Analytic Studies of Atomic Structures and the Efimov Effect

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ABSTRACT

This dissertation combines several of the results I obtained during my doctoral research under the supervision of Dirk Hundertmark and Semjon Vugalter, as well as in collaboration with Nikolaos Pattakos. The primary results of this dissertation are presented in the following manuscripts:

1. *On the Excess Charge Problem of Atoms*
2. *Why a System of Three Bosons on Separate Lines Can Not Exhibit the Confinement-Induced Efimov Effect*
3. *Conspiracy of Potential Wells and Absence of the Efimov Effect in Dimension Four*

The results presented are centered on the mathematical analysis of many–body systems in quantum mechanics. The nature of the models we studied naturally leads to intersections with various disciplines in mathematics and physics, including functional analysis, spectral theory, calculus of variations, partial differential equations, and many-body quantum mechanics. Each of the results above discusses the structure of the spectrum of many–particle Schrödinger operators. In particular, we derive criteria under which the corresponding operators will not have a discrete spectrum, or if it exists, we prove its finiteness. Our findings directly answer or improve upon open questions in the mathematical physics community.

Concerning the excess charge problem of atoms, we derive in [50] new bounds on the maximum number of electrons $N_c(Z)$ that an atom with nuclear charge Z can bind. Our main result establishes that

$$N_c(Z) < 1.1185Z + o\left(Z^{1/3}\right).$$

This finding represents a significant improvement and generalization of the argument developed by Benguria, Lieb, and Nam ([71], [81]). Notably, it highlights a fundamental distinction between fermionic and bosonic atoms in the finite Z regime: while for fermionic atoms $N_c(Z)$ satisfies the above bound, bosonic atoms exhibit a different behavior, where $\lim N_c(Z)/Z = t_c \approx 1.21$ (see [15]). Using ideas presented in [19] and [20] we are able to prove analytically $t_c < 1.47$ which directly proves new bounds on the maximal allowed excess charge in the Hartree model. We apply these improvements to obtain new bounds on $N_c(Z)$ for bosonic atoms with finite nuclear charge.
This research was conducted collaboratively with Dirk Hundertmark and Nikolaos Pattakos. Results from this manuscript were presented at the conference *Quantum Dynamics and Spectral Theory* in June 2024 at the *Institut Mittag-Leffler*. The manuscript has not yet been submitted to any Journal.

In parallel, we investigated new aspects of the Efimov effect. The research in [52] was conducted jointly with Dirk Hundertmark and Semjon Vugalter. We analyze a system of three geometrically constrained bosons. In particular, we study a system of three bosons with short-range interactions, each confined to a separate line in $\mathbb{R}^3$. Two of these lines are parallel within

a plane P. The third line intersects P at a nonzero angle and lies in a plane perpendicular to P, which intersects P in a line parallel to the first two lines. A recent prediction in the physics literature [84] suggested that such a configuration exhibits the so–called confinement–induced Efimov effect. However, we rigorously demonstrate that this prediction is incorrect by proving that the system can support at most finitely many bound states. This result is notable as it is one of the rare cases where predictions in the physics literature do not hold up to a rigorous mathematical analysis. Parts of this result were presented at the *International Congress on Mathematical Physics* in July 2024, during the *Young Researcher Symposium*. The manuscript has been submitted to *Forum of Mathematics, Sigma* and is currently under review.

We have studied particle binding mechanisms through the interplay of potential wells in dimension four. Together with Dirk Hundertmark and Semjon Vugalter, I have analyzed the asymptotic behavior of the ground-state energy of a quantum particle interacting with two separated short-range potentials. Our result refines existing lower bounds [90] for this ground-state energy. Additionally, we give a variational proof of the absence of the Efimov effect in a system of three interacting bosons in dimension four. The manuscript has not yet been submitted to any Journal.

Beyond the scope of the three aforementioned manuscripts, I have included several additional results in this dissertation that are not yet part of any planned publications. In particular, I have extended our findings on the excess charge problem to the pseudorelativistic case.
Regarding the Efimov effect, I establish pointwise bounds on the decay rates of zero-energy solutions for critical Schrödinger operators under minimal assumptions on the involved potentials. These estimates play a crucial role in the analysis of the Efimov effect and are, for instance, used in [113]. While these bounds are widely accepted in the field, to the best of our knowledge, a rigorous proof can not be found in the existing literature.

