\mathbf{y}|)^2\, d\mathbf{x} d\mathbf{y} \leq \frac{(4^3\pi)^2}{3} \frac{\beta_2^3 - \beta_1^3}{\beta_3 - \beta_2}\, \alpha^4 r^2 e^{-\alpha^{-1} r(\beta_3-\beta_2)}.$$

The proof of this estimate is given in Appendix A.

Lemma 4.3. *Let $r > 0$ and $\lambda, \nu \in (0,1)$. Let χ_- be the characteristic function of $B_{r(1-\nu)}(0)$ and χ_0 be the characteristic function of the sector $\{\mathbf{x} \in \mathbb{R}^3 : r(1-\nu) < |\mathbf{x}| < r(1+\nu)/(1-\lambda)\}$. Let η be a Lipschitz function such that $0 \leq \eta(\mathbf{x}) \leq 1$ for all $\mathbf{x} \in \mathbb{R}^3$, $\eta(\mathbf{x}) \equiv 0$ if $|\mathbf{x}| \leq r$, $\eta(\mathbf{x}) \equiv 1$ if $|\mathbf{x}| \geq r(1-\lambda)^{-1}$ and $\|\nabla\eta\|_\infty$ is bounded. Let L denote the operator with integral kernel*

$$L(\mathbf{x},\mathbf{y}) = \frac{\alpha^{-2}}{4\pi^2} \frac{(\eta(\mathbf{x}) - \eta(\mathbf{y}))(\eta(\mathbf{x})|\mathbf{x}| - \eta(\mathbf{y})|\mathbf{y}|)}{|\mathbf{x}-\mathbf{y}|^2} K_2(\alpha^{-1}|\mathbf{x}-\mathbf{y}|). \tag{49}$$

Then for every function $f \in L^2(\mathbb{R}^3)$ we have

$$\alpha^{-1}|(f, Lf)| \leq 3\, D(\eta,\lambda,r)\, \|\chi_0 f\|_2^2 + D(\eta,\lambda,r) e^{-\frac{1}{2}\alpha^{-1} r\nu} \|\chi_- f\|_2^2 + \alpha^{-1}|(f, Qf)|,$$

with $D(\eta,\lambda,r) := \|\nabla\eta\|_\infty\Big(\frac{\|\nabla\eta\|_\infty r}{1-\lambda}+1\Big)$ *and* Q *a positive semi-definite operator such that*

$$\mathrm{Tr}[Q] \le C D(\eta,\lambda,r)\alpha^{-1}r^2 e^{-\frac{1}{2}\alpha^{-1}r\nu},$$

with C *depending only on* λ *and* ν.

Proof. As a first step we decompose the operator L. We introduce a third cut-off function χ_+ such that $1=\chi_-(\mathbf{x})+\chi_0(\mathbf{x})+\chi_+(\mathbf{x})$ for all $\mathbf{x}\in\mathbb{R}^3$. We decompose the operator L with respect to these characteristic functions as follows:

$$L = \chi_- L(\chi_0+\chi_+) + (\chi_0+\chi_+)L\chi_- + \chi_0 L\chi_+ + \chi_+ L\chi_0 + \chi_0 L\chi_0.$$

We proceed similarly as in [24, Proof of Theorem 2.6 (Localization error)]. For Γ_1,Γ_2 bounded operators from $(\Gamma_1-\Gamma_2)(\Gamma_1-\Gamma_2)^*\ge 0$ it follows

$$\Gamma_1\Gamma_2^* + \Gamma_2\Gamma_1^* \le \Gamma_1\Gamma_1^* + \Gamma_2\Gamma_2^*. \tag{50}$$

We are going to use several times this inequality with different choices of Γ_1 and Γ_2.

As a first choice we consider $\Gamma_1=\sqrt{\varepsilon_1}\chi_-$ and $\Gamma_2 = 1/\sqrt{\varepsilon_1}(\chi_0+\chi_+)L\chi_-$ with $\varepsilon_1>0$ to be chosen. Using (50) we get

$$|(f,(\chi_- L(\chi_0+\chi_+)+(\chi_0+\chi_+)L\chi_-)f)| \le \varepsilon_1\|\chi_- f\|_2^2 + \frac{1}{\varepsilon_1}(f,Q_1 f), \tag{51}$$

with $Q_1 = (\chi_0+\chi_+)L\chi_-^2 L(\chi_0+\chi_+)$. We estimate now the trace of Q_1. By the definition of η,χ_-,χ_0 and χ_+ it follows that

$$\mathrm{Tr}[Q_1] = \int_{|\mathbf{x}|\le r(1-\nu)}\int_{|\mathbf{y}|\ge r} L^2(\mathbf{x},\mathbf{y})\,d\mathbf{x}d\mathbf{y} \le \tfrac{(16)^2}{3\pi^2}\tfrac{(1-\nu)^3}{\nu}D(\eta,\lambda,r)^2 r^2 e^{-\alpha^{-1}r\nu}.$$

In the last step we use the definition of L, Remark 4.2 and the definition of the constant $D(\eta,\lambda,r)$ given in the statement of the lemma.

Now we choose $\Gamma_1=\sqrt{\varepsilon_2}\chi_0$ and $\Gamma_2=1/\sqrt{\varepsilon_2}\chi_+L\chi_0$ with $\varepsilon_2>0$ to be chosen. Proceeding as above we get

$$|(f,(\chi_+L\chi_0+\chi_0L\chi_+)f)| \le \varepsilon_2\|\chi_0 f\|_2^2 + \frac{1}{\varepsilon_2}(f,Q_2 f), \tag{52}$$

with $Q_2=\chi_+L\chi_0^2L\chi_+$ and such that

$$\mathrm{Tr}[Q_2] \le \tfrac{(16)^2}{3\pi^2}\tfrac{1-(1-\nu)^3(1-\lambda)^3}{\nu(1-\lambda)^2}D(\eta,\lambda,r)^2\ r^2 e^{-\alpha^{-1}r\frac{\nu}{1-\lambda}}.$$

It remains to study the term $\chi_0L\chi_0$. This one has to be treated differently. By Schwartz's inequality one gets

$$|(f,\chi_0L\chi_0 f)| \le \tfrac{3\alpha}{2}D(\eta,\lambda,r)\int_{\mathbb{R}^3}\chi_0(\mathbf{x})|f(\mathbf{x})|^2, \tag{53}$$

since $\int_{\mathbb{R}^3}|L(\mathbf{x},\mathbf{y})|d\mathbf{x}d\mathbf{y} \le \frac{3\alpha}{2}D(\eta,\lambda,r)$.

The claim follows from (51), (52) and (53) choosing $\varepsilon_1 = D(\eta,\lambda,r)\alpha e^{-\frac{1}{2}\alpha^{-1}r\nu}$, $\varepsilon_2=\frac{3\alpha}{2}D(\eta,\lambda,r)$ and with $Q:=\frac{1}{\varepsilon_1}Q_1+\frac{1}{\varepsilon_2}Q_2$. □

Definition 4.4 (The localization function)**.** *Fix* $0<\lambda<1$ *and let* $G:\mathbb{R}^3\to\mathbb{R}$ *be given by*

$$G(\mathbf{x}) := \begin{cases} 0 & \text{if } |\mathbf{x}|\le 1,\\ \frac{\pi}{2}(|\mathbf{x}|-1)\frac{1}{(1-\lambda)^{-1}-1} & \text{if } 1\le|\mathbf{x}|\le(1-\lambda)^{-1},\\ \frac{\pi}{2} & \text{if } (1-\lambda)^{-1}\le|\mathbf{x}|. \end{cases}$$

Let $r>0$ *and define the outside localization function* $\theta_r(\mathbf{x}) := \sin(G(\frac{|\mathbf{x}|}{r}))$.

Remark 4.5. *From the definition it follows that* $\|\nabla\theta_r\|_\infty \leq \frac{\pi}{2}\frac{1-\lambda}{\lambda}r^{-1}$.

Lemma 4.6. *For all* $r>0$ *and* $\lambda,\nu\in(0,1)$ *the density* ρ^{HF} *of the minimizer satisfies*

$$\int_{|\mathbf{x}|>r(1-\lambda)^{-1}} \rho^{\mathrm{HF}}(\mathbf{x})d\mathbf{x} \quad \leq \quad 1+\tfrac{2}{\lambda}+2\sup_{|\mathbf{x}|=r(1-\lambda)} |\mathbf{x}|\Phi^{\mathrm{HF}}_{r(1-\lambda)}(\mathbf{x})+\mathcal{R}^{\frac{1}{2}}$$

with

$$\mathcal{R}=6D(\lambda)r^{-1}\int_{r(1-\nu)<|\mathbf{x}|<r\frac{1+\nu}{1-\lambda}} \rho^{\mathrm{HF}}(\mathbf{x})\,d\mathbf{x}+2D(\lambda)(r^{-1}N+Cr\alpha^{-2})e^{-\frac{1}{2}\alpha^{-1}r\nu},$$

with $D(\lambda):=(1+\pi/(2\lambda(1-\lambda)))\pi/(2\lambda)$ *and* $C=C(\lambda,\nu)$.

Proof. Let γ^{HF} be the minimizer. By the variational principle, γ^{HF} is a projection onto the subspace spanned by $u_1,\dots,u_N$. These functions u_i satisfy the Euler Lagrange equations $h_{\gamma^{\mathrm{HF}}}u_i=\varepsilon_i u_i$, $\varepsilon_i<0$, for $i=1,\dots,N$, with $h_{\gamma^{\mathrm{HF}}}$ defined in (11).

Given η a function in $C^1(\mathbb{R}^3)$ with support away from zero, we find

$$0\geq\sum_{i=1}^N\varepsilon_i\int_{\mathbb{R}^3}|u_i(\mathbf{x})|^2|\mathbf{x}|\eta^2(\mathbf{x})d\mathbf{x}=\sum_{i=1}^N\int_{\mathbb{R}^3}u_i(\mathbf{x})^*|\mathbf{x}|\eta^2(\mathbf{x})\,h_{\gamma^{\mathrm{HF}}}u_i(\mathbf{x})d\mathbf{x}.$$

Since $\eta T(\mathbf{p})u_i\in L^2(\mathbb{R}^3)$ (Theorem 1.5, (3)), using the Euler-Lagrange equations and treating all the terms, except the kinetic energy, as in [23, Formula (63)] we get

$$\begin{aligned}0 \quad\geq\quad & \alpha^{-1}\sum_{i=1}^N(u_i\eta|\cdot|,\eta T(\mathbf{p})u_i)-Z\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x}\\ &+\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\left[\rho^{\mathrm{HF}}(\mathbf{x})\rho^{\mathrm{HF}}(\mathbf{y})-\mathrm{Tr}_{\mathbb{C}^q}|\gamma^{\mathrm{HF}}(\mathbf{x},\mathbf{y})|^2\right]\frac{|\mathbf{y}|(1-\eta^2(\mathbf{x}))\eta^2(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}d\mathbf{y}\\ &+\tfrac{1}{2}\Big(\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x}\Big)^2-\tfrac{1}{2}\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x}.\end{aligned}\tag{54}$$

Now we look at the kinetic energy term. For each $i\in\{1,\dots,N\}$ we may write

$$\mathrm{Re}(u_i\eta|\cdot|,\eta T(\mathbf{p})u_i)=\mathrm{Re}(u_i\eta|\cdot|,T(\mathbf{p})(\eta u_i))+\mathrm{Re}(u_i\eta|\cdot|,[\eta,T(\mathbf{p})]u_i),\tag{55}$$

where $[A,B]$ denotes the commutator of the operators A and B. The first term on the right hand side of (55) is non-negative by the result of Lieb in [13]. Notice that here we may use that $\eta u_i\in H^1(\mathbb{R}^3)$ (see Theorem 1.5, (3)).

Hence, from (54) and (55) we find

$$\begin{aligned}0 \quad\geq\quad & \alpha^{-1}\sum_{i=1}^N\mathrm{Re}(u_i\eta|\cdot|,[\eta,T(\mathbf{p})]u_i)-Z\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x}\\ &+\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\left[\rho^{\mathrm{HF}}(\mathbf{x})\rho^{\mathrm{HF}}(\mathbf{y})-\mathrm{Tr}_{\mathbb{C}^q}|\gamma^{\mathrm{HF}}(\mathbf{x},\mathbf{y})|^2\right]\frac{|\mathbf{y}|(1-\eta^2(\mathbf{x}))\eta^2(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}d\mathbf{y}\\ &+\tfrac{1}{2}\Big(\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x}\Big)^2-\tfrac{1}{2}\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x}.\end{aligned}\tag{56}$$

By a density argument we may choose $\eta=\theta_r$ the localization function defined in Definition 4.4. Reasoning as on page 541 of [23], we get

$$\begin{aligned}0 \quad\geq\quad & \alpha^{-1}\sum_{i=1}^N\mathrm{Re}(u_i\eta|\cdot|,[\eta,T(\mathbf{p})]u_i)+\tfrac{1}{2}\Big(\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x}\Big)^2\\ &-\Big(\tfrac{1}{2}+\tfrac{1}{\lambda}+\sup_{|\mathbf{x}|=r(1-\lambda)}|\mathbf{x}|\Phi^{\mathrm{HF}}_{r(1-\lambda)}(\mathbf{x})\Big)\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x}.\end{aligned}\tag{57}$$

It remains to estimate the first term on the right hand side of (57). With the same arguments used in the proof of the IMS formula, it can be rewritten as

$$\alpha^{-1}\sum_{i=1}^{N}\mathrm{Re}(u_i\eta|\cdot|,[\eta,T(\mathbf{p})]u_i) = -\alpha^{-1}\sum_{i=1}^{N}(u_i,Lu_i), \tag{58}$$

where L is the operator defined in (49). Using Lemma 4.3 and since $\|\nabla\eta\|_\infty = \|\nabla\theta_r\|_\infty \le \pi/(2\lambda r)$ we find, with $D(\lambda)$ defined as in the statement,

$$\begin{aligned}\alpha^{-1}\Big|\sum_{i=1}^{N}(u_i,Lu_i)\Big| \;\le\;& 3D(\lambda)r^{-1}\|\chi_0\rho^{\mathrm{HF}}\|_1 + D(\lambda)r^{-1}e^{-\frac{1}{2}\alpha^{-1}r\nu}\|\chi_-\rho^{\mathrm{HF}}\|_1\\ &+CD(\lambda)r\alpha^{-2}e^{-\frac{1}{2}\alpha^{-1}r\nu},\end{aligned} \tag{59}$$

where χ_0,χ_- and C are as defined in the statement of Lemma 4.3. Hence combining (57) with (59), using the definition of χ_0 and that $\|\chi_-\rho^{\mathrm{HF}}\|_1\le N$ we have

$$\begin{aligned}0 \;\ge\;& -3D(\lambda)r^{-1}\int_{r(1-\nu)<|\mathbf{x}|<r\frac{1+\nu}{1-\lambda}}\rho^{\mathrm{HF}}(\mathbf{x})\,d\mathbf{x} - D(\lambda)r^{-1}e^{-\frac{1}{2}\alpha^{-1}r\nu}N\\ &-CD(\lambda)r\alpha^{-2}e^{-\frac{1}{2}\alpha^{-1}r\nu} + \tfrac{1}{2}\Big(\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x}\Big)^2\\ &-\Big(\tfrac{1}{2}+\tfrac{1}{\lambda}+\sup_{|\mathbf{x}|=r(1-\lambda)}|\mathbf{x}|\Phi^{\mathrm{HF}}_{r(1-\lambda)}(\mathbf{x})\Big)\int_{\mathbb{R}^3}\rho^{\mathrm{HF}}(\mathbf{x})\eta^2(\mathbf{x})d\mathbf{x}.\end{aligned}$$

The claim follows using that $x^2-Bx-C\le 0$ implies $x\le B+\sqrt{C}$. $\square$

Proof of Lemma 4.1. We proceed as in [23, page 551]. The first estimate follows directly from the equality

$$\int_{|\mathbf{x}|<r}(\rho^{\mathrm{HF}}(\mathbf{x})-\rho^{\mathrm{TF}}(\mathbf{x}))\,d\mathbf{x} = \tfrac{1}{4\pi}r\int_{S^2}(\Phi_r^{\mathrm{HF}}(r\omega)-\Phi_r^{\mathrm{TF}}(r\omega))\,d\omega,$$

and (46). To prove (48) we use Lemma 4.6. We first notice that for $0<\beta<\gamma$ and γ such that $r\gamma\le R$

$$\begin{aligned}\int_{r\beta<|\mathbf{y}|<r\gamma}\rho^{\mathrm{HF}}(\mathbf{y})\,d\mathbf{y} \;\le\;& \Big|\int_{|\mathbf{y}|<r\gamma}(\rho^{\mathrm{HF}}(\mathbf{y})-\rho^{\mathrm{TF}}(\mathbf{y}))\,d\mathbf{y}\Big|\\ &+\Big|\int_{|\mathbf{y}|<r\beta}(\rho^{\mathrm{HF}}(\mathbf{y})-\rho^{\mathrm{TF}}(\mathbf{y}))\,d\mathbf{y}\Big| + \int_{|\mathbf{y}|>r\beta}\rho^{\mathrm{TF}}(\mathbf{y})\,d\mathbf{y}\\ \le\;& Cr^{-3}\beta^{-3}(1+\sigma r^{\varepsilon'}).\end{aligned} \tag{60}$$

Here we used (47) and that by the TF-equation and (13)

$$\int_{|\mathbf{y}|>r\beta}\rho^{\mathrm{TF}}(\mathbf{y})\,d\mathbf{y} \le \tfrac{3^4 2\pi^2}{q^2}\beta^{-3}r^{-3}.$$

Since $\int_{|\mathbf{x}|>r}\rho^{\mathrm{HF}} \le \int_{|\mathbf{x}|>2r/3}\rho^{\mathrm{HF}}$ to prove the claim we estimate this second integral. By Lemma 4.6 with r replaced by $r/2$, $\lambda=\frac{1}{4}$ and $\nu=\frac{1}{2}$ we get

$$\int_{|\mathbf{x}|>2r/3}\rho^{\mathrm{HF}}(\mathbf{x})d\mathbf{x} \le 9+\tfrac{3}{4}r\sup_{|\mathbf{x}|=3r/8}\Phi^{\mathrm{HF}}_{3r/8}(\mathbf{x})+\mathcal{R}^{\frac{1}{2}},$$

with $\mathcal{R}$ defined as in the statement of Lemma 4.6. By (46) and Corollary 1.14 we find

$$\sup_{|\mathbf{x}|=3r/8} \Phi^{\mathrm{HF}}_{3r/8}(\mathbf{x}) \leq C\sigma r^{-4+\varepsilon'} + \sup_{|\mathbf{x}|=3r/8} \Phi^{\mathrm{TF}}_{3r/8}(\mathbf{x}) \leq C(1+\sigma r^{\varepsilon'})r^{-4}.$$

Moreover, from (60) with $\beta = 1/4$ and $\gamma = 1$, since $N < 2Z+1$ and the boundness of $\mathbb{R}^+ \ni x \mapsto x^p e^{-x}$ for all $p > 0$, we find

$$\mathcal{R} \leq C(r^{-4}(1+\sigma r^{\varepsilon'}) + r^{-1}).$$

The claim follows directly. □

4.2 Separating the inside from the outside

We consider the exterior part of the minimizer, i.e. the density matrix

$$\gamma_r^{\mathrm{HF}} := \theta_r \gamma^{\mathrm{HF}} \theta_r, \tag{61}$$

with θ_r as defined in Definition 4.4. This density matrix almost minimizes a new energy functional where there is no exchange term. Indeed sufficiently far away from the nucleus the electrons are far apart and hence their mutual interaction is small.

We define an auxiliary energy functional on $\mathcal{A}$ (see (8)) given by

$$\mathcal{E}^A(\gamma) := \mathrm{Tr}[(\alpha^{-1}T(\mathbf{p}) - \Phi_r^{\mathrm{HF}})\gamma] + D(\rho_\gamma). \tag{62}$$

Theorem 4.7. *Let $r > 0$ and $\lambda, \nu \in (0,1)$. Let χ_r^+ denote the characteristic function of $\mathbb{R}^3 \setminus B_r(0)$. The density matrix γ_r^{HF} defined in (61) satisfies*

$$\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) \leq \left\{\mathcal{E}^A(\gamma) : \gamma \in \mathcal{A}, \mathrm{supp}(\rho_\gamma) \subset \mathbb{R}^3 \setminus B_r(0), \|\rho_\gamma\|_1 \leq \|\rho^{\mathrm{HF}}\chi_r\|_1\right\} + \mathcal{R},$$

where

$$\begin{aligned}
\mathcal{R} \;=\;& (\tfrac{\pi}{2\lambda} + \tfrac{C}{\lambda^2} r^{-1})r^{-1} \int_{r(1-\lambda)(1-\nu)\leq|\mathbf{x}|} \rho^{\mathrm{HF}}(\mathbf{x})\, d\mathbf{x} + c'\alpha^{-2}(1+\alpha r^{-2})e^{-\frac{1}{2}\alpha^{-1}rd} \\
&+ \mathcal{E}x(\gamma_r^{\mathrm{HF}}) + C\int_{r(1-\lambda)\leq|\mathbf{x}|\leq\frac{r}{1-\lambda}} \left[\left(\Phi^{\mathrm{HF}}_{r(1-\lambda)}(\mathbf{x})\right)^{\frac{5}{2}} + \alpha^3\left(\Phi^{\mathrm{HF}}_{r(1-\lambda)}(\mathbf{x})\right)^4\right] d\mathbf{x},
\end{aligned}$$

and c', d are positive constants depending only on ν and λ.

Proof. We proceed as in [23, pages 532-6]. The first step of the proof is a localization. Once again we have to treat carefully the localization error coming from the kinetic energy. This is the main difference with [23]. For completeness we repeat the main ideas of the reasoning.

We consider the following partition of unity of $\mathbb{R}^3$: $1 = \theta_r^2(\mathbf{x}) + \theta_0^2(\mathbf{x}) + \theta_-^2(\mathbf{x})$ with θ_r defined as in Definition 4.4 and

$$\theta_0(\mathbf{x}) := \left(\theta^2_{r(1-\lambda)}(\mathbf{x}) - \theta_r^2(\mathbf{x})\right)^{\frac{1}{2}} \text{ and } \theta_-(\mathbf{x}) := \left(1 - \theta^2_{r(1-\lambda)}(\mathbf{x})\right)^{\frac{1}{2}}.$$

Associated to this partition of unity we define

$$\gamma_0^{\mathrm{HF}} := \theta_0 \gamma^{\mathrm{HF}} \theta_0 \text{ and } \gamma_-^{\mathrm{HF}} := \theta_- \gamma^{\mathrm{HF}} \theta_-.$$

We prove the claim by showing that for all density matrices $\gamma \in \mathcal{A}$ such that $\mathrm{supp}(\rho_\gamma) \subset \mathbb{R}^3 \setminus B_r(0)$ and $\|\rho_\gamma\|_1 \leq \|\rho^{\mathrm{HF}}\chi_r^+\|_1$ it holds that

$$\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) + \mathcal{E}^{\mathrm{HF}}(\gamma_-^{\mathrm{HF}}) - \mathcal{R} \leq \mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) \leq \mathcal{E}^A(\gamma) + \mathcal{E}^{\mathrm{HF}}(\gamma_-^{\mathrm{HF}}). \tag{63}$$

The proof of the upper bound in (63) is as in [23, page 533].

To prove the lower bound as a first step we localize. By Theorem 2.1 we find

$$\alpha^{-1}\operatorname{Tr}[T(\mathbf{p})\gamma^{\mathrm{HF}}] = \alpha^{-1}\operatorname{Tr}[T(\mathbf{p})(\gamma_r^{\mathrm{HF}}+\gamma_0^{\mathrm{HF}}+\gamma_-^{\mathrm{HF}})] - \alpha^{-1}\sum_{i=1}^{N}(u_i,(L_r+L_0+L_-)u_i), \tag{64}$$

where L_r, L_0 and L_- are defined as the L_i's in (14).

We first estimate the error term. The procedure is similar to the one used in the proof of Lemma 4.3. We introduce three cut-off functions: χ_- be the characteristic function of $B_{r(1-\lambda)(1-\nu)}(0)$, χ_r the characteristic function of $\mathbb{R}^3 \setminus B_{r\frac{1+\nu}{1-\lambda}}(0)$ and χ_0 defined by $\chi_0(\mathbf{x}) = 1-\chi_r(\mathbf{x})-\chi_-(\mathbf{x})$ for all $\mathbf{x}\in\mathbb{R}^3$. Notice that χ_- and χ_r are the characteristic functions of sets where θ_-, θ_0 and θ_r are constants. For $k\in\{-,0,r\}$ we have the following splitting

$$L_k = \chi_- L_k(\chi_0+\chi_r) + (\chi_0+\chi_r)L_k\chi_- + \chi_r L_k\chi_0 + \chi_0 L_k \chi_r + \chi_0 L_k\chi_0,$$

and proceeding as in the proof of Lemma 4.3 with $\varepsilon_{1,k}, \varepsilon_{2,k}$ to be chosen we find

$$\begin{aligned}(f, L_k f) \;\le\;& \varepsilon_{1,k}\|\chi_- f\|_2^2 + \varepsilon_{1,k}^{-1}(f,Q_1 f) + \varepsilon_{2,k}\|\chi_0 f\|_2^2 + \varepsilon_{2,k}^{-1}(f,Q_2 f)\\ &+\tfrac{3\alpha}{2}\|\nabla\theta_k\|_\infty^2\|\chi_0 f\|_2^2.\end{aligned}$$

with operators Q_1 and Q_2 being positive semi-definite operators with

$$\begin{aligned}\operatorname{Tr}[Q_1] &\le \tfrac{(16)^2}{3\pi^2}\tfrac{(1-\lambda)^2(1-\nu)^3}{\nu}\|\nabla\theta_k\|_\infty^4 r^2 e^{-\alpha^{-1}r\nu(1-\lambda)}\\ \operatorname{Tr}[Q_2] &\le \tfrac{(16)^2}{3\pi^2}\tfrac{1}{\nu(1-\lambda)^2}\|\nabla\theta_k\|_\infty^4 r^2 e^{-\alpha^{-1}r\frac{\nu}{1-\lambda}}.\end{aligned}$$

Choosing then

$$\varepsilon_{2,k} = \tfrac{3\alpha}{2}\|\nabla\theta_k\|_\infty^2 \text{ and } \varepsilon_{1,k} = \alpha\|\nabla\theta_k\|_\infty^2 e^{-\frac{1}{2}\alpha^{-1}r\nu(1-\lambda)},$$

since $(\|\nabla\theta_r\|_\infty^2 + \|\nabla\theta_0\|_\infty^2 + \|\nabla\theta_-\|_\infty^2) \le 3\pi^2/(4\lambda^2)r^{-2}$ and $\|\rho^{\mathrm{HF}}\chi_-\|_1 \le N$ we get

$$\begin{aligned}\alpha^{-1}\sum_{i=1}^{N}(u_i,(L_r+L_0+L_-)u_i) \;\le\;& \tfrac{3\pi^2}{4\lambda^2}r^{-2}\|\rho^{\mathrm{HF}}\chi_0\|_1 + \tfrac{3\pi^2}{4\lambda^2}r^{-2}e^{-\frac{1}{2}\alpha^{-1}r\nu(1-\lambda)}N\\ &+\; c\alpha^{-2}e^{-\frac{1}{2}\alpha^{-1}r\nu(1-\lambda)}.\end{aligned}$$

Here c is a constant that depends only on ν and λ.

Hence from (64), the inequality above and since $N\le 2Z+1$ we find

$$\begin{aligned}\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) \;\ge\;& \operatorname{Tr}\left[\left(\alpha^{-1}T(\mathbf{p}) - \frac{Z}{|\cdot|}\right)(\gamma_r^{\mathrm{HF}}+\gamma_0^{\mathrm{HF}}+\gamma_-^{\mathrm{HF}})\right] + \mathcal{D}(\gamma^{\mathrm{HF}})\\ &-\mathcal{E}x(\gamma^{\mathrm{HF}}) - \tfrac{3\pi^2}{4\lambda^2}r^{-2}\|\rho^{\mathrm{HF}}\chi_0\|_1 - c'\alpha^{-2}(1+\alpha r^{-2})e^{-\frac{1}{2}\alpha^{-1}rd}.\end{aligned}$$

The constants c', d depend only on λ and ν. Proceeding as in [23] we get

$$\begin{aligned}\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) \;\ge\;& \mathcal{E}^{\mathrm{HF}}(\gamma_-^{\mathrm{HF}}) + \mathcal{E}^{A}(\gamma_r^{\mathrm{HF}}) - \mathcal{E}x(\gamma_r^{\mathrm{HF}}) - c'\alpha^{-2}(1+\alpha r^{-2})e^{-\frac{1}{2}\alpha^{-1}rd}\\ &+\operatorname{Tr}\left[\left(\alpha^{-1}T(\mathbf{p}) - \Phi_{r(1-\lambda)}^{\mathrm{HF}}(\cdot)\right)\gamma_0^{\mathrm{HF}}\right]\\ &-\left(\tfrac{\pi}{2\lambda} + \tfrac{3\pi^2}{4\lambda^2}r^{-1}\right)r^{-1}\int_{|\mathbf{x}|\ge r(1-\lambda)(1-\nu)}\rho^{\mathrm{HF}}(\mathbf{x})\,d\mathbf{x}.\end{aligned}$$

The claim follows using Theorem 2.5. □

4.3 Comparing with an Outside Thomas Fermi

At this point we introduce an "Outside Thomas Fermi": a TF-energy functional whose minimizer approximates the HF-density at a certain distance from the nucleus.

Let $r > 0$ such that

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq \sigma |\mathbf{x}|^{-4+\varepsilon'}, \tag{65}$$

for all $|\mathbf{x}| \leq r$ for some $\sigma > 0$ and $\varepsilon' > 0$. Let V_r be the potential defined by

$$V_r(\mathbf{x}) = \chi_r^+(\mathbf{x})\Phi^{\mathrm{HF}}_r(\mathbf{x}) = \begin{cases} 0 & \text{if } |\mathbf{x}| < r, \\ \Phi^{\mathrm{HF}}_r(\mathbf{x}) & \text{if } |\mathbf{x}| \geq r. \end{cases} \tag{66}$$

Here and in the following $\chi_r^+(\mathbf{x}) := 1 - \chi_r(\mathbf{x})$, $\mathbf{x} \in \mathbb{R}^3$, where χ_r is the characteristic function of the ball of radius r centered at 0. Notice that $V_r \in L^{\frac{5}{2}}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ with

$$\inf\{\|W\|_\infty : V_r - W \in L^{\frac{5}{2}}(\mathbb{R}^3)\} = 0.$$

Let $\mathcal{E}^{\mathrm{OTF}}_r$ be the TF-functional $\mathcal{E}^{\mathrm{TF}}_{V_r}$ corresponding to the potential V_r defined in (66). Let ρ^{OTF}_r be the unique minimizer of $\mathcal{E}^{\mathrm{OTF}}_r$ under the condition

$$\int_{\mathbb{R}^3} \rho(\mathbf{x}) d\mathbf{x} \leq \int_{|\mathbf{y}| \geq r} \rho^{\mathrm{HF}}(\mathbf{y}) d\mathbf{y},$$

(see Theorem 1.9). Then ρ^{OTF}_r is solution to the OTF-equation

$$\tfrac{1}{2}\left(\tfrac{6\pi^2}{q}\right)^{\frac{2}{3}} (\rho^{\mathrm{OTF}}_r)^{\frac{2}{3}} = [\varphi^{\mathrm{OTF}}_r - \mu^{\mathrm{OTF}}_r]_+ \,, \tag{67}$$

where

$$\varphi^{\mathrm{OTF}}_r(\mathbf{x}) = V_r(\mathbf{x}) - \int_{\mathbb{R}^3} \frac{\rho^{\mathrm{OTF}}_r(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|} d\mathbf{y},$$

is the OTF-mean field potential and μ^{OTF}_r is the corresponding chemical potential. From (67) (and $\mu^{\mathrm{OTF}}_r \geq 0$) we see that the support of ρ^{OTF}_r is contained in $\mathbb{R}^3 \setminus B_r(0)$.

In the intermediary zone instead of comparing directly $\Phi^{\mathrm{HF}}_{|\mathbf{x}|}$ and $\Phi^{\mathrm{TF}}_{|\mathbf{x}|}$ we compare first the HF-density with the OTF-density and then the OTF-density with the TF-density. When comparing the TF and OTF there is no difference with the non-relativistic case and for brevity we refer for the proofs to [23].

We start by studying the behavior of the minimizer and mean field potential of the OTF. The proof of the following bounds is in [23, page 557-558] in the case $q = 2$ and it can be directly generalised to the other values of q.

Lemma 4.8 ([23, Lem.12.1]). *For all $\mathbf{y} \in \mathbb{R}^3$ we have*

$$\varphi^{\mathrm{TF}}(\mathbf{y}) \leq 3^4 2^{-1} q^{-2} \pi^2 |\mathbf{y}|^{-4} \text{ and } \rho^{\mathrm{TF}}(\mathbf{y}) \leq 3^5 2^{-1} q^{-2} \pi |\mathbf{y}|^{-6}.$$

Let β_0 be as defined in Theorem 1.12, then for all $|\mathbf{y}| \geq \beta_0 Z^{-\frac{1}{3}}$ we have

$$\varphi^{\mathrm{TF}}(\mathbf{y}) \geq C|\mathbf{y}|^{-4} \text{ and } \rho^{\mathrm{TF}}(\mathbf{y}) \geq C|\mathbf{y}|^{-6}.$$

With r, σ, ε' such that (65) holds and $\sigma r^{\varepsilon'} \leq 1$ we have for all $|\mathbf{y}| \geq r$

$$\rho^{\mathrm{OTF}}_r(\mathbf{y}) \leq C r^{-6} \text{ and } \varphi^{\mathrm{OTF}}_r(\mathbf{y}) \leq |V_r(\mathbf{y})| \leq C r^{-4}.$$

Lemma 4.9 ([23, Lem.12.2]). *With r, σ, ε' such that* (65) *holds for all $|\mathbf{x}| \le r$ we have*

$$\int_{|\mathbf{y}|\ge r} (\rho^{\mathrm{TF}}(\mathbf{y}) - \rho^{\mathrm{HF}}(\mathbf{y}))d\mathbf{y} \le \sigma r^{-3+\varepsilon'}.$$

For $\mathbf{x} \in \mathbb{R}^3$ with $|\mathbf{x}| > r$ we may write

$$\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x}) = \mathcal{A}_1(r,\mathbf{x}) + \mathcal{A}_2(r,\mathbf{x}) + \mathcal{A}_3(r,\mathbf{x}), \tag{68}$$

where

$$\begin{aligned} \mathcal{A}_1(r,\mathbf{x}) &= \varphi^{\mathrm{OTF}}_r(\mathbf{x}) - \varphi^{\mathrm{TF}}(\mathbf{x}), \\ \mathcal{A}_2(r,\mathbf{x}) &= \int_{|\mathbf{y}|>|\mathbf{x}|} \frac{\rho^{\mathrm{OTF}}_r(\mathbf{y}) - \rho^{\mathrm{TF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y} \end{aligned}$$

and

$$\mathcal{A}_3(r,\mathbf{x}) = \int_{r<|\mathbf{y}|<|\mathbf{x}|} \frac{\rho^{\mathrm{OTF}}_r(\mathbf{y}) - \rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y}.$$

4.3.1 Estimate on $\mathcal{A}_1$ and $\mathcal{A}_2$

Lemma 4.10 ([23, Lem.12.4]). *Let $N \ge Z$. Given $\varepsilon', \sigma > 0$ there exists a constant $D > 0$ such that for all r with $\beta_0 Z^{-\frac{1}{3}} \le r \le D$ for which* (65) *holds for all $|\mathbf{x}| \le r$, then $\mu^{\mathrm{OTF}}_r = 0$ and*

$$\tfrac{3^4\pi^2}{2q^2}|\mathbf{x}|^{-4}(1 + ar^{\zeta}|\mathbf{x}|^{-\zeta})^{-2} \le \varphi^{\mathrm{OTF}}_r(\mathbf{x}) \le \tfrac{3^4\pi^2}{2q^2}|\mathbf{x}|^{-4}(1 + Ar^{\zeta}|\mathbf{x}|^{-\zeta}) \quad \textit{for } |\mathbf{x}| > r,$$

where a, A are universal constants and $\zeta = (-7+\sqrt{73})/2$.

Lemma 4.11 ([23, Lem.12.5]). *Let $N \ge Z$. Given $\varepsilon', \sigma > 0$ there exists a constant $D > 0$ depending only on ε', σ such that for all r with $\beta_0 Z^{-\frac{1}{3}} \le r \le D$ for which* (65) *holds for $|\mathbf{x}| \le r$, then for all $|\mathbf{x}| \ge r$*

$$|\mathcal{A}_1(r,\mathbf{x})| \le C|\mathbf{x}|^{-4-\zeta} r^{\zeta} \quad \textit{and} \quad |\mathcal{A}_2(r,\mathbf{x})| \le C|\mathbf{x}|^{-4-\zeta} r^{\zeta},$$

with $\zeta = (-7+\sqrt{73})/2$ and C a universal constant.

The proof of the previous lemmas is in [23, p. 558-564].

4.3.2 Estimate on $\|\chi^+_r \rho^{\mathrm{HF}} - \rho^{\mathrm{OTF}}_r\|_C$

Lemma 4.12. *Let G_α be the function defined in Theorem 2.3 and $\rho^{\mathrm{HF}}_r(\mathbf{x})$ be the one-particle density of the density matrix γ^{HF}_r defined in* (61). *Let $Z\alpha = \kappa$ fixed, $0 \le \kappa < 2/\pi$ and $Z \ge 1$.*

Given constants $\varepsilon', \sigma > 0$ there exists $D < \frac{4}{5}$ such that for all r with $\beta_0 Z^{-\frac{1}{3}} \le r \le D$ for which (65) *holds for $|\mathbf{x}| \le r$, it follows that*

$$\alpha^{-1}\int_{\mathbb{R}^3} G_\alpha(\rho^{\mathrm{HF}}_r(\mathbf{x}))\, d\mathbf{x} \le \alpha^{-1}\,\mathrm{Tr}[T(\mathbf{p})\gamma^{\mathrm{HF}}_r] \le 2\mathcal{R} + Cr^{-7} + Cr^{-4}\int_{\mathbb{R}^3} \rho^{\mathrm{HF}}_r(\mathbf{x})\, d\mathbf{x},$$

with C a universal positive constant and $\mathcal{R}$ as defined in Theorem 4.7.

Proof. The first inequality follows directly from Theorem 2.3. To prove the second inequality we proceed as in Lemma 3.1. In this case we are interested only in the exterior part of the minimizer. Hence, instead of considering the HF-energy functional we consider the auxiliary functional $\mathcal{E}^A$, defined in (62), applied to the "exterior part of the minimizer" γ_r^{HF}.

Splitting the kinetic energy in two terms we find

$$\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) \geq \tfrac{1}{2}\alpha^{-1}\operatorname{Tr}[T(\mathbf{p})\gamma_r^{\mathrm{HF}}] + D(\rho_r^{\mathrm{HF}}) + \tfrac{1}{2}\operatorname{Tr}[(\alpha^{-1}T(\mathbf{p}) - 2\Phi_r^{\mathrm{HF}})\gamma_r^{\mathrm{HF}}]. \tag{69}$$

Since $\Phi_r^{\mathrm{HF}}(\mathbf{x})$ is harmonic for $|\mathbf{x}| > r$ and going to zero at infinity

$$\Phi_r^{\mathrm{HF}}(\mathbf{x}) \leq \frac{r}{|\mathbf{x}|}\sup_{|\mathbf{y}|=r}\Phi_r^{\mathrm{HF}}(\mathbf{y}) \quad \text{for } |\mathbf{x}| > r.$$

Hence, since $\operatorname{supp}(\rho_r^{\mathrm{HF}}) \subset \mathbb{R}^3 \setminus B_r(0)$ we find

$$\operatorname{Tr}[(\alpha^{-1}T(\mathbf{p}) - 2\Phi_r^{\mathrm{HF}})\gamma_r^{\mathrm{HF}}] \geq \operatorname{Tr}[(\alpha^{-1}T(\mathbf{p}) - \frac{2r}{|\cdot|}\sup_{|\mathbf{y}|=r}\Phi_r^{\mathrm{HF}}(\mathbf{y}))\gamma_r^{\mathrm{HF}}] = \dots.$$

Adding and subtracting $2D(\rho, \rho_r^{\mathrm{HF}})$ for $\rho \in L^1(\mathbb{R}^3) \cap L^{\frac{5}{3}}(\mathbb{R}^3)$, $\rho \geq 0$, to be chosen

$$\dots \;=\; \operatorname{Tr}[(\alpha^{-1}T(\mathbf{p}) - V_\rho)\gamma_r^{\mathrm{HF}}] - \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\rho_r^{\mathrm{HF}}(\mathbf{x})\rho(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{x}d\mathbf{y}. \tag{70}$$

where for simplicity of notation here and in the following V_ρ is defined as $V_\rho(\mathbf{x}) := \frac{2r}{|\mathbf{x}|}\sup_{|\mathbf{y}|=r}\Phi_r^{\mathrm{HF}}(\mathbf{y}) - \rho * \frac{1}{|\mathbf{x}|}$.

From (70), (69) and the definition of the Coulomb norm and scalar product (Definition 2.7) we find

$$\begin{aligned}
\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) \;&\geq\; \tfrac{1}{2}\alpha^{-1}\operatorname{Tr}[T(\mathbf{p})\gamma_r^{\mathrm{HF}}] + \tfrac{1}{2}D(\rho_r^{\mathrm{HF}}) + \tfrac{1}{2}\|\rho_r^{\mathrm{HF}} - \rho\|_C^2 \\
&\quad -\tfrac{1}{2}D(\rho) + \tfrac{1}{2}\operatorname{Tr}[(\alpha^{-1}T(\mathbf{p}) - V_\rho)\gamma_r^{\mathrm{HF}}] \\
&\geq\; \tfrac{1}{2}\alpha^{-1}\operatorname{Tr}[T(\mathbf{p})\gamma_r^{\mathrm{HF}}] + \tfrac{1}{2}\sum_{i=1}^{N}(\theta_r u_i, (\alpha^{-1}T(\mathbf{p}) - V_\rho)\theta_r u_i) - \tfrac{1}{2}D(\rho),
\end{aligned} \tag{71}$$

denoting by u_i the HF-orbitals.

We now choose ρ as the minimizer of the TF-energy functional of a neutral atom with Coulomb potential and nuclear charge $2r\sup_{|\mathbf{y}|=r}\Phi_r^{\mathrm{HF}}(\mathbf{y})$. Then V_ρ is the corresponding TF-mean field potential and we see that the last two terms on the right hand side of (71) are like the ones in the claim of Proposition B.2. The only difference is due to the presence of the localization function θ_r. We now prove that these terms give the TF-energy modulo lower order terms. The method is the same as that of Proposition B.2. We repeat the main steps since in this case the scaling depends on r. Notice that since $r > \beta_0 Z^{-\frac{1}{3}}$ the contribution is coming only from the "outer zone".