On the Structure of this Dissertation: This dissertation is partially cumulative, incorporating the content of the manuscripts [50], [52] and [51] as Chapters 4, 5 and 6 together with the Appendices A, B and C.
To provide some of the necessary background for these chapters, I begin in Chapter 1 with an overview of fundamental concepts in quantum mechanics, the relevant differential equations, and the basic notation used in this dissertation. More specifically, in Section 1.1 I discuss the Schrödinger equation, introducing key concepts and the specific choice of units employed in this work. Section 1.2 revisits the quadratic form approach and examines classes of physically relevant potentials that guarantee the self–adjointness of the Schrödinger operator. In Section 1.3, I discuss localization according to the IMS formula, along with Zhislin's criterion [129] for the finiteness of the discrete spectrum of a Schrödinger operator. Building on this groundwork, I introduce the concept of virtual levels in Section 1.4, following [59]. This concept is pivotal for understanding the Efimov effect, which is explored in subsequent sections. In Section 1.5, I then introduce each of the operators, which will be studied in Chapters 4, 5 and 6 and discuss the HVZ theorem for these operators.

The main results of this dissertation are summarized in Chapters 2 and 3, which provide an overview of the key findings from Chapters 4, 5, and 6. Furthermore, in Section 2.2, our results from [50] is applied to the pseudorelativistic case. Chapter 3 focuses on the Efimov effect. In Sections 3.2 and 3.3, we prove pointwise bounds on the decay rates of zero-energy solutions for critical Schrödinger operators under minimal assumptions on the involved potentials. Some of the more technical details in the proof of these estimates have been moved to Appendix D.

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I want to take a moment to acknowledge the individuals who have had the most significant impact on this thesis.

This dissertation is not just my achievement but a shared one, for no mathematician thrives in isolation. It is the result of the collective support of my teachers, peers, and the unwavering patience of my family. Together, we are proof that learning is a shared endeavor.

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Finally, this thesis, and all I have achieved, is dedicated to the most important person in my life: Annika Rosenboom.

Contents

Chapter 1

Preliminaries

1.1 Schrödinger Operator

The Schrödinger equation

$$i\hbar\partial_t\psi(x,t) = \left[\frac{P^2}{2m} + V(x)\right]\psi(x,t), \quad P = -i\hbar\nabla_x \tag{1.1.1}$$

is the fundamental equation of quantum mechanics where P denotes the quantum–mechanical momentum operator. It describes the state $\psi : \mathbb{R}^d \times \mathbb{R} \to \mathbb{C}$ of a particle of mass $m > 0$ in the potential V, where $|\psi(x,t)|^2$ is interpreted as the probability amplitude of finding the particle at a certain position $x \in \mathbb{R}^d$ at a given $t \in \mathbb{R}$. Here $\hbar = h/(2\pi)$ is the reduced Planck constant and h is the Planck constant which is one of the seven base units in the SI unit system and was set to a fixed value in 2019 (see Table 1.1). To allow for an interpretation as probability, we assume the normalization condition

$$\int_{\mathbb{R}^d} |\psi(x,t)|^2 dx = 1, \quad \forall t \in \mathbb{R}, \tag{1.1.2}$$

where $d \in \mathbb{N}$ denotes the dimension of the underlying configuration space.

Defining constant	**Symbol**	**Numerical value**	**Unit**
hyperfine transition frequency of Cs	$\Delta\nu_{\mathrm{Cs}}$	9 192 631 770	Hz
speed of light in vacuum	c	299 792 458	m s^{-1}
Planck constant	h	$6.626\,070\,15 \times 10^{-34}$	J s
elementary charge	e	$1.602\,176\,634 \times 10^{-19}$	C
Boltzmann constant	k	$1.380\,649 \times 10^{-23}$	J K^{-1}
Avogadro constant	N_A	$6.022\,140\,76 \times 10^{23}$	mol^{-1}
luminous efficacy	K_{cd}	683	lm W^{-1}

TABLE 1.1: Fundamental physical constants with their symbols, numerical values, and units according to the 2019 revision of the SI unit system [21].

Remark 1.1.1. *The natural choice is $d = 3$, but also any other choice for $d \in \mathbb{N}$ allows us to derive a corresponding Schrödinger equation in* (1.1.1) *by the so-called correspondence principle.*

Of particular interest are observables, i.e., self-adjoint operators that are connected to the Schrödinger equation. In comparison to classical mechanics (Hamilton approach), we denote by

$$T = \frac{P^2}{2m} = \frac{-\hbar^2}{2m}\Delta$$

the *kinetic energy* observable and for a given state $\psi \in L^2(\mathbb{R}^d)$

$$\langle \psi, T\psi \rangle = \frac{\hbar^2}{2m}\int_{\mathbb{R}^3} |\nabla\psi|^2 dx$$

the expectation value of the kinetic energy. Similarly for any potential $V : \mathbb{R}^d \to \mathbb{R}$

$$\langle \psi, V\psi \rangle = \int_{\mathbb{R}^3} V|\psi|^2 dx$$

denotes the expectation of the *potential energy*. Said this, it is natural to define the (one-particle) Schrödinger operator on $L^2(\mathbb{R}^d)$