Let $g \in C_0^\infty(\mathbb{R}^3)$ be spherically symmetric, normalized in $L^2(\mathbb{R}^3)$ and with support in $B_1(0)$. Let us define $g_r(\mathbf{x}) := r^{-3}g(\mathbf{x}r^{-2})$ and $\psi_r := g_r^2$. Since V_ρ is subharmonic on $|\mathbf{x}| > 0$, we see from the support properties of ψ_r and θ_r that

$$\sum_{i=1}^{N}(\theta_r u_i, (\alpha^{-1}T(\mathbf{p}) - V_\rho)\theta_r u_i) \geq \sum_{i=1}^{N}(\theta_r u_i, (\alpha^{-1}T(\mathbf{p}) - V_\rho * \psi_r)\theta_r u_i) = \dots.$$

For $\mathbf{p}, \mathbf{q} \in \mathbb{R}^3$ we define the coherent states $g_r^{\mathbf{p},\mathbf{q}}(\mathbf{x}) := g_r(\mathbf{x}-\mathbf{q})e^{i\mathbf{p}\cdot\mathbf{x}}$. By the formulas (B16) and (B17) with $L_{\mathbf{q}}$ the operator defined in the equation below (B17) we get

$$\begin{aligned} \ldots \quad = \quad & \tfrac{1}{(2\pi)^3}\alpha^{-1}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} d\mathbf{p}d\mathbf{q}\,(T(\mathbf{p})-\alpha V_\rho(\mathbf{q}))\sum_{i=1}^N\sum_{j=1}^q |(\theta_r u_i^j, g_r^{\mathbf{p},\mathbf{q}})|^2 \\ & -\alpha^{-1}\sum_{i=1}^N\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} d\mathbf{x}d\mathbf{q}\,\overline{(\theta_r u_i)}(\mathbf{x})(L_{\mathbf{q}}\theta_r u_i)(\mathbf{x})\,, \end{aligned} \tag{72}$$

where u_i^j denotes the j-th spin component of the orbital u_i. By the choice of the function g_r and with the same arguments that led to (B19) in the appendix we find

$$\begin{aligned} & \alpha^{-1}\sum_{i=1}^N\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} d\mathbf{x}d\mathbf{q}\,\overline{(\theta_r u_i)}(\mathbf{x})(L_{\mathbf{q}}\theta_r u_i)(\mathbf{x}) \\ \leq \quad & 3\sum_{i=1}^N \|\theta_r u_i\|_2^2\|\nabla g_r\|_\infty^2 Vol(\mathrm{supp}(g_r)) \leq Cr^{-4}\|\rho_r^{\mathrm{HF}}\|_1. \end{aligned} \tag{73}$$

In the first term on the right hand side of (72) the integrand is zero if $|\mathbf{q}| < \frac{1}{4}r^2$ since in this case $\mathrm{supp}(\theta_r)\cap\mathrm{supp}(g_r^{\mathbf{q},\mathbf{p}}) = \emptyset$ (by the choice $D < 4/5$). To estimate it further from below we consider only the negative part of the integrand

$$\begin{aligned} & \tfrac{1}{(2\pi)^3}\alpha^{-1}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} d\mathbf{p}d\mathbf{q}\,(T(\mathbf{p})-\alpha V_\rho(\mathbf{q}))\sum_{i=1}^N\sum_{j=1}^q |(\theta_r u_i^j, g_r^{\mathbf{p},\mathbf{q}})|^2 \\ \geq \quad & \tfrac{q}{(2\pi)^3}\alpha^{-1}\iint_{\substack{|\mathbf{q}|>\frac{1}{4}r^2 \\ T(\mathbf{p})\leq\alpha V_\rho(\mathbf{q})}} d\mathbf{p}d\mathbf{q}\,(T(\mathbf{p})-\alpha V_\rho(\mathbf{q}))\,, \end{aligned} \tag{74}$$

where we have used that $0 \leq \sum_{i=1}^N |(\theta_r u_i^j, g_r^{\mathbf{p},\mathbf{q}})|^2 \leq 1$ (Bessel's inequality). We split the domain of integration in $\mathbf{p}$ as follows

$$\{\mathbf{p}\in\mathbb{R}^3 : T(\mathbf{p}) \leq \alpha V_\rho(\mathbf{q})\} = \Sigma_1 \cup \Sigma_2$$

with Σ_1, Σ_2 disjoint and $\Sigma_1 = \{\mathbf{p}\in\mathbb{R}^3 : \frac{1}{2}|\mathbf{p}|^2 \leq V_\rho(\mathbf{q})\}$. We treat these two contributions separately. We have

$$\alpha^{-1}\iint_{\substack{|\mathbf{q}|>\frac{1}{4}r^2 \\ \mathbf{p}\in\Sigma_2}} d\mathbf{p}d\mathbf{q}\,(T(\mathbf{p})-\alpha V_\rho(\mathbf{q})) \geq -\iint_{\substack{|\mathbf{q}|>\frac{1}{4}r^2 \\ \mathbf{p}\in\Sigma_2}} d\mathbf{p}d\mathbf{q}\,[V_\rho(\mathbf{q})]_+ = \ldots$$

and computing the integral, using that $(1+x)^{\frac{3}{2}} \leq 1+\frac{3}{2}x+\frac{3}{8}x^2$

$$\cdots \geq -C\int_{|\mathbf{q}|>\frac{1}{4}r^2} d\mathbf{q}\,(\alpha^2[V_\rho(\mathbf{q})]_+^{\frac{7}{2}} + \alpha^4[V_\rho(\mathbf{q})]_+^{\frac{9}{2}}) \geq -C\alpha^2 r^{-\frac{23}{2}} - C\alpha^4 r^{-\frac{33}{2}}. \tag{75}$$

In the last step we used that $[V_\rho(\mathbf{q})]_+ \leq 2\frac{r}{|\mathbf{q}|}\sup_{|\mathbf{x}|=r}\Phi_r^{\mathrm{HF}}(\mathbf{x})$ and that by the hypothesis and Corollary 1.14

$$r\sup_{|\mathbf{x}|=r}\Phi_r^{\mathrm{HF}}(\mathbf{x}) \leq Cr^{-3}, \tag{76}$$

choosing D such that $\sigma r^{\varepsilon'} \leq 1$.

Since $T(\mathbf{p}) \geq \frac{1}{2}\alpha|\mathbf{p}|^2 - \frac{1}{8}\alpha^3|\mathbf{p}|^4$ we find

$$\begin{aligned}
&\alpha^{-1}\iint_{\substack{|\mathbf{q}|>\frac{1}{4}r^2\\ \mathbf{p}\in\Sigma_1}} d\mathbf{p}d\mathbf{q}\,(T(\mathbf{p})-\alpha V_\rho(\mathbf{q}))\\
&\geq \iint_{\substack{|\mathbf{q}|>\frac{1}{4}r^2\\ \frac{1}{2}|\mathbf{p}|^2\leq V_\rho(\mathbf{q})}} d\mathbf{p}d\mathbf{q}\,(\frac{1}{2}|\mathbf{p}|^2 - V_\rho(\mathbf{q})) - \tfrac{1}{8}\alpha^2\iint_{\substack{|\mathbf{q}|>\frac{1}{4}r^2\\ \frac{1}{2}|\mathbf{p}|^2\leq V_\rho(\mathbf{q})}} d\mathbf{p}d\mathbf{q}\,|\mathbf{p}|^4. \qquad (77)
\end{aligned}$$

Computing the last integral we find

$$\alpha^2\iint_{\substack{|\mathbf{q}|>\frac{1}{4}r^2\\ \frac{1}{2}|\mathbf{p}|^2\leq V_\rho(\mathbf{q})}} d\mathbf{p}d\mathbf{q}\,|\mathbf{p}|^4 \leq C\alpha^2 r^{-1}(2r\sup_{|\mathbf{x}|=r}\Phi_r^{\mathrm{HF}}(\mathbf{x}))^{\frac{7}{2}} \leq C\alpha^2 r^{-\frac{23}{2}}. \qquad (78)$$

While for the first term on the right hand side of (77), computing the integral with respect to $\mathbf{p}$, we get

$$\iint_{\substack{|\mathbf{q}|>\frac{1}{4}r^2\\ \frac{1}{2}|\mathbf{p}|^2\leq V_\rho(\mathbf{q})}} d\mathbf{p}d\mathbf{q}\,(\tfrac{1}{2}|\mathbf{p}|^2 - V_\rho(\mathbf{q})) = -4\pi\frac{2^{\frac{5}{2}}}{15}\int_{|\mathbf{q}|>\frac{1}{4}r^2} d\mathbf{q}\,[V_\rho(\mathbf{q})]_+^{\frac{5}{2}}.$$

Hence collecting together (72), (73), (74) (75), (78) and the inequality above we find

$$\mathrm{Tr}[(\alpha^{-1}T(\mathbf{p}) - V_\rho)\gamma_r^{\mathrm{HF}}] \geq -\frac{2^{\frac{3}{2}}q}{15\pi^2}\int_{\mathbb{R}^3} d\mathbf{x}\,[V_\rho(\mathbf{x})]_+^{\frac{5}{2}} - Cr^{-4}\|\rho_r^{\mathrm{HF}}\|_1 - Cr^{-\frac{11}{2}} = \ldots.$$

since $\beta_0 Z^{-\frac{1}{3}} \leq r$ implies $\beta_0\alpha^{\frac{1}{3}} \leq \kappa^{\frac{1}{3}}r$. From the TF-equation that ρ satisfies it follows that

$$\begin{aligned}
\ldots &= \tfrac{3}{10}(\tfrac{6\pi^2}{q})^{\frac{2}{3}}\int_{\mathbb{R}^3} d\mathbf{x}\,\rho(\mathbf{x})^{\frac{5}{3}} - \int_{\mathbb{R}^3}\rho(\mathbf{x})V_\rho(\mathbf{x})\,d\mathbf{x} - Cr^{-4}\|\rho_r^{\mathrm{HF}}\|_1 - Cr^{-\frac{11}{2}}\\
&= \mathcal{E}^{\mathrm{TF}}(\rho) + D(\rho) - Cr^{-4}\|\rho_r^{\mathrm{HF}}\|_1 - Cr^{-\frac{11}{2}}.
\end{aligned}$$

Hence from (71) and the inequality above we get using (12) and (76)

$$\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) \geq \tfrac{1}{2}\alpha^{-1}\,\mathrm{Tr}[T(\mathbf{p})\gamma^{\mathrm{HF}}] - Cr^{-7} - Cr^{-4}\|\rho_r^{\mathrm{HF}}\|_1.$$

The claim follows since $\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) \leq \mathcal{R}$ by the result of Theorem 4.7 considering as a trial density matrix $\gamma \equiv 0$. $\square$

Lemma 4.13. *Let $N' \in \mathbb{N}$ and $Z\alpha = \kappa$ be fixed, $0 \leq \kappa < 2/\pi$ and $Z \geq 1$. Let e_j be the first N' negative eigenvalues of the operator $\alpha^{-1}T(\mathbf{p}) - \varphi_r^{\mathrm{OTF}}$ acting on functions with support on $\{\mathbf{x} \in \mathbb{R}^3 : |\mathbf{x}| \geq r\}$.*

Given constants $\varepsilon', \sigma > 0$ there exists $D < 4/5$ such that for all r with $\beta_0 Z^{-\frac{1}{3}} \leq r \leq D$ for which (65) holds for $|\mathbf{x}| \leq r$, for all $\mu \in (0,1)$ and $s < r$ we have

$$\begin{aligned}
\sum_{j=1}^{N'} e_j &\geq -(\tfrac{2}{1-\mu})^{\frac{3}{2}}\tfrac{1}{15\pi^2}\int_{|\mathbf{q}|>r}[\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+^{\frac{5}{2}}\,d\mathbf{q} - Cr^{-8}s\mu^{-\frac{3}{2}} - C\mu^{-3}r^{-5}s\\
&\quad - C(1-\mu)^{-\frac{7}{2}}r^{-5} - C(1-\mu)s^{-2}N',
\end{aligned}$$

with C a positive constant.

Proof. Let f_j be the eigenfunctions (normalized in $L^2(\mathbb{R}^3, \mathbb{C}^q)$) corresponding to the eigenvalues e_j, $j = 1, .., N'$. Let $g \in C_0^\infty(\mathbb{R}^3)$ with support in $B_1(0)$ and define $g_s(\mathbf{x}) = s^{-\frac{3}{2}} g(\mathbf{x}/s)$ for a positive parameter s, $s < r$. We then write for $\mu \in (0,1)$

$$\sum_{j=1}^{N'} e_j = \sum_{j=1}^{N'} (f_j, (\alpha^{-1} T(\mathbf{p}) - \varphi_r^{\mathrm{OTF}}) f_j) = \mathcal{B}_1 + \mathcal{B}_2,$$

where

$$\begin{aligned} \mathcal{B}_1 &= \sum_{j=1}^{N'} (f_j, ((1-\mu)\alpha^{-1} T(\mathbf{p}) - \varphi_r^{\mathrm{OTF}} * g_s^2) f_j), \\ \mathcal{B}_2 &= \sum_{j=1}^{N'} (f_j, (\mu\alpha^{-1} T(\mathbf{p}) - \varphi_r^{\mathrm{OTF}} + \varphi_r^{\mathrm{OTF}} * g_s^2) f_j). \end{aligned}$$

We estimate these two terms separately. Considering for $\mathbf{p}, \mathbf{q} \in \mathbb{R}^3$ the coherent states $g_s^{\mathbf{p},\mathbf{q}}(\mathbf{x}) := e^{i\mathbf{p}.\mathbf{x}} g_s(\mathbf{x} - \mathbf{q})$ using (B16) and (B17), we find

$$\begin{aligned} \mathcal{B}_1 &= \tfrac{1}{(2\pi)^3} \iint ((1-\mu)\alpha^{-1} T(\mathbf{p}) - \varphi_r^{\mathrm{OTF}}(\mathbf{q})) \sum_{j=1}^{N} |(f_j, g_s^{\mathbf{p},\mathbf{q}})|^2 \, d\mathbf{q} d\mathbf{p} \\ &\quad - (1-\mu)\alpha^{-1} \sum_{j=1}^{N'} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} d\mathbf{x} d\mathbf{q} \overline{f_j(\mathbf{x})} (L_{\mathbf{q}} f_j)(\mathbf{x}) \,. \end{aligned} \tag{79}$$

Estimating the error term as done in (B32) and previous inequalities we get

$$(1-\mu)\alpha^{-1} \sum_{j=1}^{N'} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} d\mathbf{x} d\mathbf{q} \overline{f_j(\mathbf{x})} (L_{\mathbf{q}} f_j)(\mathbf{x}) \leq C(1-\mu) s^{-2} N'.$$

Since we are interested in an estimate from below and $\varphi_r^{\mathrm{OTF}}(\mathbf{q}) \leq 0$ for $|\mathbf{q}| < r$, from (79) we find

$$\begin{aligned} \mathcal{B}_1 &\geq \tfrac{1}{(2\pi)^3} \iint_{|\mathbf{q}|>r} ((1-\mu)\alpha^{-1} T(\mathbf{p}) - \varphi_r^{\mathrm{OTF}}(\mathbf{q})) \sum_{j=1}^{N} |(f_j, g_s^{\mathbf{p},\mathbf{q}})|^2 \, d\mathbf{q} d\mathbf{p} \\ &\quad - C(1-\mu) s^{-2} N'. \end{aligned} \tag{80}$$

We estimate now the first term on the right hand side of (80). Considering only the negative part of the integrand and since $\sum_{j=1}^{N'} |(f_j, g_s^{\mathbf{p},\mathbf{q}})|^2 \leq 1$ we get

$$\begin{aligned} &\tfrac{1}{(2\pi)^3} \iint_{|\mathbf{q}|>r} ((1-\mu)\alpha^{-1} T(\mathbf{p}) - \varphi_r^{\mathrm{OTF}}(\mathbf{q})) \sum_{j=1}^{N'} |(f_j, g_s^{\mathbf{p},\mathbf{q}})| \, d\mathbf{q} d\mathbf{p} \\ \geq\ &\tfrac{1}{(2\pi)^3} \iint_{\substack{|\mathbf{q}|>r, \\ (1-\mu)\alpha^{-1} T(\mathbf{p}) \leq \varphi_r^{\mathrm{OTF}}(\mathbf{q})}} ((1-\mu)\alpha^{-1} T(\mathbf{p}) - \varphi_r^{\mathrm{OTF}}(\mathbf{q})) \, d\mathbf{p} d\mathbf{q}. \end{aligned}$$

Now we split the domain of integration in $\mathbf{p}$ as follows

$$\{\mathbf{p} \in \mathbb{R}^3 : \alpha^{-1}(1-\mu) T(\mathbf{p}) \leq \varphi_r^{\mathrm{OTF}}(\mathbf{q})\} = \Sigma_1 \cup \Sigma_2,$$

with Σ_1, Σ_2 disjoint and $\Sigma_1 = \{\mathbf{p} \in \mathbb{R}^3 : (1-\mu)|\mathbf{p}|^2/2 \leq \varphi_r^{\mathrm{OTF}}(\mathbf{q})\}$. We treat these two contributions separately. Then

$$\begin{aligned} &\tfrac{1}{(2\pi)^3} \iint_{\substack{|\mathbf{q}|>r,\\ \mathbf{p}\in\Sigma_2}} ((1-\mu)\alpha^{-1}T(\mathbf{p}) - \varphi_r^{\mathrm{OTF}}(\mathbf{q}))d\mathbf{p}d\mathbf{q} \\ \geq\ & -\tfrac{1}{(2\pi)^3} \iint_{\substack{|\mathbf{q}|>r,\\ \mathbf{p}\in\Sigma_2}} [\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+ d\mathbf{p}d\mathbf{q} = \dots \end{aligned}$$

and since in the domain of integration

$$\tfrac{2}{1-\mu}[\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+ \leq |\mathbf{p}|^2 \leq \tfrac{2}{1-\mu}[\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+(1 + \tfrac{1}{2(1-\mu)}\alpha^2[\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+)$$

we get

$$\begin{aligned} \dots\ &\geq\ -\tfrac{C}{(1-\mu)^{\frac{5}{2}}}\alpha^2 \int_{|\mathbf{q}|>r} d\mathbf{q}\ ([\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+^{\frac{7}{2}} + \tfrac{\alpha^2}{8(1-\mu)}[\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+^{\frac{9}{2}}) \\ &\geq\ -\tfrac{C}{(1-\mu)^{\frac{5}{2}}}\alpha^2(r^{-11} + \tfrac{\alpha^2}{1-\mu}r^{-15}), \end{aligned} \tag{81}$$

using Lemma 4.10 in the last step.

Since $\sqrt{1+t^2} \geq 1 + (1/2)t^2 - (1/8)t^4$, we get

$$\begin{aligned} &\tfrac{1}{(2\pi)^3} \iint_{\substack{|\mathbf{q}|>r,\\ \mathbf{p}\in\Sigma_1}} ((1-\mu)\alpha^{-1}T(\mathbf{p}) - \varphi_r^{\mathrm{OTF}}(\mathbf{q}))d\mathbf{p}d\mathbf{q} \\ \geq\ & \tfrac{1}{(2\pi)^3} \iint_{\substack{|\mathbf{q}|>r,\\ \mathbf{p}\in\Sigma_1}} ((1-\mu)\tfrac{1}{2}|\mathbf{p}|^2 - \varphi_r^{\mathrm{OTF}}(\mathbf{q}) - \tfrac{1}{8}(1-\mu)\alpha^2|\mathbf{p}|^4)d\mathbf{p}d\mathbf{q}. \end{aligned}$$

The last term gives by Lemma 4.10

$$\alpha^2 \iint_{\substack{|\mathbf{q}|>r\\ \mathbf{p}\in\Sigma_1}} d\mathbf{p}d\mathbf{q}\ |\mathbf{p}|^4 = \alpha^2\tfrac{4\pi}{7} \int_{|\mathbf{q}|>r} d\mathbf{q}\ (\tfrac{2}{1-\mu})^{\frac{7}{2}}[\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+^{\frac{7}{2}} \leq C\alpha^2(\tfrac{2}{1-\mu})^{\frac{7}{2}}r^{-11}. \tag{82}$$

While for the other terms computing the integral with respect to $\mathbf{p}$, we get

$$\tfrac{1}{(2\pi)^3} \iint_{\substack{|\mathbf{q}|>r,\\ \mathbf{p}\in\Sigma_1}} ((1-\mu)\tfrac{1}{2}|\mathbf{p}|^2 - \varphi_r^{\mathrm{OTF}}(\mathbf{q}))d\mathbf{p}d\mathbf{q} = -(\tfrac{2}{1-\mu})^{\frac{3}{2}}\tfrac{1}{15\pi^2} \int_{|\mathbf{q}|>r} d\mathbf{q}\ [\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+^{\frac{5}{2}}. \tag{83}$$

For the term $\mathcal{B}_2$ using Theorem 2.5 and Remark 2.6 we find

$$\mathcal{B}_2 \geq -Cq(\mu^{-\frac{3}{2}}\|[\varphi_r^{\mathrm{OTF}} - \varphi_r^{\mathrm{OTF}} * g_s^2]_+\|_{\frac{5}{2}}^{\frac{5}{2}} + \alpha^3\mu^{-3}\|[\varphi_r^{\mathrm{OTF}} - \varphi_r^{\mathrm{OTF}} * g_s^2]_+\|_4^4).$$

From the choice of g_s it follows that $\varphi_r^{\mathrm{OTF}} - \varphi_r^{\mathrm{OTF}} * g_s^2 \leq V_r - V_r * g_s^2$ and the term $V_r - V_r * g_s^2$ is non-zero only for $r - s \leq |\mathbf{x}| \leq r + s$. Hence by Lemma 4.8 and since $s < r$

$$\|[\varphi_r^{\mathrm{OTF}} - \varphi_r^{\mathrm{OTF}} * g_s^2]_+\|_{\frac{5}{2}}^{\frac{5}{2}} \leq \int_{r-s\leq|\mathbf{x}|\leq r+s} [V_r(\mathbf{x}) - V_r * g^2(\mathbf{x})]_+^{\frac{5}{2}} d\mathbf{x} \leq Cr^{-8}s, \tag{84}$$

and similarly $\|[\varphi_r^{\mathrm{OTF}} - \varphi_r^{\mathrm{OTF}} * g_s^2]_+\|_4^4 \leq Cr^{-14}s$. The claim follows from (80), (81), (82), (83) and (84) using that $\beta_0\alpha^{\frac{1}{3}} \leq \kappa^{\frac{1}{3}}r$. $\square$

Lemma 4.14. *Let G_α be the function defined in Theorem 2.3 and $\rho_r^{\mathrm{HF}}(\mathbf{x})$ the one-particle density of the density matrix γ_r^{HF} defined in (61). Let $Z\alpha = \kappa$ be fixed, $0 \le \kappa < 2/\pi$ and $Z \ge 1$.*

There exists $\alpha_0 > 0$ such that given $\varepsilon', \sigma > 0$ there exists $D < 1/4$ such that for all $\alpha \le \alpha_0$ and r with $\beta_0 Z^{-\frac{1}{3}} \le r \le D$ for which (65) holds for $|\mathbf{x}| \le r$, we have

$$\begin{aligned} &\|\chi_r^+ \rho^{\mathrm{HF}} - \rho_r^{\mathrm{OTF}}\|_C \le C r^{-\frac{7}{2}+\frac{1}{6}} \qquad \text{and} \\ &\alpha^{-1}\int_{\mathbb{R}^3} G_\alpha(\chi_r^+ \rho^{\mathrm{HF}}(\mathbf{x}))d\mathbf{x} \le C r^{-7}, \quad \alpha^{-1}\,\mathrm{Tr}[T(\mathbf{p})\gamma_r^{\mathrm{HF}}] \le C r^{-7}, \end{aligned} \tag{85}$$

with C a universal positive constant.

Proof. The idea of the proof is the same as that of Lemma 3.1. In this case we are interested only in the exterior part of the minimizer. Hence, instead of considering the HF-energy functional we estimate from above and below the auxiliary one $\mathcal{E}^A$, defined in (62), applied on the "exterior part of the minimizer" γ_r^{HF}.

Step I. Estimate from above on $\mathcal{E}^A(\gamma_r^{\mathrm{HF}})$. Let us consider γ the density matrix that acts identically on the spin components and on each as

$$\gamma^j = \tfrac{1}{(2\pi)^3}\iint_{\frac{1}{2}|\mathbf{p}|^2 \le \varphi_r^{\mathrm{OTF}}(\mathbf{q})} \Pi_{\mathbf{p},\mathbf{q}}\, d\mathbf{p}d\mathbf{q},$$

where $j \in \{1,\dots,q\}$ is the spin index, $\Pi_{\mathbf{p},\mathbf{q}}$ is the projection onto the space spanned by $h_s^{\mathbf{p},\mathbf{q}}(\mathbf{x}) = h_s(\mathbf{x}-\mathbf{q})e^{i\mathbf{p}.\mathbf{x}}$ where h_s is the ground state for the Dirichlet Laplacian on the ball of radius s for $0 < s < r$. By the OTF-equation (67) and since $\mu_r^{\mathrm{OTF}} = 0$ (see Lemma 4.10) we see that $\rho_\gamma(\mathbf{x}) = \rho_r^{\mathrm{OTF}} * |h_s|^2(\mathbf{x})$. Moreover, by Lemma 4.10

$$\mathrm{Tr}[-\tfrac{1}{2}\Delta\gamma] = \tfrac{3}{10}(\tfrac{6\pi^2}{q})^{\frac{2}{3}}\int_{\mathbb{R}^3}(\rho_r^{\mathrm{OTF}}(\mathbf{x}))^{\frac{5}{3}}\,d\mathbf{x} + Cs^{-2}r^{-3}. \tag{86}$$

Since $[\Phi_r^{\mathrm{HF}}]_+ \in L^{\frac{5}{2}}_{loc}(\mathbb{R}^3)$, by [23, Lemma 8.5] for $\lambda' \in (0,1)$ we may find $\tilde\gamma$ such that $\mathrm{supp}(\rho_{\tilde\gamma}) \subset \{\mathbf{x} : |\mathbf{x}| \ge r\}$, $\rho_{\tilde\gamma}(\mathbf{x}) \le \rho_\gamma(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^3$ and

$$\begin{aligned} \mathrm{Tr}[(-\tfrac{1}{2}\Delta - \Phi_r^{\mathrm{HF}})\tilde\gamma] \;&\le\; \mathrm{Tr}[(-\tfrac{1}{2}\Delta - \chi_r^+\Phi_r^{\mathrm{HF}})\gamma] + L_1\int_{|\mathbf{x}|\le\frac{r}{1-\lambda'}}[V_r(\mathbf{x})]_+^{\frac{5}{2}}\,d\mathbf{x} \\ &\quad + \tfrac{1}{2}(\tfrac{\pi}{2\lambda' r})^2\int_{|\mathbf{x}|\le\frac{r}{1-\lambda'}}\rho_\gamma(\mathbf{x})\,d\mathbf{x}. \end{aligned} \tag{87}$$

Since $\int\rho_{\tilde\gamma} \le \int\rho_\gamma = \int\rho_r^{\mathrm{OTF}} \le \int\chi_r^+\rho^{\mathrm{HF}}$ we may choose $\tilde\gamma$ as a trial density matrix in Theorem 4.7 and we find for λ, ν to be chosen

$$\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) \le \mathcal{E}^A(\tilde\gamma) + \mathcal{R} \le \mathrm{Tr}[(-\tfrac{1}{2}\Delta - \Phi_r^{\mathrm{HF}})\tilde\gamma] + \mathcal{R} + D(\rho_{\tilde\gamma}),$$

since $\alpha^{-1}T(\mathbf{p}) \le \frac{1}{2}|\mathbf{p}|^2$. Notice that $\mathcal{R}$ depends on λ and ν. From (87) it follows that

$$\begin{aligned} \mathcal{E}^A(\gamma_r^{\mathrm{HF}}) \;&\le\; \mathrm{Tr}[(-\tfrac{1}{2}\Delta - \chi_r^+\Phi_r^{\mathrm{HF}})\gamma] + L_1\int_{|\mathbf{x}|\le\frac{r}{1-\lambda'}}[V_r(\mathbf{x})]_+^{\frac{5}{2}}\,d\mathbf{x} \\ &\quad + \tfrac{1}{2}(\tfrac{\pi}{2\lambda' r})^2\int_{|\mathbf{x}|\le\frac{r}{1-\lambda'}}\rho_\gamma(\mathbf{x})\,d\mathbf{x} + \mathcal{R} + D(\rho_{\tilde\gamma}). \end{aligned} \tag{88}$$

From the OTF-equation (67) and Lemma 4.10 we get

$$\int_{|\mathbf{x}|\le\frac{r}{1-\lambda'}}\rho_\gamma(\mathbf{x})\,d\mathbf{x} \le \int_{|\mathbf{x}|\le\frac{2-\lambda'}{1-\lambda'}r}\rho_r^{\mathrm{OTF}}(\mathbf{x})\,d\mathbf{x} \le Cr^{-3}.$$

While since $V_r(\mathbf{y}) \leq Cr^{-4}$ (Lemma 4.8) and is non-zero only for $|\mathbf{y}| > r$

$$\int_{|\mathbf{x}|\leq \frac{r}{1-\lambda'}} [V_r(\mathbf{x})]_+^{\frac{5}{2}} \, d\mathbf{x} \leq Cr^{-7} \tfrac{\lambda'}{(1-\lambda')^3}.$$

Hence, from (86) and (88) and the inequalities above we find choosing $\lambda' = r^{\frac{2}{3}}$

$$\begin{aligned}\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) \quad &\leq \quad \tfrac{3}{10}(\tfrac{6\pi^2}{q})^{\frac{2}{3}} \int_{\mathbb{R}^3} (\rho_r^{\mathrm{OTF}}(\mathbf{x}))^{\frac{5}{3}} \, d\mathbf{x} - \int_{\mathbb{R}^3} V_r(\mathbf{x}) \rho_\gamma(\mathbf{x}) \, d\mathbf{x} + Cs^{-2}r^{-3} \\ &\quad +Cr^{-7+\frac{2}{3}} + \mathcal{R} + D(\rho_{\tilde{\gamma}}) = \ldots .\end{aligned}$$

Here we used that $\lambda' \leq 1/2$ which follows by the bound on D. Since $\rho_{\tilde{\gamma}} \leq \rho_\gamma$, $D(\rho_{\tilde{\gamma}}) \leq D(\rho_\gamma)$. Moreover by Newton's Theorem $D(\rho_\gamma) \leq D(\rho_r^{\mathrm{OTF}})$. Hence we get

$$\begin{aligned}\ldots \quad \leq \quad &\mathcal{E}^{\mathrm{OTF}}(\rho_r^{\mathrm{OTF}}) + \int_{\mathbb{R}^3} V_r(\mathbf{x})(\rho_r^{\mathrm{OTF}}(\mathbf{x}) - \rho_\gamma(\mathbf{x})) \, d\mathbf{x} + Cs^{-2}r^{-3} \\ &+Cr^{-7+\frac{2}{3}} + \mathcal{R}.\end{aligned} \tag{89}$$

We study now the second term on the right hand side of (89). Since $\rho_\gamma = \rho^{\mathrm{OTF}} * |h_s|^2$, rewriting

$$\int_{\mathbb{R}^3} V_r(\mathbf{x})(\rho_r^{\mathrm{OTF}}(\mathbf{x}) - \rho_\gamma(\mathbf{x})) \, d\mathbf{x} = \int_{\mathbb{R}^3} \rho_r^{\mathrm{OTF}}(\mathbf{x})(V_r(\mathbf{x}) - V_r * |h_s|^2(\mathbf{x})) \, d\mathbf{x}.$$

Since $s < r$, V_r is harmonic on $|\mathbf{x}| > r$ and ρ_r^{OTF} vanishes for $|\mathbf{x}| < r$ one sees that the integrand on the right hand side of the equation above is non-zero only for $r < |\mathbf{x}| < r + s$. Hence by Lemma 4.8

$$\int_{\mathbb{R}^3} V_r(\mathbf{x})(\rho_r^{\mathrm{OTF}}(\mathbf{x}) - \rho_\gamma(\mathbf{x})) \, d\mathbf{x} \leq \int_{r<|\mathbf{x}|<r+s} \rho_r^{\mathrm{OTF}}(\mathbf{x}) V_r(\mathbf{x}) \, d\mathbf{x} \leq Cr^{-8}s.$$

Choosing $s = r^{\frac{5}{3}}$ we find from (89) that

$$\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) \leq \mathcal{E}^{\mathrm{OTF}}(\rho_r^{\mathrm{OTF}}) + Cr^{-7+\frac{2}{3}} + \mathcal{R}. \tag{90}$$

It remains to estimate $\mathcal{R}$. From Lemma 4.1, choosing $\lambda, \nu \leq 1/2$ and D such that $\sigma r^{\varepsilon'} \leq 1$ we find

$$(\tfrac{\pi}{2\lambda r} + \tfrac{C}{\lambda^2 r^2}) \int_{|\mathbf{x}|\geq r(1-\lambda)(1-\nu)} \rho^{\mathrm{HF}}(\mathbf{x}) \, d\mathbf{x} \leq Cr^{-5}\lambda^{-2}.$$

By Lemma 4.8, (66) and since $\lambda \leq 1/2$ we get

$$\int_{r(1-\lambda)\leq|\mathbf{x}|\leq\frac{r}{1-\lambda}} (\Phi_{r(1-\lambda)}^{\mathrm{HF}}(\mathbf{x}))^{\frac{5}{2}} \, d\mathbf{x} \leq Cr^{-7}\lambda,$$

and similarly

$$\alpha^3 \int_{r(1-\lambda)\leq|\mathbf{x}|\leq\frac{r}{1-\lambda}} (\Phi_{r(1-\lambda)}^{\mathrm{HF}}(\mathbf{x}))^4 \, d\mathbf{x} \leq Cr^{-4}\lambda,$$

since $r \geq \beta_0 Z^{-\frac{1}{3}}$ implies $\alpha r^{-3} \leq \beta_0^{-3}\kappa$. Hence from the expression of $\mathcal{R}$ and the boundness of $t^p e^{-t}$ for $t > 0$, we find

$$\mathcal{R} \leq \mathcal{E}x(\gamma_r^{\mathrm{HF}}) + Cr^{-5}\lambda^{-2} + Cr^{-7}\lambda. \tag{91}$$

We estimate now the exchange term. By the exchange inequality ([15] or [23, Th.6.4]) and proceeding as in (27) we find by Lemma 4.1 and Lemma 4.12

$$\begin{aligned}\mathcal{E}x(\gamma_r^{\mathrm{HF}}) &\leq C\int_{\mathbb{R}^3} G_\alpha(\rho_r^{\mathrm{HF}}(\mathbf{x}))d\mathbf{x} + Cr^{-\frac{3}{2}}\Big(\alpha^{-1}\int_{\mathbb{R}^3} G_\alpha(\rho_r^{\mathrm{HF}}(\mathbf{x}))d\mathbf{x}\Big)^{\frac{1}{2}}\\ &\leq C\alpha\mathcal{R} + C\alpha r^{-7} + Cr^{-\frac{3}{2}}(\mathcal{R}+r^{-7})^{\frac{1}{2}}.\end{aligned}$$

Hence choosing α_0 such that $1 - C\alpha \geq 1/2$ for all $\alpha \leq \alpha_0$ we get from the inequality above and (91)

$$\tfrac{1}{2}\mathcal{R} \leq Cr^{-\frac{3}{2}}(\mathcal{R}+r^{-7})^{\frac{1}{2}} + Cr^{-5}\lambda^{-2} + Cr^{-7}\lambda\,,$$

that gives

$$\mathcal{R} \leq C(r^{-5}\lambda^{-2} + \lambda r^{-7})\,. \tag{92}$$

The second two inequalities in (85) follow from the estimate above and lemmas 4.1 and 4.12 choosing $\lambda = 1/2$ and replacing r with $r/2$.

Step II. Estimate from below on $\mathcal{E}^A(\gamma_r^{\mathrm{HF}})$. Adding and subtracting $D(\rho_r^{\mathrm{OTF}})$ and $\mathrm{Tr}[\rho_r^{\mathrm{OTF}} * \frac{1}{|\cdot|}\gamma_r^{\mathrm{HF}}]$ we write

$$\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) = \mathrm{Tr}[(\alpha^{-1}T(\mathbf{p}) - \varphi_r^{\mathrm{OTF}})\gamma_r^{\mathrm{HF}}] + \|\rho_r^{\mathrm{OTF}} - \rho_r^{\mathrm{HF}}\|_C^2 - D(\rho_r^{\mathrm{OTF}}), \tag{93}$$

using that $V_r = \Phi_r^{\mathrm{HF}}$ on the support of ρ_r^{HF}. The first term on the right hand side of (93) is estimated from below by the sum of the first N' eigenvalues of the operator $\alpha^{-1}T(\mathbf{p}) - \varphi_r^{\mathrm{OTF}}$ acting on the functions with support on $\{\mathbf{x} : |\mathbf{x}| \geq r\}$. Here N' denotes the smallest integer bigger than $\mathrm{Tr}[\gamma_r^{\mathrm{HF}}]$. Hence by Lemma 4.13 we find for $\mu \in (0,1)$ and $s < r$

$$\begin{aligned}\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) \geq\ & -(\tfrac{2}{1-\mu})^{\frac{3}{2}}\tfrac{q}{15\pi^2}\int_{\mathbb{R}^3}[\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+^{\frac{5}{2}}\,d\mathbf{q} - Cr^{-8}s\mu^{-\frac{3}{2}} - C\mu^{-3}r^{-5}s\\ & -C(1-\mu)^{-\frac{7}{2}}r^{-5} - C(1-\mu)s^{-2}\Big(\int_{\mathbb{R}^3}\rho_r^{\mathrm{HF}}(\mathbf{x})\,d\mathbf{x} + 1\Big)\\ & +\|\rho_r^{\mathrm{OTF}} - \rho_r^{\mathrm{HF}}\|_C^2 - D(\rho_r^{\mathrm{OTF}}) = \ldots,\end{aligned}$$

Notice the factor q due to spin. Choosing D such that $\sigma r^{\varepsilon'} \leq 1$, by lemmas 4.1 and 4.10 we find

$$\int_{\mathbb{R}^3}\rho_r^{\mathrm{HF}}(\mathbf{x})\,d\mathbf{x} \leq Cr^{-3} \text{ and } \int_{\mathbb{R}^3}[\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+^{\frac{5}{2}}\,d\mathbf{q} \leq Cr^{-7}.$$

Hence considering $\mu \leq 1/2$

$$\begin{aligned}\ldots \geq\ & -2^{\frac{3}{2}}\tfrac{q}{15\pi^2}\int_{\mathbb{R}^3}[\varphi_r^{\mathrm{OTF}}(\mathbf{q})]_+^{\frac{5}{2}}\,d\mathbf{q} - Cr^{-7} - Cr^{-8}s\mu^{-\frac{3}{2}} - C\mu^{-3}r^{-5}s\\ & -Cs^{-2}r^{-3} + \|\rho_r^{\mathrm{OTF}} - \rho_r^{\mathrm{HF}}\|_C^2 - D(\rho_r^{\mathrm{OTF}}) = \ldots.\end{aligned}$$

By the OTF-equation (67) and since ρ_r^{OTF} has support where $\varphi_r^{\mathrm{OTF}} \geq 0$ we find

$$\cdots = \mathcal{E}^{\mathrm{OTF}}(\rho_r^{\mathrm{OTF}}) - Cr^{-7+\frac{1}{3}} + \|\rho_r^{\mathrm{OTF}} - \rho_r^{\mathrm{HF}}\|_C^2,$$

choosing $\mu = \frac{1}{2}r^{-\frac{2}{5}}s^{\frac{2}{5}}$ and $s = r^{\frac{11}{6}}$.

Hence combining the inequality above with (90) and (92) we find

$$\|\rho_r^{\mathrm{OTF}} - \rho_r^{\mathrm{HF}}\|_C^2 \leq Cr^{-7+\frac{1}{3}} + C(r^{-5}\lambda^{-2} + \lambda r^{-7}). \tag{94}$$

We study now $\|\chi_r^+\rho^{\mathrm{HF}}-\rho_r^{\mathrm{HF}}\|_C$. By Hardy-Littlewood-Sobolev inequality we find

$$\|\chi_r^+\rho^{\mathrm{HF}}-\rho_r^{\mathrm{HF}}\|_C \le C\|\chi_r^+\rho^{\mathrm{HF}}-\rho_r^{\mathrm{HF}}\|_{\frac{6}{5}} \le C\Big(\int_{r\le|\mathbf{x}|\le\frac{r}{1-\lambda}}\rho^{\mathrm{HF}}(\mathbf{x})^{\frac{6}{5}}\,d\mathbf{x}\Big)^{\frac{5}{6}}. \tag{95}$$

To estimate the last term in (95) we are going to use the second estimate in (85) that we have just proved. With Σ defined as in (26) we find by Hölder's inequality

$$\begin{aligned}\int_{r\le|\mathbf{x}|\le\frac{r}{1-\lambda}}\rho^{\mathrm{HF}}(\mathbf{x})^{\frac{6}{5}}\,d\mathbf{x} &\le \Big(\int_{\substack{r\le|\mathbf{x}|,\\ \mathbf{x}\in\Sigma}}\rho^{\mathrm{HF}}(\mathbf{x})^{\frac{4}{3}}\,d\mathbf{x}\Big)^{\frac{9}{10}}\Big(\int_{r\le|\mathbf{x}|\le\frac{r}{1-\lambda}}1\,d\mathbf{x}\Big)^{\frac{1}{10}}\\ &\quad+\Big(\int_{\substack{r\le|\mathbf{x}|,\\ \mathbf{x}\in\mathbb{R}^3\setminus\Sigma}}\rho^{\mathrm{HF}}(\mathbf{x})^{\frac{5}{3}}\,d\mathbf{x}\Big)^{\frac{18}{25}}\Big(\int_{r\le|\mathbf{x}|\le\frac{r}{1-\lambda}}1\,d\mathbf{x}\Big)^{\frac{7}{25}}\\ &\le Cr^{-\frac{33}{10}}\lambda^{\frac{1}{10}}+Cr^{-\frac{21}{5}}\lambda^{\frac{7}{25}}.\end{aligned}$$

From the estimate above, (94) and (95) it then follows

$$\begin{aligned}\|\chi_r^+\rho^{\mathrm{HF}}-\rho_r^{\mathrm{OTF}}\|_C &\le \|\chi_r^+\rho^{\mathrm{HF}}-\rho_r^{\mathrm{HF}}\|_C+\|\rho_r^{\mathrm{HF}}-\rho_r^{\mathrm{OTF}}\|_C\\ &\le Cr^{-\frac{7}{2}+\frac{1}{6}}+C(r^{-5}\lambda^{-2}+\lambda r^{-7})^{\frac{1}{2}}+C(r^{-\frac{11}{4}}\lambda^{\frac{1}{12}}+r^{-\frac{7}{2}}\lambda^{\frac{7}{30}}),\end{aligned}$$

that gives the claim choosing $\lambda=r^{\frac{5}{7}}$ □

4.3.3 Estimate on $\mathcal{A}_3$

Lemma 4.15. *Let G_α be the function defined in Theorem 2.3. Let $Z\alpha=\kappa$ fixed, $0\le\kappa<2/\pi$ and $Z\ge1$.*

There exists $\alpha_0>0$ such that given $\varepsilon',\sigma>0$ there exists a constant $D<1/4$ depending only on ε' and σ such that if (65) holds for all $|\mathbf{x}|\le D$, then for all $\alpha\le\alpha_0$

$$\alpha^{-1}\int_{|\mathbf{y}|\ge|\mathbf{x}|}G_\alpha(\rho^{\mathrm{HF}}(\mathbf{y}))d\mathbf{y}\le C|\mathbf{x}|^{-7}\ \textit{for all}\ |\mathbf{x}|\le D,$$

with C a universal positive constant.

Proof. If $|\mathbf{x}|<\beta_0Z^{-\frac{1}{3}}$ we find by Lemma 3.1

$$\alpha^{-1}\int_{|\mathbf{y}|>|\mathbf{x}|}G_\alpha(\rho^{\mathrm{HF}}(\mathbf{y}))d\mathbf{y}\le\alpha^{-1}\int_{\mathbb{R}^3}G_\alpha(\rho^{\mathrm{HF}}(\mathbf{y}))d\mathbf{y}\le CZ^{\frac{7}{3}}\le C|\mathbf{x}|^{-7}.$$

While if $D\ge|\mathbf{x}|\ge\beta_0Z^{-\frac{1}{3}}$ the claim follows from the second estimate in (85). □

Lemma 4.16. *Let $Z\alpha=\kappa$ fixed, $0\le\kappa<2/\pi$, $Z\ge1$ and $0<\mu<\frac{1}{109}$.*

There exists α_0 such that given $\varepsilon',\sigma>0$ there exists a constant $D<1/4$ depending only on ε' and σ such that for all $\alpha\le\alpha_0$ and for all r with $\beta_0Z^{-\frac{1-\mu}{3}}\le r\le D$ for which (65) holds for $|\mathbf{x}|\le r$, then for all $\mathbf{x}$ with $|\mathbf{x}|\ge r$

$$|\mathcal{A}_3(r,\mathbf{x})|\le C\Big(\frac{|\mathbf{x}|}{r}\Big)^{\frac{1}{12}}r^{-4+\frac{3\mu}{1-\mu}},$$

with $C>0$ a universal constant.