$$H \coloneqq T + V\,. \tag{1.1.3}$$

As for T and V we denote by

$$\langle \psi, H\psi \rangle = \frac{\hbar^2}{2m}\int_{\mathbb{R}^3} |\nabla\psi|^2 dx + \int_{\mathbb{R}^3} V|\psi|^2 dx$$

the expectation of the energy associated with $\psi \in L^2(\mathbb{R}^d)$ at a given time $t \in \mathbb{R}$. A first step in the understanding of the time–dependent Schrödinger equation (1.1.1) is the study of the spectrum of the Schrödinger operator in (1.1.3) which is the focus of this dissertation. Of particular interest is the corresponding eigenvalue problem, namely the (stationary) Schrödinger equation

$$H\psi = E\psi\,. \tag{1.1.4}$$

Of course, H is not a self–adjoint operator for arbitrary potential V, however it turns out to be self–adjoint for almost any physically relevant situation. It is often convenient to work in terms of so-called quadratic forms rather than operators, which we discuss in Section 1.2.
In order to discuss magnetic fields, we can add a vector potential, namely a function $A : \mathbb{R}^d \to \mathbb{R}^d$, which determines the magnetic field $B = \nabla \wedge A$ (which is the curl of A in dimension $d = 3$). From classical mechanics in dimension $d = 3$ and in comparison to the Lorenz force $F_L = -e/c\,(\dot{x} \times B(x))$ of a single particle of charge e we define the magnetic

momentum operator and magnetic kinetic energy as

$$P_A = P + \frac{e}{c}A, \quad T_A = \frac{P_A^2}{2m} = \frac{1}{2m}\left(P + \frac{e}{c}A\right)^2 .$$

with e is the elementary charge and c the speed of light. Any of these physical constants $\hbar, e, c$ are measurable and have been set to the given fixed number as the fundamental base of the SI–Unit system.
The explicit values of the physical constants in Table 1.1 are of little importance for spectral properties of $H_A = T_A^2 + V$. Consider the rescaling $\psi_\lambda(x) = \lambda^{-d/2}\psi(\lambda^{-1}x)$, then

$$\langle \psi_\lambda, H_A\psi_\lambda\rangle = \left\langle \psi, \left[\lambda^{-2}\frac{\hbar^2}{2m}\left(-i\nabla + \lambda^2\frac{e}{\hbar c}A(\lambda x)\right)^2 + V(\lambda x)\right]\psi\right\rangle .$$

Choosing $\lambda = \lambda_c = \hbar/(mc)$ the Compton wave–length then we obtain the units

$$[\lambda_c] = \mathrm{m} \quad \text{and} \quad \left[\lambda_c^{-2}\frac{\hbar^2}{2m}\right] = \left[\frac{m^2c}{2}\right] = \mathrm{kg}\cdot\mathrm{m}^2/\mathrm{s}^2 = \mathrm{J}\,. \tag{1.1.5}$$

For example, $\lambda_c x$ has the unit of a length whenever $x \in \mathbb{R}$ is dimension–free. Note that $e^2/(\hbar c) = \alpha$ is the fine–structure constant that is dimension–free. Therefore, it is convenient to choose $\hbar = m = c = 1$ and consequently $\lambda_c = 1$ leading to a dimension-free description where all lengths and energies are implicitly measured with respect to the units defined in (1.1.5). The only remaining relevant physical constant is $e = \sqrt{\alpha}$. In the following, we will work in this dimension–free unit system. Consequently the corresponding one-particle Schrödinger operator is

$$H_A = T_A + V, \quad T_A = \frac{1}{2}(-i\nabla + \sqrt{\alpha}A)^2 .$$

For a particle with high kinetic energies, we keep track of the physical constants more carefully. It is well known that the relativistic kinetic energy has an asymptotically linear behavior in the momentum. It is usual to include the mass $m \geq 0$ in this description since the case $m \to 0$ covers a case called the ultrarelativistic case. From relativistic mechanics, we know the dispersion relation of a particle of mass $m > 0$

$$E_{kin} = \sqrt{c^2p^2 + (mc^2)^2} - mc^2 . \tag{1.1.6}$$

The simplest pseudorelativistic model is the Chandrasekhar operator C_A, which is obtained by replacing p in (1.1.6) with the magnetic momentum operator P_A, where the (positive) unique square root of an unbounded positive operator can be defined by the spectral theorem of unbounded operators. By a similar change of coordinates as in the non–relativistic case, we can pass to an operator with a dimensionless description, i.e., the Chandrasekhar operator

$$C_A = T_A^{\mathrm{rel}} + V, \quad T_A^{\mathrm{rel}} = \sqrt{\alpha^{-2}P_A^2 + \alpha^{-4}} - \alpha^{-2} \tag{1.1.7}$$

where $\alpha = e^2/(\hbar c)$ is the fine–structure constant defined above. Note that the pseudorelativistic kinetic energy is always smaller than the non–relativistic one since

$$\sqrt{\alpha^{-2}P_A^2 + \alpha^{-4}} - \alpha^{-2} = \alpha^{-2}\left(\sqrt{1+\alpha^2 P_A^2} - 1\right) \le \frac{1}{2}P_A^2 .$$