Proof. We proceed similarly as in Theorem 3.3. By the formula for $\mathcal{A}_3$, Proposition 2.8 and Lemma 4.14 we get

$$|\mathcal{A}_3(r,\mathbf{x})| \leq \int_{A(|\mathbf{x}|,k)} \chi_r^+(\mathbf{y}) \frac{|\rho_r^{\mathrm{OTF}}(\mathbf{y}) - \rho^{\mathrm{HF}}(\mathbf{y})|}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y} + Ck^{-1}|\mathbf{x}|^{-\frac{1}{2}} r^{-\frac{7}{2}+\frac{1}{6}}. \tag{96}$$

By Hölder's inequality, Lemma 4.10, the OTF-equation (67) and (33) we find

$$\int_{A(|\mathbf{x}|,k)} \frac{\rho_r^{\mathrm{OTF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y} \leq C r^{-\frac{21}{5}} |\mathbf{x}|^{\frac{1}{5}} k^{\frac{1}{5}}. \tag{97}$$

Once again, to estimate $\int_{A(|\mathbf{x}|,k)} \frac{\chi_r^+(\mathbf{y})\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y}$ we have to proceed differently than in [23, Lem.12.7] since ρ^{HF} is not in $L^{\frac{5}{3}}(\mathbb{R}^3)$. We consider the following splitting

$$\int_{A(|\mathbf{x}|,k)} \chi_r^+(\mathbf{y}) \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y} = \int_{\substack{A(|\mathbf{x}|,k)\\ |\mathbf{x}-\mathbf{y}|>R, |\mathbf{y}|>r}} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y} + \int_{\substack{|\mathbf{y}|>r,\\ |\mathbf{x}-\mathbf{y}|<R}} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y}, \tag{98}$$

for $R>0$ to be chosen. By Hölder's inequality, Theorem 2.3, Remark 2.4, (33) and Lemma 4.14 we get

$$\int_{\substack{A(|\mathbf{x}|,k)\\ |\mathbf{x}-\mathbf{y}|>R, |\mathbf{y}|>r}} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y} \leq C\alpha^{\frac{3}{4}} R^{-\frac{3}{8}} |\mathbf{x}|^{\frac{1}{8}} k^{\frac{1}{8}} r^{-\frac{21}{4}} + C r^{-\frac{21}{5}} |\mathbf{x}|^{\frac{1}{5}} k^{\frac{1}{5}}. \tag{99}$$

It remains to study the second term on the right hand side of (98). Let $\nu \in \mathbb{R}^+$ be such that $\nu\alpha \leq 2/\pi$. We consider the density matrix $\gamma_{r/2}^{\mathrm{HF}}$ defined in (61) with $\lambda = 1/2$. From Theorem 2.10 it follows that for $\mathbf{x}$ such that $|\mathbf{x}| \geq r$

$$\mathrm{Tr}[(\alpha^{-1}T(\mathbf{p}) - \frac{\nu}{|\cdot - \mathbf{x}|}\chi_{B_R(\mathbf{x})}(\cdot))\gamma_{r/2}^{\mathrm{HF}}] \geq -C(\nu^{\frac{5}{2}} R^{\frac{1}{2}} + \nu^4\alpha^2).$$

Hence we find

$$\begin{aligned} \nu \int_{|\mathbf{y}-\mathbf{x}|<R} \chi_r^+(\mathbf{y}) \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y} &\leq \nu \int_{|\mathbf{y}-\mathbf{x}|<R} \frac{\rho_{r/2}^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y} \\ &\leq \mathrm{Tr}[\alpha^{-1}T(\mathbf{p})\gamma_{r/2}^{\mathrm{HF}}] + C(\nu^{\frac{5}{2}} R^{\frac{1}{2}} + \nu^4\alpha^2) \end{aligned}$$

and by Lemma 4.14

$$\int_{|\mathbf{y}-\mathbf{x}|<R} \chi_r^+(\mathbf{y}) \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y} \leq C\nu^{-1} r^{-7} + C(\nu^{\frac{3}{2}} R^{\frac{1}{2}} + \nu^3\alpha^2). \tag{100}$$

Hence from (96), (97), (99) and (100) it follows that

$$\begin{aligned} |\mathcal{A}_3(r,\mathbf{x})| \leq\; & C\nu^{-1} r^{-7} + C(\nu^{\frac{3}{2}} R^{\frac{1}{2}} + \nu^3\alpha^2) + C\alpha^{\frac{3}{4}} R^{-\frac{3}{8}} |\mathbf{x}|^{\frac{1}{8}} k^{\frac{1}{8}} r^{-\frac{21}{4}} \\ & + C r^{-\frac{21}{5}} |\mathbf{x}|^{\frac{1}{5}} k^{\frac{1}{5}} + Ck^{-1} |\mathbf{x}|^{-\frac{1}{2}} r^{-\frac{7}{2}+\frac{1}{6}}. \end{aligned}$$

So choosing $\nu = 1/2(\beta_0 r^{-1})^{\frac{3}{1-\mu}}$ (that gives $\nu\alpha < 2/\pi$), k such that $r^{-\frac{21}{5}}|\mathbf{x}|^{\frac{1}{5}}k^{\frac{1}{5}} = k^{-1}|\mathbf{x}|^{-\frac{1}{2}} r^{-\frac{7}{2}+\frac{1}{6}}$, i.e. $k = |\mathbf{x}|^{-\frac{7}{12}} r^{\frac{13}{18}}$ and R such that $\alpha^{\frac{3}{4}} R^{-\frac{3}{8}} |\mathbf{x}|^{\frac{1}{8}\frac{5}{12}} r^{-\frac{21}{4}+\frac{1}{8}\frac{13}{18}} = r^{-4-\frac{1}{18}}|\mathbf{x}|^{\frac{1}{12}}$, i.e. $R = \alpha^2 |\mathbf{x}|^{-\frac{1}{12}} r^{-\frac{5}{18}}$

$$|\mathcal{A}_3(r,\mathbf{x})| \leq C(r^{-4+\frac{3\mu}{1-\mu}} + |\mathbf{x}|^{-\frac{1}{24}} r^{-\frac{5}{36}-\frac{9}{2(1-\mu)}}\alpha + r^{-\frac{9}{1-\mu}}\alpha^2 + |\mathbf{x}|^{\frac{1}{12}} r^{-4-\frac{1}{18}}).$$

Finally since $r^{-1}\alpha^{\frac{1-\mu}{3}} \leq \beta_0^{-1}\kappa^{\frac{1-\mu}{3}}$, the claim follows for $|\mathbf{x}| \geq r$ and $\mu < 1/(109)$. $\square$

4.4 The intermediate region

Here we prove the main estimate in Theorem 1.17 up to a fixed distance independent of Z.

Lemma 4.17 (Iterative step). *Let $Z\alpha = \kappa$ fixed with $0 \le \kappa < 2/\pi$. Consider $\mu = \frac{1}{11}\frac{1}{49}$ and assume $N \ge Z \ge 1$.*

Then there exists $\alpha_0 > 0$ such that for all $\delta, \varepsilon', \sigma > 0$ with $\delta < \delta_0$, where δ_0 is some universal constant, there exists constants $\varepsilon_2, C'_\phi > 0$ depending only on δ and a constant $D = D(\varepsilon', \sigma) > 0$ depending only on ε', σ with the following property. For all $\alpha \le \alpha_0$ and $R_0 < D$ satisfying that $\beta_0 Z^{-\frac{1-\mu}{3}} \le R_0^{1+\delta}$ and that (65) holds for all $|\mathbf{x}| \le R_0$, there exists $R'_0 > R_0$ such that

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \le C'_\Phi |\mathbf{x}|^{-4+\varepsilon_2}$$

for all $\mathbf{x}$ with $R_0 < |\mathbf{x}| < R'_0$.

Proof. Let $D > 0$ depending on σ, ε' be the smaller of the values of D occurring in Lemma 4.11 and Lemma 4.16. Given $\delta > 0$. We consider $R_0 < D$ satisfying $\beta_0 Z^{-\frac{1-\mu}{3}} \le R_0^{1+\delta}$ and such that (65) holds for all $|\mathbf{x}| \le R_0$.

Set $R'_0 = R_0^{1-\delta}$ and $r = R_0^{1+\delta}$. Then we have $\beta_0 Z^{-\frac{1}{3}} \le \beta_0 Z^{-\frac{1-\mu}{3}} \le r \le R_0 < D$ we can therefore apply Lemma 4.11 and Lemma 4.16. From (68) we obtain that for all $|\mathbf{x}| \ge r$ and all $\alpha \le \alpha_0$

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \le C|\mathbf{x}|^{-4-\zeta} r^{\zeta} + C\Big(\frac{|\mathbf{x}|}{r}\Big)^{\frac{1}{12}} r^{-4+\frac{3\mu}{1-\mu}}.$$

Since for $R_0 < |\mathbf{x}| < R'_0$ we have

$$|\mathbf{x}|^{\frac{2\delta}{1-\delta}} \le \frac{r}{|\mathbf{x}|} \le |\mathbf{x}|^{\delta}$$

and thus

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \le C|\mathbf{x}|^{-4+\delta\zeta} + C|\mathbf{x}|^{-4+3\frac{\mu}{1-\mu}} |\mathbf{x}|^{-\frac{\delta}{1-\delta}(8+\frac{1}{6}-\frac{6\mu}{1-\mu})}.$$

Hence choosing δ_0 sufficiently small there are C'_Φ and ε_2 such that the claim holds. □

Lemma 4.18. *Let $Z\alpha = \kappa$ fixed with $0 \le \kappa < 2/\pi$. Assume $N \ge Z \ge 1$.*

Then there exist universal constants α_0, $\varepsilon \in (0,4)$ and $D, C_\Phi > 0$, $D < 1/4$, such that for all $\alpha \le \alpha_0$ and $\mathbf{x}$ with $|\mathbf{x}| \le D$ we have

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \le C_\Phi |\mathbf{x}|^{-4+\varepsilon}.$$

Proof. We fix $\mu = \frac{1}{11}\frac{1}{49}$ as in Lemma 4.17. Since $\mu < \frac{2}{11}\frac{1}{49}$, by Theorem 3.3 we know that there exists constants $a, b, c > 0$ such that for all $|\mathbf{x}| \le \beta Z^{-\frac{1-\mu}{3}}$

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \le C(1 + \beta^2 + \beta^{5/2} + \beta^b |\mathbf{x}|^c)\beta^{2-a} |\mathbf{x}|^{-4+a}. \tag{101}$$

We first show that we may choose δ small enough such that if we choose $\tilde{R}^{1+\delta} = \beta_0 Z^{-\frac{1-\mu}{3}}$ we have for all $|\mathbf{x}| < \tilde{R}$ that

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \le C''_\Phi |\mathbf{x}|^{-4+\frac{a}{2}}. \tag{102}$$

Let $\beta > 0$ be such that $(\beta Z^{-\frac{1-\mu}{3}})^{1+\delta} = \beta_0 Z^{-\frac{1-\mu}{3}}$, i.e. $\beta^{1+\delta} = \beta_0 Z^{\delta\frac{1-\mu}{3}}$. Hence from (101) we find for all $|\mathbf{x}| \le \beta Z^{-\frac{1-\mu}{3}}$

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \le C(1 + \beta^2 + \beta^{5/2} + \beta^b |\mathbf{x}|^c)\beta^{2-\frac{a}{2}} Z^{-\frac{a}{2}\frac{1-\mu}{3}} |\mathbf{x}|^{-4+\frac{a}{2}},$$

and by the choice of β (and $\beta_0 < 1$)

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \le C(1 + Z^{2\frac{\delta}{1+\delta}\frac{1-\mu}{3}} + Z^{\frac{5}{2}\frac{\delta}{1+\delta}\frac{1-\mu}{3}} + Z^{\frac{\delta}{1+\delta}\frac{1-\mu}{3}(b+c)}Z^{-c\frac{1-\mu}{3}}) \\ Z^{(2-\frac{a}{2})\frac{1-\mu}{3}\frac{\delta}{1+\delta}}Z^{-\frac{a}{2}\frac{1-\mu}{3}}|\mathbf{x}|^{-4+\frac{a}{2}}.$$

Hence if δ is small enough we may choose a universal constant C''_Φ such that (102) holds.

Let now δ be small enough so that we may apply Lemma 4.17. This give constant ε_2 and C'_Φ (depending only on δ) and for all $\sigma, \varepsilon' > 0$ a constant $D < 1/4$. Now choose $\sigma = \max\{C'_\Phi, C''_\Phi\}$ and $\varepsilon' = \min\{a/2, \varepsilon_2\}$. Now σ, ε' and D are universal constants. To prove the claim we shall prove that for all $|\mathbf{x}| \le D$

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \le \sigma|\mathbf{x}|^{-4+\varepsilon'}. \tag{103}$$

We have to prove that D belongs to the set

$$\mathcal{M} = \{0 < R \le 1/4 : \text{ Inequality (103) holds for all } |\mathbf{x}| \le R\}.$$

We reason by contradiction. If this was not true then $D > R_0 = \sup \mathcal{M}$ and in particular $R_0 < 1/4$. From (102) and the choice of σ and ε' it follows that either $\tilde{R} > 1/4$ or $\tilde{R} \in \mathcal{M}$. In the first case then $R_0 = \sup \mathcal{M} = 1/4 > D$ that contradicts our hypothesis. On the other hand if $\tilde{R} \in \mathcal{M}$, then $R_0^{1+\delta} \ge \tilde{R}^{1+\delta} = \beta_0 Z^{-\frac{1-\mu}{3}}$. It then follows from Lemma 4.17 that there exists $R'_0 \in \mathcal{M}$ with $R'_0 > R_0$. This contradicts also our hypothesis. □

4.5 The outer zone and proof of Theorem 1.17

The proof of Theorem 1.17 follows directly from Lemma 4.18 and the following result.

Lemma 4.19. *Let $Z\alpha = \kappa$, $0 \le \kappa < 2/\pi$. Assume $N \ge Z \ge 1$. Let D, ε and C_Φ be the constants introduced in Lemma 4.18.*

Then there exist $\alpha_0 > 0$ and a universal constant $C_M > 0$ such that for all $\alpha \le \alpha_0$ and $\mathbf{x}$ with $|\mathbf{x}| \ge D$ we have

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \le C_M.$$

Proof. Here C_i, $i = 1, \ldots, 6$ denote positive universal constants. We write

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \le |\Phi^{\mathrm{HF}}_{D}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{D}(\mathbf{x})| + \int_{D<|\mathbf{y}|<|\mathbf{x}|} \frac{\rho^{\mathrm{TF}}(\mathbf{y}) + \rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y}. \tag{104}$$

Since $\Phi^{\mathrm{HF}}_{D}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{D}(\mathbf{x})$ is harmonic for $|\mathbf{x}| > D$ and tends to zero at infinity we have by Lemma 4.18

$$|\Phi^{\mathrm{HF}}_{D}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{D}(\mathbf{x})| \le \sup_{|\mathbf{x}|=D} |\Phi^{\mathrm{HF}}_{D}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{D}(\mathbf{x})| \le C_\phi D^{-4+\varepsilon}. \tag{105}$$

For the second term on the right hand side of (104) we write

$$\int_{D<|\mathbf{y}|<|\mathbf{x}|} \frac{\rho^{\mathrm{TF}}(\mathbf{y}) + \rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y} \\ \le \int_{\substack{|\mathbf{x}-\mathbf{y}|<D/4 \\ |\mathbf{y}|>D}} \frac{\rho^{\mathrm{TF}}(\mathbf{y}) + \rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y} + \frac{4}{D}\int_{D<|\mathbf{y}|} (\rho^{\mathrm{TF}}(\mathbf{y}) + \rho^{\mathrm{HF}}(\mathbf{y}))\, d\mathbf{y}. \tag{106}$$

By Lemma 4.1, Lemma 4.18, estimate (13) and the TF-equation we find

$$\int_{D<|\mathbf{y}|} (\rho^{\mathrm{TF}}(\mathbf{y}) + \rho^{\mathrm{HF}}(\mathbf{y}))\, d\mathbf{y} \le C_1(1 + C_\Phi D^{\varepsilon})(1 + D^{-3}) + C_1 D^{-3}. \tag{107}$$

It remains to estimate the first term on the right hand side of (106). By Hölder's inequality, estimate (13) and the TF-equation we get

$$\int_{\substack{|\mathbf{x}-\mathbf{y}|<D/4\\|\mathbf{y}|>D}} \frac{\rho^{\mathrm{TF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{y} \le C_2\Big(\int_{|\mathbf{y}|>D}(\rho^{\mathrm{TF}}(\mathbf{y}))^{\frac{5}{3}}\,d\mathbf{y}\Big)^{\frac{3}{5}} D^{\frac{1}{5}} \le C_3 D^{-4}. \tag{108}$$

To estimate the term with the HF-density we use Theorem 2.10. Let γ_D^{HF} be the exterior HF-density matrix as defined in (61) with $r = D/2$ and $\lambda = 1/2$. Then by Theorem 2.10 with $\nu = \beta_0^3 D^{-3}$

$$\alpha^{-1}\,\mathrm{Tr}[(T(\mathbf{p}) - \frac{\nu\alpha}{|\mathbf{x}-\cdot|}\chi_{B_{\frac{D}{4}}(\mathbf{x})}(\cdot))\gamma_{D/2}^{\mathrm{HF}}] \ge -C_4(D^{\frac{1}{2}}\nu^{\frac{5}{2}} + \nu^4\alpha^2),$$

and thus

$$\int_{|\mathbf{x}-\mathbf{y}|<D/4} \frac{\rho_{D/2}^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{y} \le C_5 D^3\alpha^{-1}\,\mathrm{Tr}[T(\mathbf{p})\gamma_{D/2}^{\mathrm{HF}}] + C_6 D^{-4},$$

Here we use that $D > 2\beta_0 Z^{-\frac{1}{3}}$ (for $\alpha \le \alpha_0$) and $D < 1/4$. By Lemma 4.14 we conclude

$$\int_{|\mathbf{x}-\mathbf{y}|<D/4} \chi_D^+(\mathbf{y})\frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{y} \le \int_{|\mathbf{x}-\mathbf{y}|<D/4} \frac{\rho_{D/2}^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{y} \le C_7 D^{-4}. \tag{109}$$

The claim follows collecting together formula (104) to formula (109). □

5 Proofs of Theorems 1.1, 1.18, 1.19 and 1.20

In this section we always assume the following: $Z\alpha = \kappa$ with $0 \le \kappa < 2/\pi$ and $N \ge Z \ge 1$.

Proof of Theorem 1.1. Assume that a HF-minimizer exists with $\int \rho^{\mathrm{HF}} = N$. Let ρ^{TF} be the minimizer of the TF-energy functional of the neutral atom with nuclear charge Z. Then for $R > 0$ to be chosen

$$N = \int_{|\mathbf{x}|<R} \rho^{\mathrm{TF}}(\mathbf{x})\,d\mathbf{x} + \int_{|\mathbf{x}|<R}(\rho^{\mathrm{HF}}(\mathbf{x}) - \rho^{\mathrm{TF}}(\mathbf{x}))\,d\mathbf{x} + \int_{|\mathbf{x}|>R}\rho^{\mathrm{HF}}(\mathbf{x})\,d\mathbf{x}. \tag{110}$$

By Theorem 1.17 we know that there exist universal positive constants $\varepsilon, \alpha_0, C_M$ and C_Φ such that for all $\alpha \le \alpha_0$ and $\mathbf{x} \in \mathbb{R}^3$

$$|\Phi_{|\mathbf{x}|}^{\mathrm{HF}}(\mathbf{x}) - \Phi_{|\mathbf{x}|}^{\mathrm{TF}}(\mathbf{x})| \le C_\Phi|\mathbf{x}|^{-4+\varepsilon} + C_M. \tag{111}$$

Let Z_0 be such that $Z_0\alpha_0 = \kappa$. Then $\alpha \le \alpha_0$ corresponds to $Z \ge Z_0$. Let us choose R such that $C_\Phi R^{-4+\varepsilon} = C_M$. Then from (110), (111) and Lemma 4.1 for all $Z \ge Z_0$ we find

$$N \le \int_{|\mathbf{x}|<R}\rho^{\mathrm{TF}}(\mathbf{x})\,d\mathbf{x} + 2C_\Phi R^{-3+\varepsilon} + C(1 + C_\Phi R^\varepsilon)(R^{-3}+1) < Z + \tilde{Q}.$$

The claim follows choosing $Q = \max\{\tilde{Q}, Z_0 + 1\}$. □

Proof of Theorem 1.18. Let ρ^{HF} be the density of the HF-minimizer in the neutral case $N = Z$. We have

$$\begin{aligned}
\Big|\int_{|\mathbf{x}|>R}(\rho^{\mathrm{HF}}(\mathbf{x}) - \rho^{\mathrm{TF}}(\mathbf{x}))d\mathbf{x}\Big| &= \Big|\int_{|\mathbf{x}|<R}(\rho^{\mathrm{HF}}(\mathbf{x}) - \rho^{\mathrm{TF}}(\mathbf{x}))d\mathbf{x}\Big| \\
&= \Big|\frac{R}{4\pi}\int_{S^2} d\omega(\Phi_R^{\mathrm{HF}}(R\omega) - \Phi_R^{\mathrm{TF}}(R\omega))\Big| \\
&\le C_\Phi R^{-3+\varepsilon} + C_M R,
\end{aligned}$$

where in the last step we have used Theorem 1.17. Notice that for Z sufficiently big $\alpha \leq \alpha_0$ where α_0 is the constant given in Theorem 1.17. By the TF-equation, Theorem 1.12 we then find

$$3^4 \frac{2\pi^2}{q^2} R^{-3} - C_\Phi R^{-3+\varepsilon} - C_M R \leq \int_{|\mathbf{x}|>R} \rho^{\mathrm{HF}}(\mathbf{x}) d\mathbf{x} \leq 3^4 \frac{2\pi^2}{q^2} R^{-3} + C_\Phi R^{-3+\varepsilon} + C_M R,$$

from which the claim follows directly by the definition of HF-radius. □

Proof of Theorem 1.19. Since $E^{\mathrm{HF}}(Z-1,Z) \geq E^{\mathrm{HF}}(Z,Z)$ the ionization energy is bounded from below by zero. If Z is smaller than a universal constant then we can also bound the ionization energy with a universal constant using Theorem 2.11.

It remains to estimate from above the ionization energy when Z is larger than a universal constant. We first construct a density matrix γ such that $\mathrm{Tr}[\gamma] \leq Z-1$. Let $\theta_- := (1-\theta^2_{r(1-\lambda)})^{\frac{1}{2}}$ for r, λ positive parameters and θ_r defined in Definition 4.4. We consider the density matrix $\gamma_-^{\mathrm{HF}} := \theta_- \gamma^{\mathrm{HF}} \theta_-$ where γ^{HF} is the HF-minimizer in the neutral case. By an opportune choice of r we will then have $\mathrm{Tr}[\gamma_-^{\mathrm{HF}}] \leq Z-1$. Indeed,

$$\mathrm{Tr}[\gamma_-^{\mathrm{HF}}] = \int_{\mathbb{R}^3} \rho^{\mathrm{HF}}(\mathbf{x})\, d\mathbf{x} - \int_{\mathbb{R}^3} \theta^2_{r(1-\lambda)}(\mathbf{x}) \rho^{\mathrm{HF}}(\mathbf{x})\, d\mathbf{x} \leq Z - \int_{|\mathbf{x}|>r} \rho^{\mathrm{HF}}(\mathbf{x})\, d\mathbf{x}.$$

We now choose $\lambda = \frac{1}{2}$. Let $R>0$ be such that $C_M = C_\Phi R^{-4+\varepsilon}$ where C_M, C_Φ, ε are the constants in Theorem 1.17. Then R is a universal constant. We consider Z large enough so that $\beta_0 Z^{-\frac{1}{3}} < R$ where β_0 is the constant in Theorem 1.12. This gives that Z has to be larger than some universal constant. For r such that $\beta_0 Z^{-\frac{1}{3}} < r < R$ by Theorem 1.17 we find

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq 2C_\Phi |\mathbf{x}|^{-4+\varepsilon} \text{ for all } |\mathbf{x}| \leq r.$$

Since $\int \rho^{\mathrm{TF}} = \int \rho^{\mathrm{HF}}$, by the choice of r and Lemma 4.1 we get

$$\begin{aligned}
\int_{|\mathbf{x}|>r} \rho^{\mathrm{HF}}(\mathbf{x})\, d\mathbf{x} &= \int_{|\mathbf{x}|>r} \rho^{\mathrm{TF}}(\mathbf{x})\, d\mathbf{x} + \int_{|\mathbf{x}|<r} (\rho^{\mathrm{TF}}(\mathbf{x}) - \rho^{\mathrm{HF}}(\mathbf{x}))\, d\mathbf{x} \\
&\geq \int_{|\mathbf{x}|>r} \rho^{\mathrm{TF}}(\mathbf{x})\, d\mathbf{x} - 2C_\Phi r^{-3+\varepsilon} \geq C r^{-3} - 2C_\Phi r^{-3+\varepsilon}.
\end{aligned} \tag{112}$$

In the last step we used the TF-equation, Corollary 1.13 and that $r > \beta_0 Z^{-\frac{1}{3}}$. Finally, it follows from (112) by choosing r sufficiently small that $\int_{|\mathbf{x}|>r} \rho^{\mathrm{HF}} > 1$ and hence that $\mathrm{Tr}[\gamma_-^{\mathrm{HF}}] \leq Z-1$. We may choose r sufficiently small by taking Z large enough. Notice that r can be choosen universally and so Z has to be larger than some universal constant.

By the last estimate in the proof of Theorem 4.7 we find

$$\mathcal{E}^{\mathrm{HF}}(\gamma_-^{\mathrm{HF}}) \leq \mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) - \mathcal{E}^A(\gamma_r^{\mathrm{HF}}) + \mathcal{R},$$

with $\mathcal{R}$ and γ_r^{HF} as defined in the statement of Theorem 4.7. Since $\mathcal{E}^{\mathrm{HF}}(\gamma_-^{\mathrm{HF}}) \geq E^{\mathrm{HF}}(Z-1,Z)$ and $\mathcal{E}^{\mathrm{HF}}(\gamma^{\mathrm{HF}}) = E^{\mathrm{HF}}(Z,Z)$ it remains to prove that $-\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) + \mathcal{R}$ is bounded from above by some universal constant. Here we use repeteadly that r is a universal constant. By estimate (92) we see that $\mathcal{R} \leq Cr^{-7}$ a universal constant. To estimate from below $\mathcal{E}^A(\gamma_r^{\mathrm{HF}})$ we first leave out the kinetic energy term and the direct term since these are positive. Moreover, since Φ_r^{HF} is harmonic for $|\mathbf{x}| > r$ and tends to zero at infinity we see that

$$\Phi_r^{\mathrm{HF}}(\mathbf{x}) \leq \frac{r}{|\mathbf{x}|} \sup_{|\mathbf{y}|=r} \Phi_r^{\mathrm{HF}}(\mathbf{y}) \leq \frac{r}{|\mathbf{x}|} \sup_{|\mathbf{y}|=r} \Phi_r^{\mathrm{TF}}(\mathbf{y}) + \frac{r}{|\mathbf{x}|} \sup_{|\mathbf{y}|=r} |\Phi_r^{\mathrm{TF}}(\mathbf{y}) - \Phi_r^{\mathrm{HF}}(\mathbf{y})|,$$

which is bounded by $C'/|\mathbf{x}|$, C' a universal constant, by Theorem 1.17 and Corollary 1.14. It then follows that

$$\mathcal{E}^A(\gamma_r^{\mathrm{HF}}) \geq -\operatorname{Tr}[\frac{C'}{|\cdot|}\gamma_r^{\mathrm{HF}}] \geq -\frac{C'}{r}\int_{|\mathbf{x}|>r}\rho^{\mathrm{HF}}(\mathbf{x})\,d\mathbf{x},$$

that is bounded from below by a universal constant using Lemma 4.1. □

Proof of Theorem 1.20. Let α_0 be the constant appearing in Theorem 1.17 and Z_0 be such that $\alpha_0 Z_0 = \kappa$. The claim follows directly for $Z \leq Z_0$ since both functions are bounded for $|\mathbf{x}|$ large, while for $|\mathbf{x}|$ small the functions are bounded by a constant times $|\mathbf{x}|^{-1}$.

The case $Z > Z_0$ corresponds to $\alpha < \alpha_0$ and for such values of α we can use the result in Theorem 1.17. We separate the case small $\mathbf{x}$, intermediate $\mathbf{x}$ and large $\mathbf{x}$. Once again, comparing with the proof in the non-relativistic case ([23]) we have to do an extra splitting for small $\mathbf{x}$.

By the definition of the mean field potential and Proposition 2.8 we find

$$|\varphi^{\mathrm{TF}}(\mathbf{x}) - \varphi^{\mathrm{HF}}(\mathbf{x})| \leq \int_{|\mathbf{x}-\mathbf{y}|<s}(\rho^{\mathrm{TF}}(\mathbf{y}) + \rho^{\mathrm{HF}}(\mathbf{y}))\Big(\frac{1}{|\mathbf{x}-\mathbf{y}|} - \frac{1}{s}\Big) + \frac{\sqrt{2}}{s^{\frac{1}{2}}}\|\rho^{\mathrm{TF}} - \rho^{\mathrm{HF}}\|_C.$$

Since ρ^{TF} is bounded in $L^{\frac{5}{3}}$-norm, we find using Hölder's inequality, Corollary 1.15 and Lemma 3.1 that

$$|\varphi^{\mathrm{TF}}(\mathbf{x}) - \varphi^{\mathrm{HF}}(\mathbf{x})| \leq \int_{|\mathbf{x}-\mathbf{y}|<s}\rho^{\mathrm{HF}}(\mathbf{y})\Big(\frac{1}{|\mathbf{x}-\mathbf{y}|} - \frac{1}{s}\Big) + C(s^{\frac{1}{5}}Z^{\frac{7}{5}} + s^{-\frac{1}{2}}Z^{1+\frac{3}{22}}). \tag{113}$$

For the integral with the HF-density we need to split the region where the HF-density is bounded in $L^{\frac{4}{3}}$-norm from the one where it is bounded in $L^{\frac{5}{3}}$-norm. Proceeding as in the proof of Lemma 3.2 (from (35) to (37) replacing the integrals on $A(|\mathbf{x}|,k)$ with integrals on $|\mathbf{x}-\mathbf{y}| < s$) using the results of Lemma 3.1 we get with $R \in (0,s)$ to be chosen

$$\int_{|\mathbf{x}-\mathbf{y}|<s}\rho^{\mathrm{HF}}(\mathbf{y})\Big(\frac{1}{|\mathbf{x}-\mathbf{y}|} - \frac{1}{s}\Big) \leq C(Z^{\frac{7}{5}}s^{\frac{1}{5}} + R^{-\frac{1}{4}}(\alpha Z^{\frac{7}{3}})^{\frac{3}{4}} + Z^{\frac{4}{3}} + R^{\frac{1}{2}}Z^{\frac{3}{2}}). \tag{114}$$

Recall that $Z\alpha = \kappa$ is fixed. Choosing s such that $Z^{\frac{7}{5}}s^{\frac{1}{5}} = Z^{\frac{4}{3}}$ (i.e. $s = Z^{-\frac{1}{3}}$) and R such that $R^{-\frac{1}{4}}Z = R^{\frac{1}{2}}Z^{\frac{3}{2}}$ (i.e $R = Z^{-\frac{2}{3}}$; notice that $R < s$) we get from (113) and (114)

$$|\varphi^{\mathrm{TF}}(\mathbf{x}) - \varphi^{\mathrm{HF}}(\mathbf{x})| \leq C(Z^{\frac{4}{3}} + Z^{\frac{7}{6}}).$$

The claim follows from this inequality for $\mathbf{x} \in \mathbb{R}^3$ such that $|\mathbf{x}| \leq \beta_0 Z^{-\frac{1+\gamma}{3}}$ for $\gamma > 0$. We consider $\gamma < \frac{1}{263}$.

If $|\mathbf{x}| \geq \beta_0 Z^{-\frac{1+\gamma}{3}}$ then proceeding as for very small $\mathbf{x}$ and as in the proof of Theorem 3.3 up to inequality (43) we get for $t \in (\frac{1+\gamma}{3}, \frac{3}{5})$, $l > t$ and $R < \beta_0 Z^{-l}$

$$|\varphi^{\mathrm{TF}}(\mathbf{x}) - \varphi^{\mathrm{HF}}(\mathbf{x})| \leq C(s^{\frac{1}{5}}Z^{\frac{7}{5}} + s^{-\frac{1}{2}}Z^{1+\frac{3}{22}} + R^{-\frac{3}{8}}s^{\frac{1}{8}}Z + Z^{\frac{1}{2}(3-t)}).$$

Here we have also used that $Z\alpha$ is a constant. So choosing s such that $s^{\frac{1}{5}}Z^{\frac{7}{5}} = Z^{\frac{1}{2}(3-t)}$ (i.e. $s = Z^{\frac{1}{2}-\frac{5}{2}t}$), R such that $R^{-\frac{3}{8}}Z^{1+\frac{1}{16}-\frac{5}{16}t} = Z^{\frac{1}{2}(3-t)}$ (i.e. $R = Z^{-\frac{7}{6}+\frac{1}{2}t}$) and optimizing in t (i.e. $t = \frac{1}{3} + \frac{4}{3}\frac{1}{77}$) we obtain

$$|\varphi^{\mathrm{TF}}(\mathbf{x}) - \varphi^{\mathrm{HF}}(\mathbf{x})| \leq CZ^{\frac{4}{3}-\frac{2}{3}\frac{1}{77}}. \tag{115}$$

Notice that $t > \frac{1+\gamma}{3}$, $R < s$ by the choice of t and that R satisfies the condition $R < \beta_0 Z^{-l}$, $l > t$, for Z sufficiently big. The claim then follows from (115) for $\mathbf{x} \in \mathbb{R}^3$ such that $|\mathbf{x}|^{1+\delta} \leq \beta_0 Z^{-\frac{1}{3}}$ for $\delta < \frac{1}{153}$. We fix $\delta = \frac{1}{2}\frac{1}{153}$.

We turn now to study intermediate $\mathbf{x}$. Let $D \leq 1$ be such that $C_M \leq C_\Phi D^{-4+\varepsilon}$ with C_M, C_Φ, ε the constants in Theorem 1.17. Then for all $\mathbf{x}$ such that $|\mathbf{x}| \leq D$

$$|\Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x})| \leq 2C_\Phi |\mathbf{x}|^{-4+\varepsilon}.$$

Moreover we choose D such that Lemma 4.11 holds. Let $\mathbf{x}$ be such that $\beta_0 Z^{-\frac{1}{3}} \leq |\mathbf{x}|^{1+\delta} \leq D^{\frac{1+\delta}{1+\mu}}$ with $0 < \mu \leq \delta$. We set $r = |\mathbf{x}|^{1+\mu}$. Then $\beta_0 Z^{-\frac{1}{3}} \leq r \leq D$. We write $\varphi^{\mathrm{TF}}(\mathbf{x}) - \varphi^{\mathrm{HF}}(\mathbf{x}) = \varphi^{\mathrm{TF}}(\mathbf{x}) - \varphi_r^{\mathrm{OTF}}(\mathbf{x}) + \varphi_r^{\mathrm{OTF}}(\mathbf{x}) - \varphi^{\mathrm{HF}}(\mathbf{x})$ with φ_r^{OTF} the mean field potential of the OTF-problem defined in Subsection 4.3. By the choice of r and D and Lemma 4.11 we get since $|\mathbf{x}| \geq r = |\mathbf{x}|^{1+\mu}$

$$|\varphi^{\mathrm{TF}}(\mathbf{x}) - \varphi_r^{\mathrm{OTF}}(\mathbf{x})| \leq C|\mathbf{x}|^{-4-\zeta} r^{\zeta}, \tag{116}$$

for $|\mathbf{x}| \geq r$ with $\zeta = (7+\sqrt{73})/2$. For the other two terms we see

$$\varphi^{\mathrm{HF}}(\mathbf{x}) - \varphi_r^{\mathrm{OTF}}(\mathbf{x}) = \int \frac{\rho_r^{\mathrm{OTF}}(\mathbf{y}) - \chi_r^+(\mathbf{y})\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y},$$

and proceeding as for small $\mathbf{x}$ with the Coulomb-norm estimate Proposition 2.8, by Lemma 4.14 and inequality (100)

$$|\varphi^{\mathrm{HF}}(\mathbf{x}) - \varphi_r^{\mathrm{OTF}}(\mathbf{x})| \leq C\Big(\frac{s^{\frac{1}{5}}}{r^{\frac{21}{5}}} + \frac{r^{-\frac{7}{2}+\frac{1}{6}}}{s^{\frac{1}{2}}} + R^{-\frac{1}{4}}(\alpha r^{-7})^{\frac{3}{4}} + \nu^{-1} r^{-7} + \nu^{\frac{3}{2}} R^{\frac{1}{2}} + \nu^3 \alpha^2\Big).$$

Choosing $\nu = \beta_0^3 r^{-3\frac{1+\delta}{1+\mu}}$, so that $\nu\alpha \leq \kappa < 2/\pi$, s such that $s^{\frac{1}{5}} r^{-\frac{21}{5}} = r^{-\frac{7}{2}+\frac{1}{6}} s^{-\frac{1}{2}}$ (i.e. $s = r^{1+\frac{5}{21}}$), and choosing R such that the two terms where it appears are equal (i.e. $R = r^{2+9\frac{\delta-\mu}{1+\mu}}$; notice that $R < s$) we get

$$|\varphi^{\mathrm{HF}}(\mathbf{x}) - \varphi_r^{\mathrm{OTF}}(\mathbf{x})| \leq C(r^{-4+\frac{1}{21}} + r^{-4+3\frac{\delta-\mu}{1+\mu}}),$$

since $\alpha r^{-3\frac{1+\delta}{1+\mu}}$ is bounded and $r \leq 1$. Collecting together the inequality above and (116) and using that $r = |\mathbf{x}|^{1+\mu}$ the claim follows for $\beta_0 Z^{-\frac{1}{3}} \leq |\mathbf{x}|^{1+\delta} \leq D^{\frac{1+\delta}{1+\mu}}$. We fix $\mu = \delta/2$.

It remains to study the case of large $\mathbf{x}$, i.e. $|\mathbf{x}| \geq D^{\frac{1+\delta}{1+\mu}}$ with D, δ, μ universal constants. For simplicity of notation we fix the universal constant $A := D^{\frac{1+\delta}{1+\mu}}$. We first notice that

$$\varphi^{\mathrm{HF}}(\mathbf{x}) - \varphi^{\mathrm{TF}}(\mathbf{x}) = \Phi^{\mathrm{HF}}_{|\mathbf{x}|}(\mathbf{x}) - \Phi^{\mathrm{TF}}_{|\mathbf{x}|}(\mathbf{x}) + \int_{|\mathbf{y}|>|\mathbf{x}|} \frac{\rho^{\mathrm{TF}}(\mathbf{y}) - \rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y}.$$

The difference of the first two terms is bounded by a universal constant for $|\mathbf{x}| \geq A$ by the result in Theorem 1.17. To estimate the last integral we split it as follows

$$\begin{aligned}\int_{|\mathbf{y}|>|\mathbf{x}|} \frac{|\rho^{\mathrm{TF}}(\mathbf{y}) - \rho^{\mathrm{HF}}(\mathbf{y})|}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y} \quad &\leq \quad \int_{\substack{|\mathbf{y}|>|\mathbf{x}| \\ |\mathbf{x}-\mathbf{y}|<1}} \frac{\rho^{\mathrm{TF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y} + \int_{\substack{|\mathbf{y}|>|\mathbf{x}| \\ |\mathbf{x}-\mathbf{y}|<1}} \frac{\rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y} \\ &\quad + \int_{|\mathbf{y}|>|\mathbf{x}|} (\rho^{\mathrm{TF}}(\mathbf{y}) + \rho^{\mathrm{HF}}(\mathbf{y}))\, d\mathbf{y}.\end{aligned}$$

Since $|\mathbf{x}| \geq A$ the third term on the right hand side is bounded by a universal constant by Lemma 4.1 (for ρ^{HF}) and Corollary 1.13 (for ρ^{TF}). We estimate the first term by Hölder's inequality and Corollary 1.15. We get a bound on the second term proceeding as in (100) (using Theorem 2.10) and choosing $\nu = \frac{1}{2}$ and $R = 1$. We obtain

$$\int_{\substack{|\mathbf{y}|>|\mathbf{x}| \\ |\mathbf{x}-\mathbf{y}|<1}} \frac{\rho^{\mathrm{TF}}(\mathbf{y}) + \rho^{\mathrm{HF}}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y} \leq C(A^{-\frac{21}{5}} + A^{-7} + \alpha^2).$$

Then there exists a universal contant A' such that $|\varphi^{\mathrm{HF}}(\mathbf{x}) - \varphi^{\mathrm{TF}}(\mathbf{x})| \leq A'$ for $|\mathbf{x}| \geq A$. $\square$

A Technical lemmas

Proof of (16) By the definition of the function G_α the inequalities in (16) are equivalent to the following ones

$$\tfrac{3}{5}t^4\min\{\tfrac{2}{5}t,1\} \le g(t) - \tfrac{8}{3}t^3 \le 2t^4\min\{\tfrac{2}{5}t,1\} \text{ for } t \ge 0. \tag{A1}$$

As before we use the substitution $t = \alpha(\rho/C)^{\frac{1}{3}}$.

The estimates in (A1) follow directly from the study of the function g separating the cases $t < \frac{5}{2}$ and $t \ge \frac{5}{2}$.

Proof of Remark 4.2 Using the estimate on K_2 given in (15) we find

$$\begin{aligned}
&\iint_{\substack{\mathbf{x}\in\Sigma_r(\beta_1,\beta_2)\\ \mathbf{y}\in\Sigma_r(\beta_3,\beta_4)}} K_2(\alpha^{-1}|\mathbf{x}-\mathbf{y}|)^2\,d\mathbf{x}d\mathbf{y}\\
\le\;& (16)^2\alpha^4 \iint_{\substack{\mathbf{x}\in\Sigma_r(\beta_1,\beta_2)\\ \mathbf{y}\in\Sigma_r(\beta_3,\beta_4)}} \frac{e^{-\alpha^{-1}|\mathbf{x}-\mathbf{y}|}}{|\mathbf{x}-\mathbf{y}|^4}\,d\mathbf{x}d\mathbf{y}\\
\le\;& (16)^2\alpha^4 e^{-\alpha^{-1}r(\beta_3-\beta_2)}4\pi\int_{r(\beta_3-\beta_2)}^{\infty}\rho^{-2}d\rho\int_{\Sigma_r(\beta_1,\beta_2)}d\mathbf{x},
\end{aligned}$$

since $|\mathbf{x}-\mathbf{y}| \ge (\beta_3-\beta_2)r$. The claim follows computing the two integrals.

A.1 Fourier transform

In the present sub-section we present our notation for the Fourier transform (as in [20]). Given $f \in L^2(\mathbb{R}^3)$ we denote its Fourier transform by

$$\hat f(\mathbf{p}) = \mathcal{F}(f)(\mathbf{p}) := \tfrac{1}{(2\pi)^{\frac{3}{2}}}\int_{\mathbb{R}^3} e^{i\mathbf{p}\cdot x} f(\mathbf{x})d\mathbf{x}.$$

Let $f, g \in L^2(\mathbb{R}^3)$. The following formulas hold:

1. $\mathcal{F}(f*g)(\mathbf{p}) = (2\pi)^{\frac{3}{2}}\hat f(\mathbf{p})\hat g(\mathbf{p})$;
2. $\mathcal{F}(fg)(\mathbf{p}) = (2\pi)^{-\frac{3}{2}}(\hat f * \hat g)(\mathbf{p})$;
3. if $g(\mathbf{x}) = e^{-\lambda|\mathbf{x}|^2}$ then $\hat g(\mathbf{p}) = (2\lambda)^{-\frac{3}{2}}e^{-|\mathbf{p}|^2/(4\lambda)}$;
4. $|\mathbf{x}|^{-\alpha} = \pi^{\frac{\alpha}{2}}(\Gamma(\frac{\alpha}{2}))^{-1}\int_0^{+\infty} e^{-\pi|\mathbf{x}|^2\lambda}\lambda^{\frac{\alpha}{2}-1}d\lambda$ for $0 < \alpha < n$ (see [14, page 130]).

Moreover,

$$\mathcal{F}\Big(\frac{f(\mathbf{x})}{|\mathbf{x}|}\Big)(\mathbf{k}) = \tfrac{1}{2\pi^2}\int_{\mathbb{R}^3}\frac{\hat f(\mathbf{p})}{|\mathbf{k}-\mathbf{p}|^2}d\mathbf{p}.$$

B Large Z-behavior of the energy

In [21] the author studies the large Z-behavior of the ground state energy for problem (1). In this work we are going to use the same construction in several points (Lemmas 3.1, 4.12, Theorem 3.3, ...) and with, in certain cases, a slightly different Hamiltonian. For convenience we repeat here the main ideas of the proof. We do it as it is needed in the proof of Theorem 3.3 since in this case the proof is more involved. We remark that in our proof we use a localisation less than in

[21]. Thanks to Theorem 2.10 and [24, Theorem 2.8] it is sufficient to consider the region near the nuclei and the one far away from the nuclei. There is no need for an intermediate region.

Proposition B.1. *Let $Z\alpha = \kappa$ be fixed with $0 \le \kappa < 2/\pi$ and $Z \ge 1$. Let us consider $\mathbf{P} \in \mathbb{R}^3$, with $|\mathbf{P}| \ge \beta Z^{-\frac{1+\mu}{3}}$ for $\beta > 0$ and $\mu \in (0, 4/5)$. Let $Z \ge \nu > 0$ and $R > 0$ be such that $R < \beta Z^{-l}/4$ for some $\frac{1+\mu}{3} < l$. Moreover, let ρ^{TF} denote the minimizer of the TF-energy functional of a neutral atom with nucleus of charge Z. Consider the Hamiltonian*

$$H_{\mathbf{P}} := \sum_{i=1}^{N} \left(\alpha^{-1} T(\mathbf{p}_i) - \frac{Z}{|\mathbf{x}_i|} - \frac{\nu}{|\mathbf{x}_i - \mathbf{P}|}\chi_{B_R(\mathbf{P})}(\mathbf{x}_i)\right) + \sum_{i<j} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|}, \tag{B2}$$

acting on $\wedge_{i=1}^{N} L^2(\mathbb{R}^3; \mathbb{C}^q)$.

Then for all $t \in (\frac{1+\mu}{3}, \min\{l, \frac{3}{5}\})$ and $\psi \in \wedge_{i=1}^{N} L^2(\mathbb{R}^3)$, with $\|\psi\|_2 = 1$,

$$\langle \psi, H_{\mathbf{p}} \psi \rangle \ge \mathcal{E}^{\mathrm{TF}}(\rho^{\mathrm{TF}}) - C(\beta^{\frac{1}{2}} + \beta^{-2}) Z^{\frac{5}{2} - \frac{1}{2}t},$$

with C depending only on q and κ.

Proof. Since $\mathcal{E}^{\mathrm{TF}}(\rho^{\mathrm{TF}}) = -e_0 Z^{\frac{7}{3}}$ (see (12)) to prove the claim it is sufficient to show that the TF-energy gives a lower bound to the quantum energy modulo lower order terms. In the proof we first reduce to a one-particle operator. Then we localize the energy separating the contribution from the regions near the nuclei from the contribution from the region far away from them. Finally we study the contribution of each of these terms. The main contribution to the energy is given by the region far away from the nuclei. This region will give the TF-energy.

In the following, $s = (3 - t)/4$ ($t < s < 2/3$).

In the proof C denotes a generic positive constant depending only on q and κ.

Reduction to a one-particle problem. We are going to estimate from below $H_{\mathbf{P}}$ by a one-particle operator. This allows us to consider only Slater determinants when minimizing the energy.

Let $g \in C_0^\infty(\mathbb{R}^3)$, $g \ge 0$ be spherically symmetric with $\mathrm{supp}(g) \subset B_1(0)$ and such that $\|g\|_2 = 1$. Starting from these g we define $\Phi_s(\mathbf{x}) := (\beta/(8Z^s))^{-3} g^2(8Z^s\mathbf{x}/\beta)$. Then by Newton's theorem

$$\begin{aligned}
\sum_{i<j} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|} &\ge \sum_{i<j} \iint \frac{\Phi_s(\mathbf{x}_i - \mathbf{x})\Phi_s(\mathbf{x}_j - \mathbf{y})}{|\mathbf{x} - \mathbf{y}|}\, d\mathbf{x} d\mathbf{y} = \\
= \tfrac{1}{2} \sum_{i,j=1}^{N} &\iint \frac{\Phi_s(\mathbf{x}_i - \mathbf{x})\Phi_s(\mathbf{x}_j - \mathbf{y})}{|\mathbf{x} - \mathbf{y}|}\, d\mathbf{x} d\mathbf{y} - \tfrac{N}{2} \iint \frac{\Phi_s(\mathbf{x})\Phi_s(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|}\, d\mathbf{x} d\mathbf{y} = \dots
\end{aligned}$$

and introducing $\rho \in L^1(\mathbb{R}^3) \cap L^{\frac{5}{3}}(\mathbb{R}^3)$, $\rho \ge 0$, to be chosen

$$\begin{aligned}
\dots \quad &= \tfrac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{(\sum_{i=1}^{N} \Phi_s(\mathbf{x}_i - \mathbf{x}) - \rho(\mathbf{x}))(\sum_{j=1}^{N} \Phi_s(\mathbf{x}_j - \mathbf{y}) - \rho(\mathbf{y}))}{|\mathbf{x} - \mathbf{y}|}\, d\mathbf{x} d\mathbf{y} \\
&+ \sum_{i=1}^{N} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\Phi_s(\mathbf{x}_i - \mathbf{x})\rho(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|}\, d\mathbf{x} d\mathbf{y} - D(\rho) - \tfrac{N}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\Phi_s(\mathbf{x})\Phi_s(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|}\, d\mathbf{x} d\mathbf{y} \\
&\ge \sum_{i=1}^{N} \rho * \Phi_s * \frac{1}{|\mathbf{x}_i|} - D(\rho) - C\|g^2\|_{\frac{6}{5}}^2 N \beta^{-1} Z^s.
\end{aligned} \tag{B3}$$

In the last inequality we use that the first term on the left hand side of (B3) is non-negative and that

$$\begin{aligned}
\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\Phi_s(\mathbf{x})\Phi_s(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|}\, d\mathbf{x} d\mathbf{y} &= C\beta^{-1} Z^s \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{g^2(\mathbf{x}) g^2(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|}\, d\mathbf{x} d\mathbf{y} \\
&\le C\beta^{-1} Z^s \|g^2\|_{6/5}^2,
\end{aligned}$$

by definition of Φ_s and Hardy-Littlewood-Sobolev's inequality. Hence

$$\begin{aligned} H_{\mathbf{P}} \quad \geq \quad & \sum_{i=1}^{N} \big(\alpha^{-1}T(\mathbf{p}_i) - \frac{Z}{|\mathbf{x}_i|} - \frac{\nu}{|\mathbf{x}_i - \mathbf{P}|}\chi_{B_R(\mathbf{P})}(\mathbf{x}_i) + \rho * \Phi_s * \frac{1}{|\mathbf{x}_i|}\big) \\ & -D(\rho) - C\|g^2\|_{\frac{6}{5}}^2 N\beta^{-1}Z^s. \end{aligned} \tag{B4}$$

Choice of the localization. The localization will be given by the following functions $\chi_1, \chi_2 \in C_0^\infty(\mathbb{R}^3)$:

$$\chi_1(\mathbf{x}) := \begin{cases} 1 & \text{if } |\mathbf{x}| < \frac{1}{4}\beta Z^{-t}, \\ 0 & \text{if } |\mathbf{x}| > \frac{1}{2}\beta Z^{-t}, \end{cases} \quad \chi_2(\mathbf{x}) := \begin{cases} 1 & \text{if } |\mathbf{x} - \mathbf{P}| < \frac{1}{4}\beta Z^{-t}, \\ 0 & \text{if } |\mathbf{x} - \mathbf{P}| > \frac{1}{2}\beta Z^{-t} \end{cases} \tag{B5}$$

and $\chi_3 \in C^\infty(\mathbb{R}^3)$ such that $\sum_{i=1}^3 \chi_i^2(\mathbf{x}) = 1$ for all $\mathbf{x} \in \mathbb{R}^3$. Moreover we ask that

$$\|\nabla\chi_1\|_\infty, \|\nabla\chi_2\|_\infty, \|\nabla\chi_3\|_\infty \leq 2^5\beta^{-1}Z^t. \tag{B6}$$

Here t is the parameter given in the statement of the proposition. Notice that by the assumptions on R and $\mathbf{P}$ the functions defined above give a well defined partition of unity of $\mathbb{R}^3$. Moreover, $B_R(\mathbf{P})$ is a subset of $\{\mathbf{x} \in \mathbb{R}^3 : \chi_2(\mathbf{x}) = 1\}$.

The localization in the energy expectation. We insert now the localization in the energy expectation. As already observed, since we reduced the operator to a one-particle operator in the energy expectation it is sufficient to consider Slater determinants: i.e. $\psi = u_1 \wedge \cdots \wedge u_N$ with $\{u_i\}_{i=1}^N$ orthonormal functions in $L^2(\mathbb{R}^3, \mathbb{C}^q)$. We may assume that $u_i \in H^{\frac{1}{2}}(\mathbb{R}^3, \mathbb{C}^q)$ for $i = 1, \ldots, N$.

From (B4) and Theorem 2.1 we find with $\psi = u_1 \wedge \cdots \wedge u_N$

$$\begin{aligned} \langle\psi, H_{\mathbf{P}}\psi\rangle \quad \geq \quad & \sum_{i=1}^{N}\sum_{j=1}^{3}(\chi_j u_i, h\chi_j u_i) - D(\rho) - C\|g^2\|_{\frac{6}{5}}^2 N\beta^{-1}Z^s \\ & -\alpha^{-1}\sum_{i=1}^{N}\sum_{j=1}^{3}(u_i, L_j u_i), \end{aligned} \tag{B7}$$

with

$$h := \alpha^{-1}T(\mathbf{p}) - \frac{Z}{|\cdot|} - \frac{\nu\, \chi_{B_R(\mathbf{P})}(\cdot)}{|\cdot - \mathbf{P}|} + \rho * \Phi_s * \frac{1}{|\cdot|},$$

and L_j is the operator (defined in Theorem 2.1) that gives the error due to the localization in the kinetic energy. We first estimate this error term. Using the definition of L_j we find for all $j \in \{1, 2, 3\}$, $i \in \{1, \ldots, N\}$

$$(u_i, L_j u_i) \leq \frac{\alpha^{-2}}{4\pi^2}\|\nabla\chi_j\|_\infty^2 \iint K_2(\alpha^{-1}|\mathbf{x} - \mathbf{y}|)|u_i(\mathbf{y})||u_i(\mathbf{x})|\, d\mathbf{x}d\mathbf{y}.$$

We then obtain by using Schwarz's inequality

$$\alpha^{-1}\sum_{i=1}^{N}\sum_{j=1}^{3}(u_i, L_j u_i) \leq \frac{\alpha^{-3}}{4\pi^2}\sum_{j=1}^{3}\|\nabla\chi_j\|_\infty^2 \sum_{i=1}^{N}\int K_2(\alpha^{-1}|\mathbf{z}|)d\mathbf{z} \leq CN\beta^{-2}Z^{2t}, \tag{B8}$$

since from (15)

$$\int_{\mathbb{R}^3} K_2(\alpha^{-1}|\mathbf{z}|)\, d\mathbf{z} = \alpha^3\int_{\mathbb{R}^3} K_2(|\mathbf{z}|)\, d\mathbf{z} = 4\pi\alpha^3\int_0^\infty t^2K_2(t)\, dt = 6\pi^2\alpha^3. \tag{B9}$$

Collecting together (B7) and (B8) we get

$$\langle\psi, H_{\mathbf{P}}\psi\rangle \geq \sum_{i=1}^{N}\sum_{j=1}^{3}(\chi_j u_i, h\chi_j u_i) - D(\rho) - C\beta^{-2}Z^{1+2t} - C\beta^{-1}Z^{7/4-t/4}. \tag{B10}$$

Here we used that $N \leq 2Z+1$, the choice of s and that we may choose g such that $\|\nabla g\|_2^2 \leq 2\pi$.

Near the nuclei. When $j = 1$ in the summation in the first term on the right hand side of (B10) we find

$$\sum_{i=1}^{N}(\chi_1 u_i, h\chi_1 u_i) \geq \sum_{i=1}^{N}(\chi_1 u_i, (\alpha^{-1}T(\mathbf{p}) - \frac{Z}{|\cdot|})\chi_1 u_i),$$

since $\chi_{B_R(\mathbf{P})}\chi_1 \equiv 0$ by the choice of χ_1, and the term $\Phi_s * \rho * \frac{1}{|\cdot|}$ is non-negative. Then by Theorem 2.10 we find

$$\begin{aligned}\sum_{i=1}^{N}(\chi_1 u_i, h\chi_1 u_i) &\geq \operatorname{Tr}[\alpha^{-1}T(\mathbf{p}) - \frac{Z}{|\cdot|}\chi_{|\mathbf{x}|<\frac{1}{2}\beta Z^{-t}}]_- \\ &\geq -C\beta^{1/2}Z^{5/2-t/2} - C\kappa^2 Z^2.\end{aligned} \tag{B11}$$

To estimate from below the term corresponding to $j = 2$ in the sum on the right hand side of (B10) we use [24, Theorem 2.8]. Here we need the result in [24] (instead of Theorem 2.10) because of the presence of the two nuclei. Notice that Theorem 2.10 can be extended to include also different nuclei. We have

$$\begin{aligned}\sum_{i=1}^{N}(\chi_2 u_i, h\chi_2 u_i) &\geq \sum_{i=1}^{N}(\chi_2 u_i, (\alpha^{-1}T(\mathbf{p}) - \frac{Z}{|\mathbf{x}|} - \frac{\nu}{|\mathbf{x}-\mathbf{P}|}\chi_{B_R(\mathbf{P})})\chi_2 u_i) \\ &\geq \operatorname{Tr}[\alpha^{-1}T(\mathbf{p}) - \frac{Z}{|\mathbf{x}|}\chi_{|\mathbf{x}-\mathbf{P}|<\frac{1}{2}\beta Z^{-t}} - \frac{\nu}{|\mathbf{x}-\mathbf{P}|}\chi_{B_R(\mathbf{P})}]_-,\end{aligned}$$

and by [24, Theorem 2.8] we get

$$\begin{aligned}\sum_{i=1}^{N}(\chi_2 u_i, h\chi_2 u_i) &\geq -CZ^{5/2}\alpha^{1/2} - C\int_{\frac{1}{2}\beta Z^{-t}>|\mathbf{x}-\mathbf{P}|>\alpha}\left(\frac{Z^{5/2}}{|\mathbf{x}|^{5/2}} + \alpha^3\frac{Z^4}{|\mathbf{x}|^4}\right)\,d\mathbf{x} \\ &\quad -C\int_{R>|\mathbf{x}-\mathbf{P}|>\alpha}\left(\frac{\nu^{5/2}}{|\mathbf{x}-\mathbf{P}|^{5/2}} + \alpha^3\frac{\nu^4}{|\mathbf{x}-\mathbf{P}|^4}\right)\,d\mathbf{x} \\ &\geq -C\kappa^{1/2}Z^2 - C\beta^{1/2}Z^{5/2-t/2} - C\kappa^2 Z^2.\end{aligned} \tag{B12}$$

Here we used that $t < l$ and $Z\alpha = \kappa$.

The outer zone. This region gives the main contribution to the energy. The term in (B10) that we still have to study is

$$\sum_{i=1}^{N}(\chi_3 u_i, h\chi_3 u_i) - D(\rho) \tag{B13}$$

We start by estimating the first term in (B13) using coherent states.

We consider again the function $g \in \mathcal{C}_0^\infty(\mathbb{R}^3)$ introduced at the beginning of the proof and we define the function

$$g_s(\mathbf{x}) := (\beta/(8Z^s))^{-\frac{3}{2}}g(8Z^s\mathbf{x}/\beta) = \Phi_s^{\frac{1}{2}}(\mathbf{x}), \tag{B14}$$

with s the same parameter as before. For simplicity of notation we write $\tilde V := Z/|\mathbf{x}| - \rho * 1/|\mathbf{x}|$. Then

$$\frac{Z}{|\mathbf{x}|} - \rho * \Phi_s * \frac{1}{|\mathbf{x}|} = \tilde V * \Phi_s - Z\Phi_s * \frac{1}{|\mathbf{x}|} + \frac{Z}{|\mathbf{x}|}.$$

Since $\mathrm{supp}(g_s) \cap \mathrm{supp}(\chi_3) = \emptyset$ by Newton's Theorem we find

$$\sum_{i=1}^N (\chi_3 u_i, h\chi_3 u_i) = \sum_{i=1}^N (\chi_3 u_i, (\alpha^{-1}T(\mathbf{p}) - \tilde V * \Phi_s)\chi_3 u_i). \tag{B15}$$

We consider the coherent states $g_s^{\mathbf{p},\mathbf{q}}$ defined for $\mathbf{p}, \mathbf{q} \in \mathbb{R}^3$ by

$$g_s^{\mathbf{p},\mathbf{q}}(\mathbf{x}) = g_s(\mathbf{x} - \mathbf{q})e^{-i\mathbf{p}.\mathbf{x}}.$$

The following formulas hold for $f \in H^{\frac12}(\mathbb{R}^3, \mathbb{C})$

$$\begin{aligned} (f, f) &= \tfrac{1}{(2\pi)^3} \int_{\mathbb{R}^3} d\mathbf{p} \int_{\mathbb{R}^3} d\mathbf{q}\, (f, g_s^{\mathbf{p},\mathbf{q}})\, (g_s^{\mathbf{p},\mathbf{q}}, f), \\ (f, V * g_s^2 f) &= \tfrac{1}{(2\pi)^3} \int_{\mathbb{R}^3} d\mathbf{p} \int_{\mathbb{R}^3} d\mathbf{q}\, V(\mathbf{q})\, (f, g_s^{\mathbf{p},\mathbf{q}})\, (g_s^{\mathbf{p},\mathbf{q}}, f) \end{aligned} \tag{B16}$$

and

$$\begin{aligned} (f, T(\mathbf{p})f) &= \tfrac{1}{(2\pi)^3} \int_{\mathbb{R}^3} d\mathbf{p} \int_{\mathbb{R}^3} d\mathbf{q}\, T(\mathbf{p})\, (f, g_s^{\mathbf{p},\mathbf{q}})\, (g_s^{\mathbf{p},\mathbf{q}}, f) \\ &\quad - \int_{\mathbb{R}^3} d\mathbf{x} \int_{\mathbb{R}^3} d\mathbf{q} \overline{f(\mathbf{x})}(L_q f)(\mathbf{x}), \end{aligned} \tag{B17}$$

where L_q has integral kernel

$$L_q(\mathbf{x}, \mathbf{y}) = \frac{\alpha^{-2}}{4\pi^2} |g_s(\mathbf{x} - \mathbf{q}) - g_s(\mathbf{y} - \mathbf{q})|^2 \frac{K_2(\alpha^{-1}|\mathbf{x} - \mathbf{y}|)}{|\mathbf{x} - \mathbf{y}|^2}.$$

Using these formulas we can rewrite (B15) as follows

$$\begin{aligned} &\sum_{i=1}^N (\chi_3 u_i, (\alpha^{-1}T(\mathbf{p}) - \tilde V * \Phi_s)\chi_3 u_i) \\ = \;& \tfrac{1}{(2\pi)^3}\alpha^{-1} \int_{\mathbb{R}^3} d\mathbf{p} \int_{\mathbb{R}^3} d\mathbf{q} (T(\mathbf{p}) - \alpha \tilde V(\mathbf{q})) \sum_{j=1}^q \sum_{i=1}^N |(\chi_3 u_i^j, g_s^{\mathbf{p},\mathbf{q}})|^2 \\ &- \alpha^{-1} \sum_{i=1}^N \int_{\mathbb{R}^3} d\mathbf{x} \int_{\mathbb{R}^3} d\mathbf{q}\, \overline{\chi_3 u_i(\mathbf{x})} (L_{\mathbf{q}} \chi_3 u_i)(\mathbf{x}), \end{aligned} \tag{B18}$$

Here u_i^j is the j-th spin component of u_i. We start by estimating the error term, the last term on the right hand side of (B18). From the definition of $L_{\mathbf{q}}$ it follows

$$L_q(\mathbf{x}, \mathbf{y}) \le \frac{\alpha^{-2}}{4\pi^2} \|\nabla g_s\|_\infty^2 K_2(\alpha^{-1}|\mathbf{x} - \mathbf{y}|)(\chi_{\mathrm{supp}(g_s)}(\mathbf{x} - \mathbf{q}) + \chi_{\mathrm{supp}(g_s)}(\mathbf{y} - \mathbf{q})),$$

and by the definition of the function g_s

$$\int_{\mathbb{R}^3} L_q(\mathbf{x}, \mathbf{y})\, d\mathbf{q} \le C\|\nabla g\|_\infty^2 \alpha^{-2}\beta^{-2} Z^{2s} K_2(\alpha^{-1}|\mathbf{x} - \mathbf{y}|).$$

By the estimate above, Schwarz's inequality, (B9) and the choice of s we find

$$\alpha^{-1}\sum_{i=1}^{N}\int_{\mathbb{R}^3} d\mathbf{x}\int_{\mathbb{R}^3} d\mathbf{q}\ \overline{\chi_3 u_i(\mathbf{x})}(L_{\mathbf{q}}\chi_3 u_i)(\mathbf{x}) \le C\|\nabla g\|_\infty^2 \beta^{-2} Z^{3/2-t/2} N. \tag{B19}$$

It remains to study the first term on the right hand side of (B18). In order to get an estimate from below we consider only the negative part of the integrand. Moreover, since if $|\mathbf{q}| < \beta Z^{-t}/8$ then $\mathrm{supp}(\chi_3 g_s^{\mathbf{p},\mathbf{q}}) = \emptyset$ (because $Z^{-t} > Z^{-s}$ since $s > t$) we find

$$\begin{aligned} &\tfrac{1}{(2\pi)^3}\alpha^{-1}\int_{\mathbb{R}^3} d\mathbf{p}\int_{\mathbb{R}^3} d\mathbf{q}\ (T(\mathbf{p}) - \alpha\tilde V(\mathbf{q}))\sum_{j=1}^{q}\sum_{i=1}^{N}|(\chi_3 u_i^j, g_s^{\mathbf{p},\mathbf{q}})|^2 \\ \ge\ & \tfrac{q}{(2\pi)^3}\alpha^{-1}\int_{|\mathbf{q}|\ge\frac18\beta Z^{-t}} d\mathbf{q}\int_{T(\mathbf{p})-\alpha\tilde V(\mathbf{q})\le 0} d\mathbf{p}\ (T(\mathbf{p}) - \alpha\tilde V(\mathbf{q})) = \dots, \end{aligned} \tag{B20}$$

where we also use that $\sum_{i=1}^N |(\chi_3 u_i^j, g_s^{\mathbf{p},\mathbf{q}})|^2 \le 1$ (Bessel's inequality). We split now the integral as a sum of two terms

$$\begin{aligned} \dots\ =\ & \tfrac{q}{(2\pi)^3}\alpha^{-1}\iint_{\substack{\frac12|\mathbf{p}|^2-\tilde V(\mathbf{q})\le 0\\ |\mathbf{q}|\ge\frac18\beta Z^{-t}}} d\mathbf{q}d\mathbf{p}\ (T(\mathbf{p}) - \alpha\tilde V(\mathbf{q})) \\ +\ & \tfrac{q}{(2\pi)^3}\alpha^{-1}\iint_{\substack{\frac{\alpha}{2}|\mathbf{p}|^2\ge\alpha\tilde V(\mathbf{q})\ge T(\mathbf{p})\\ |\mathbf{q}|\ge\frac18\beta Z^{-t}}} d\mathbf{q}d\mathbf{p}\ (T(\mathbf{p}) - \alpha\tilde V(\mathbf{q})). \end{aligned} \tag{B21}$$

We consider these two terms separately. The second term in (B21) gives a lower order contribution. Indeed

$$\begin{aligned} &\tfrac{q}{(2\pi)^3}\alpha^{-1}\iint_{\substack{\frac{\alpha}{2}|\mathbf{p}|^2\ge\alpha\tilde V(\mathbf{q})\ge T(\mathbf{p})\\ |\mathbf{q}|\ge\frac18\beta Z^{-t}}} d\mathbf{q}d\mathbf{p}\ (T(\mathbf{p}) - \alpha\tilde V(\mathbf{q})) \\ \ge\ & -\tfrac{q}{(2\pi)^3}\iint_{\substack{(\alpha^2[\tilde V(\mathbf{q})]_+^2+2[\tilde V(\mathbf{q})]_+)^{\frac12}\ge|\mathbf{p}|\ge(2[\tilde V(\mathbf{q})]_+)^{\frac12}\\ |\mathbf{q}|\ge\frac18\beta Z^{-t}}} d\mathbf{q}d\mathbf{p}\ [\tilde V(\mathbf{q})]_+ = \dots, \end{aligned}$$

and computing the $\mathbf{p}$-integral

$$\dots = -C\int_{|\mathbf{q}|\ge\frac18\beta Z^{-t}} d\mathbf{q}\ [\tilde V(\mathbf{q})]_+^{\frac52}((1+\frac{\alpha^2}{2}[\tilde V(\mathbf{q})]_+)^{\frac32} - 1) = \dots .$$

Using $(1+x)^{\frac32} \le 1 + \frac32 x + \frac38 x^2$ and that $[\tilde V(\mathbf{q})]_+ \le Z/|\mathbf{q}|$ we get computing the integral

$$\begin{aligned} \dots\ =\ & -C\alpha^2\textstyle\int_{|\mathbf{q}|\ge\frac18\beta Z^{-t}} d\mathbf{q}\ [\tilde V(\mathbf{q})]_+^{\frac72}(1+\frac{\alpha^2}{8}[\tilde V(\mathbf{q})]_+) \\ \ge\ & -C\beta^{-\frac12}\kappa^2 Z^{3/2+t/2} - C\kappa^4\beta^{-\frac32}Z^{1/2+3t/2}. \end{aligned} \tag{B22}$$

Here we use that $Z\alpha = \kappa$.

Since $\sqrt{1+x} \ge 1 + x/2 - x^3/8$ for all $x > 0$, we have

$$T(\mathbf{p}) \ge \alpha\tfrac12|\mathbf{p}|^2 - \alpha^3\tfrac18|\mathbf{p}|^4,$$

and, for the first term on the right hand side of (B21), we obtain

$$\begin{aligned} &\tfrac{q}{(2\pi)^3}\alpha^{-1}\iint_{\substack{\frac12|\mathbf{p}|^2-\tilde V(\mathbf{q})\le 0\\ |\mathbf{q}|\ge\frac18\beta Z^{-t}}} d\mathbf{q}d\mathbf{p}\ (T(\mathbf{p}) - \alpha\tilde V(\mathbf{q})) \ge \\ \ge\ & \tfrac{q}{(2\pi)^3}\iint_{\substack{\frac12|\mathbf{p}|^2-\tilde V(\mathbf{q})\le 0\\ |\mathbf{q}|\ge\frac18\beta Z^{-t}}} d\mathbf{q}d\mathbf{p}\ (\tfrac12|\mathbf{p}|^2 - \tfrac18\alpha^2|\mathbf{p}|^4 - \tilde V(\mathbf{q})) = \dots . \end{aligned}$$

Computing now the integral with respect to $\mathbf{p}$, we find

$$\cdots = -\frac{2^{\frac{3}{2}}q}{15\pi^2}\int_{|\mathbf{q}|>\frac{1}{8}\beta Z^{-t}}[\tilde{V}(\mathbf{q})]_+^{\frac{5}{2}}\,d\mathbf{q} - C\alpha^2\int_{|\mathbf{q}|>\frac{1}{8}\beta Z^{-t}}[\tilde{V}(\mathbf{q})]_+^{\frac{7}{2}}\,d\mathbf{q}. \tag{B23}$$

We see that the second term on the right hand side of (B23) gives a lower order contribution since it is of the same order as the one in (B22).

Collecting together (B10), (B11), (B12), (B15), (B18), (B19), (B22) and (B23)

$$\langle\psi, H_{\mathbf{P}}\psi\rangle \;\; \geq \;\; -C(\beta^{\frac{1}{2}}+\beta^{-2})Z^{5/2-t/2} - \frac{2^{\frac{3}{2}}q}{15\pi^2}\int_{\mathbb{R}^3}[\tilde{V}(\mathbf{q})]_+^{\frac{5}{2}}\,d\mathbf{q} - D(\rho)\,. \tag{B24}$$

Here we used also that $N < 2Z+1$, the choice of s and that $t \leq 3/5$.

Now we choose $\rho = \rho^{\mathrm{TF}}$ the minimizer of the TF-energy functional of a neutral atom with Coulomb potential and nuclear charge Z. Hence ρ^{TF} satisfies the TF-equation

$$\tfrac{1}{2}\big(\tfrac{6\pi^2}{q}\big)^{\frac{2}{3}}\rho^{\mathrm{TF}}(\mathbf{x})^{\frac{2}{3}} = [\tilde{V}(\mathbf{x})]_+,$$

since $\tilde{V}$ is the TF-mean field potential. Notice that here we use that the chemical potential of a neutral atom is zero. By the choice of ρ from the TF-equation it follows from (B24) that

$$\begin{aligned}\langle\psi, H_{\mathbf{P}}\psi\rangle \;\; &\geq \;\; -C(\beta^{\frac{1}{2}}+\beta^{-2})Z^{5/2-t/2} + \tfrac{3}{10}\big(\tfrac{6\pi^2}{q}\big)^{\frac{2}{3}}\int_{\mathbb{R}^3}d\mathbf{x}\,\rho^{\mathrm{TF}}(\mathbf{x})^{\frac{5}{3}} \\ &\quad -Z\int_{\mathbb{R}^3}\frac{\rho^{\mathrm{TF}}(\mathbf{x})}{|\mathbf{x}|}\,d\mathbf{x} + D(\rho^{\mathrm{TF}}) \\ &= \;\; \mathcal{E}^{\mathrm{TF}}(\rho^{\mathrm{TF}}) - C(\beta^{\frac{1}{2}}+\beta^{-2})Z^{5/2-t/2}\,.\end{aligned}$$

The claim follows. □

Proposition B.2. *Let ρ^{TF} be the minimizer of the TF-energy functional of a neutral atom with nuclear charge Z. Let $Z\alpha = \kappa$ be fixed with $0 \leq \kappa < 2/\pi$ and $Z \geq 1$.*

Then there is a constant depending only on κ and q such that for all $\{u_i\}_{i=1}^N \subset H^{\frac{1}{2}}(\mathbb{R}^3;\mathbb{C}^q)$ orthonormal in $L^2(\mathbb{R}^3)$ we have

$$\sum_{i=1}^{N}(u_i,(\alpha^{-1}T(\mathbf{p}) - \varphi^{\mathrm{TF}})u_i) - D(\rho^{\mathrm{TF}}) \geq \mathcal{E}^{\mathrm{TF}}(\rho^{\mathrm{TF}}) - CZ^{2+\frac{1}{5}}\,,$$

with $D(\cdot) = D(\cdot,\cdot)$ the Coulomb scalar product.

Proof. Since $\mathcal{E}^{\mathrm{TF}}(\rho^{\mathrm{TF}}) = -e_0 Z^{\frac{7}{3}}$ (see (12)) to prove the claim it is sufficient to show that the TF-energy gives a lower bound to the quantum energy modulo lower order terms. In the proof we localize the energy separating the contribution from the region near the nucleus to the one far away. The region far away from the nuclei will give the TF-energy.

In the proof C denotes a generic universal positive constant.

Choice of the localization. The localization will be given by the functions $\chi_1 \in C_0^\infty(\mathbb{R}^3)$ and $\chi_2 \in C^\infty(\mathbb{R}^3)$ such that: $0 \leq \chi_1, \chi_2 \leq 1$, $\chi_1^2 + \chi_2^2 = 1$ in $\mathbb{R}^3$,

$$\chi_1(\mathbf{x}) := \begin{cases} 1 & \text{if } |\mathbf{x}| < 2Z^{-3/5}, \\ 0 & \text{if } |\mathbf{x}| > 3Z^{-3/5}. \end{cases} \tag{B25}$$

Moreover we ask that

$$\|\nabla\chi_1\|_\infty, \|\nabla\chi_2\|_\infty \leq 2^2 Z^{3/5}. \tag{B26}$$

The localization in the energy expectation. We insert now the localization in the energy expectation. From Theorem 2.1 we find

$$\begin{aligned}&\sum_{i=1}^{N}(u_i,(\alpha^{-1}T(\mathbf{p})-\varphi^{\mathrm{TF}})u_i)-D(\rho^{\mathrm{TF}}) \\ \geq\ &\sum_{i=1}^{N}\sum_{j=1}^{2}(\chi_j u_i,(\alpha^{-1}T(\mathbf{p})-\varphi^{\mathrm{TF}})\chi_j u_i)-D(\rho^{\mathrm{TF}})-\alpha^{-1}\sum_{i=1}^{N}\sum_{j=1}^{2}(u_i,L_j u_i),\end{aligned} \tag{B27}$$

with L_j is the operator (defined in Theorem 2.1) that gives the error due to the localization in the kinetic energy. We first estimate this error term. Since $N \leq 2Z+1$ we find as in (B8) that

$$\alpha^{-1}\sum_{i=1}^{N}\sum_{j=1}^{2}(u_i,L_j u_i)\leq CZ^{6/5}N\leq CZ^{2+1/5}\,. \tag{B28}$$

Near the nucleus. Since

$$\sum_{i=1}^{N}(\chi_1 u_i,(\alpha^{-1}T(\mathbf{p})-\varphi^{\mathrm{TF}})\chi_1 u_i)\geq \mathrm{Tr}[\alpha^{-1}T(\mathbf{p})-\varphi^{\mathrm{TF}}\chi_{|\mathbf{x}|<3Z^{-3/5}}]_-,$$

by Theorem 2.10 with $R=3Z^{-3/5}$ we find

$$\sum_{i=1}^{N}(\chi_1 u_i,(\alpha^{-1}T(\mathbf{p})-\varphi^{\mathrm{TF}})\chi_1 u_i)\geq -CZ^{2+1/5}-C\kappa^2 Z^2. \tag{B29}$$

Here we use that $Z\alpha=\kappa$.

The outer zone. This region gives the main contribution to the energy.

Let $g\in C_0^\infty(\mathbb{R}^3)$, $g\geq 0$ be spherically symmetric with $\mathrm{supp}(g)\subset B_1(0)$ and such that $\|g\|_2=1$. Starting from these g we define $\Phi_Z(\mathbf{x}):=(Z^{-3/5})^{-3}g^2(\mathbf{x}Z^{3/5})$ and

$$g_Z(\mathbf{x}):=(Z^{-3/5})^{-\frac{3}{2}}g(\mathbf{x}Z^{3/5})=\Phi_Z^{\frac{1}{2}}(\mathbf{x}).$$

Since $\mathrm{supp}(g_Z)\cap\mathrm{supp}(\chi_2)=\emptyset$ by Newton's Theorem we find

$$\sum_{i=1}^{N}(\chi_2 u_i,(\alpha^{-1}T(\mathbf{p})-\varphi^{\mathrm{TF}})\chi_2 u_i)=\sum_{i=1}^{N}(\chi_2 u_i,(\alpha^{-1}T(\mathbf{p})-\varphi^{\mathrm{TF}}*\Phi_Z)\chi_2 u_i). \tag{B30}$$

We consider the coherent states $g_Z^{\mathbf{p},\mathbf{q}}$ defined for $\mathbf{p},\mathbf{q}\in\mathbb{R}^3$ by

$$g_Z^{\mathbf{p},\mathbf{q}}(\mathbf{x})=g_Z(\mathbf{x}-\mathbf{q})e^{-i\mathbf{p}.\mathbf{x}}.$$

Using formulas (B16) and (B17) we can rewrite (B30) as follows

$$\begin{aligned}&\sum_{i=1}^{N}(\chi_2 u_i,(\alpha^{-1}T(\mathbf{p})-\varphi^{\mathrm{TF}}*g_Z^2)\chi_2 u_i) \\ =\ &\tfrac{1}{(2\pi)^3}\alpha^{-1}\int_{\mathbb{R}^3}d\mathbf{p}\int_{\mathbb{R}^3}d\mathbf{q}(T(\mathbf{p})-\alpha\varphi^{\mathrm{TF}}(\mathbf{q}))\sum_{j=1}^{q}\sum_{i=1}^{N}|(\chi_2 u_i^j,g_Z^{\mathbf{p},\mathbf{q}})|^2 \\ &-\alpha^{-1}\sum_{i=1}^{N}\int_{\mathbb{R}^3}d\mathbf{x}\int_{\mathbb{R}^3}d\mathbf{q}\,\overline{\chi_2 u_i(\mathbf{x})}(L_{\mathbf{q}}\chi_2 u_i)(\mathbf{x}),\end{aligned} \tag{B31}$$

Here u_i^j is the j-th spin component of u_i. We start by estimating the error term, the last term on the right hand side of (B31). We find as in (B19) that

$$\alpha^{-1}\sum_{i=1}^{N}\int_{\mathbb{R}^3} d\mathbf{x}\int_{\mathbb{R}^3} d\mathbf{q}\;\overline{\chi_2 u_i(\mathbf{x})}(L_{\mathbf{q}}\chi_2 u_i)(\mathbf{x}) \le C\|\nabla g\|_\infty^2 Z^{6/5}N. \tag{B32}$$

It remains to study the first term on the right hand side of (B31). In order to get an estimate from below we consider only the negative part of the integrand. Moreover, since if $|\mathbf{q}|<Z^{-3/5}$ then $\mathrm{supp}(\chi_2 g_Z^{\mathbf{p},\mathbf{q}})=\emptyset$ we find

$$\begin{aligned}
&\tfrac{1}{(2\pi)^3}\alpha^{-1}\int_{\mathbb{R}^3} d\mathbf{p}\int_{\mathbb{R}^3} d\mathbf{q}\;(T(\mathbf{p})-\alpha\varphi^{\mathrm{TF}}(\mathbf{q}))\sum_{j=1}^{q}\sum_{i=1}^{N}|(\chi_2 u_i^j, g_Z^{\mathbf{p},\mathbf{q}})|^2\\
\ge\;& \tfrac{q}{(2\pi)^3}\alpha^{-1}\int_{|\mathbf{q}|\ge Z^{-3/5}} d\mathbf{q}\int_{T(\mathbf{p})-\alpha\varphi^{\mathrm{TF}}(\mathbf{q})\le 0} d\mathbf{p}\;(T(\mathbf{p})-\alpha\varphi^{\mathrm{TF}}(\mathbf{q})) = \ldots,
\end{aligned}\tag{B33}$$

where we also use that $\sum_{i=1}^N |(\chi_3 u_i^j, g_Z^{\mathbf{p},\mathbf{q}})|^2\le 1$ (Bessel's inequality). We split now the integral as a sum of two terms

$$\begin{aligned}
\ldots \;=\;& \tfrac{q}{(2\pi)^3}\alpha^{-1}\iint_{\substack{\frac12|\mathbf{p}|^2-\varphi^{\mathrm{TF}}(\mathbf{q})\le 0\\ |\mathbf{q}|\ge Z^{-3/5}}} d\mathbf{q}d\mathbf{p}\;(T(\mathbf{p})-\alpha\varphi^{\mathrm{TF}}(\mathbf{q}))\\
+\;& \tfrac{q}{(2\pi)^3}\alpha^{-1}\iint_{\substack{\frac{\alpha}{2}|\mathbf{p}|^2\ge\alpha\varphi^{\mathrm{TF}}(\mathbf{q})\ge T(\mathbf{p})\\ |\mathbf{q}|\ge Z^{-3/5}}} d\mathbf{q}d\mathbf{p}\;(T(\mathbf{p})-\alpha\varphi^{\mathrm{TF}}(\mathbf{q})).
\end{aligned}\tag{B34}$$

We consider these two terms separately. The second term in (B34) gives a lower order contribution. Indeed

$$\begin{aligned}
&\tfrac{q}{(2\pi)^3}\alpha^{-1}\iint_{\substack{\frac{\alpha}{2}|\mathbf{p}|^2\ge\alpha\varphi^{\mathrm{TF}}(\mathbf{q})\ge T(\mathbf{p})\\ |\mathbf{q}|\ge Z^{-3/5}}} d\mathbf{q}d\mathbf{p}\;(T(\mathbf{p})-\alpha\varphi^{\mathrm{TF}}(\mathbf{q}))\\
\ge\;& -\tfrac{q}{(2\pi)^3}\iint_{\substack{(\alpha^2[\varphi^{\mathrm{TF}}]_+^2+2[\varphi^{\mathrm{TF}}]_+)^{\frac12}\ge|\mathbf{p}|\ge(2[\varphi^{\mathrm{TF}}(\mathbf{q})]_+)^{\frac12}\\ |\mathbf{q}|\ge Z^{-3/5}}} d\mathbf{q}d\mathbf{p}\;[\varphi^{\mathrm{TF}}(\mathbf{q})]_+ = \ldots,
\end{aligned}$$

and computing the integral in $\mathbf{p}$

$$\cdots = -C\int_{|\mathbf{q}|\ge Z^{-3/5}} d\mathbf{q}\;[\varphi^{\mathrm{TF}}(\mathbf{q})]_+^{\frac52}((1+\frac{\alpha^2}{2}[\varphi^{\mathrm{TF}}(\mathbf{q})]_+)^{\frac32}-1) = \ldots.$$

Using $(1+x)^{\frac32}\le 1+\frac32 x+\frac38 x^2$ and that $[\varphi^{\mathrm{TF}}(\mathbf{q})]_+\le Z/|\mathbf{q}|$ we get computing the integral

$$\begin{aligned}
\ldots \;=\;& -C\alpha^2\int_{|\mathbf{q}|\ge Z^{-3/5}} d\mathbf{q}\;[\varphi^{\mathrm{TF}}]_+^{\frac72}(1+\frac{\alpha^2}{8}[\varphi^{\mathrm{TF}}(\mathbf{q})]_+)\\
\ge\;& -C\kappa^2 Z^{2-\frac15}-C\kappa^4 Z^{\frac75}.
\end{aligned}\tag{B35}$$

Since $\sqrt{1+x}\ge 1+x/2-x^3/8$ for all $x\ge 0$, we have

$$T(\mathbf{p})\ge \alpha\tfrac12|\mathbf{p}|^2-\alpha^3\tfrac18|\mathbf{p}|^4,$$

and, for the first term on the right hand side of (B34), we obtain

$$\begin{aligned}
&\tfrac{q}{(2\pi)^3}\alpha^{-1}\iint_{\substack{\frac12|\mathbf{p}|^2-\varphi^{\mathrm{TF}}(\mathbf{q})\le 0\\ |\mathbf{q}|\ge Z^{-3/5}}} d\mathbf{q}d\mathbf{p}\;(T(\mathbf{p})-\alpha\varphi^{\mathrm{TF}}(\mathbf{q}))\ge\\
\ge\;& \tfrac{q}{(2\pi)^3}\iint_{\substack{\frac12|\mathbf{p}|^2-\varphi^{\mathrm{TF}}(\mathbf{q})\le 0\\ |\mathbf{q}|\ge Z^{-3/5}}} d\mathbf{q}d\mathbf{p}\;(\tfrac12|\mathbf{p}|^2-\tfrac18\alpha^2|\mathbf{p}|^4-\varphi^{\mathrm{TF}}(\mathbf{q})) = \ldots.
\end{aligned}$$

Computing now the integral with respect to $\mathbf{p}$, we find

$$\cdots = -\frac{2^{\frac{3}{2}}q}{15\pi^2}\int_{|\mathbf{q}|>Z^{-3/5}}[\varphi^{\mathrm{TF}}(\mathbf{q})]_+^{\frac{5}{2}}\,d\mathbf{q} - C\alpha^2\int_{|\mathbf{q}|>Z^{-3/5}}[\varphi^{\mathrm{TF}}(\mathbf{q})]_+^{\frac{7}{2}}\,d\mathbf{q}. \tag{B36}$$

We see that the second term on the right hand side of (B36) gives a lower order contribution since it is of the same order as the one in (B35).

Starting from (B27), by (B28), (B29), (B32), (B35) and (B36) we find

$$\begin{aligned}&\sum_{i=1}^{N}(u_i,(\alpha^{-1}T(\mathbf{p})-\varphi^{\mathrm{TF}})u_i)-D(\rho^{\mathrm{TF}}) \qquad\qquad (\mathrm{B37})\\ \geq\ & -C(Z^{2+1/5}+Z^2+Z^{2-1/5}+Z^{7/5})-\frac{2^{\frac{3}{2}}q}{15\pi^2}\int_{\mathbb{R}^3}[\varphi^{\mathrm{TF}}(\mathbf{q})]_+^{\frac{5}{2}}\,d\mathbf{q}-D(\rho^{\mathrm{TF}}).\end{aligned}$$

The result follows from the TF-equation. □

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