In the limit $\alpha \to 0$ (or $c \to \infty$) the pseudorelativistic expression converges to the non–relativistic operator. A fundamental example of a Schrödinger operator is the Bohr atom, which describes a single particle in a Coulomb potential, $V(x) \sim |x|^{-1}$. Specifically, for a single electron interacting with a nucleus of charge Z, the Schrödinger operator is

$$H_{\mathrm{Bohr}} = T - \frac{Z\alpha}{|x|} .$$

To model a pseudorelativistic hydrogen atom or incorporate magnetic fields (neglecting spin), the operator T can be replaced by the corresponding (pseudorelativistic) magnetic kinetic energy.
Note that the non–relativistic operator H_{Bohr} is bounded from below for any values of $Z\alpha \ge 0$, which can be shown by the Hardy inequality. In the pseudorelativistic case the situation is more complicated. By the ultrarelativistic uncertainty principle (see [76, Lemma 8.2] for a proof)

Lemma 1.1.2 (Fractional–Hardy Inequality)**.** *Let $d \ge 2$ and let $f \ge 0$ in $H^{1/2}(\mathbb{R}^d)$, then*

$$\langle f, (-\Delta_x)^{1/2} f\rangle \ge 2\frac{\Gamma^2(\frac{d+1}{4})}{\Gamma^2(\frac{d-1}{4})} \iint_{\mathbb{R}^d} \frac{|f(x)|^2}{|x|} dx .$$

Remark 1.1.3. *In dimension $d = 3$, the ultrarelativistic Bohr atom is bounded from below (in fact positive) for $Z\alpha \le 2/\pi$ and for $d = 2$, we need $Z\alpha \le 4\pi^2/\Gamma(1/4)^{-4}$, see [45]. Since*

$$|p| - 1 \le \sqrt{|p|^2 + 1} - 1 \le |p| \quad \forall p \in \mathbb{R}^3$$

the same bounds on $Z\alpha$ can be applied in the pseudorelativistic case.

1.2 Quadratic Forms

Under suitable restrictions on the potential $V : \mathbb{R}^d \to \mathbb{R}$, any of the operators in Section 1.1 have a (densely) defined self-adjoint realization on $L^2(\mathbb{R}^d)$. Sometimes, it is necessary or just more convenient to speak about quadratic forms and the corresponding *form domain* of these operators instead of the operator itself. Following Simon [104] and [114] , we explain this approach for the Schrödinger operator $H = T+V$. For the pseudorelativistic and ultrarelativistic cases, the ideas remain the same. Let $\mathcal{H}$ be a Hilbert space.

Definition 1.2.1. *Let $q : Q(q) \times Q(q) \to \mathbb{C}$ be a sesquilinearform and $Q(q)$ dense in $\mathcal{H}$. Then the mapping*

$$q : \psi \in Q(q) \mapsto q(\psi, \psi)$$

is the quadratic form associated with the sesquilinear form q.

If $q(\varphi, \varphi) \geq 0$ for any $\varphi \in Q(q)$, the quadratic form is called positive. It is called closed if $Q(q)$ is complete in the norm

$$\|\varphi\|_q := \left[q(\varphi, \varphi) + \|\varphi\|_{\mathcal{H}}^2\right]^{1/2} .$$

We say q is closable if it has a closed extension. For any densely defined linear operator A, we can define on its domain $D(A)$ a quadratic form by

$$\psi \in D(A) \mapsto (\psi, \psi)_A := \langle \psi, A\psi \rangle .$$

If A is essentially self–adjoint and bounded from below, then $(\cdot, \cdot)_A$ is closable, and its closure, denoted by q_A, is called the quadratic form of A. Moreover, the domain $Q(A)$ of this quadratic form is called the form domain of A. An important theorem for which a proof can be found in [115, Theorem 2.5.18] or [114, Theorem 2.14] states

Theorem 1.2.2. *If a quadratic form q is positive and closed, then it is the form of a unique self–adjoint positive operator. More generally, a closed quadratic form which is lower semi–bounded, is the form of a unique self–adjoint lower semi–bounded operator and the lower bounds coincide.*

Theorem 1.2.2 allows us to make sense of the kinetic energies from Section 1.1 on $L^2(\mathbb{R}^d)$. Still, we would like to define a Schrödinger operator, which is a sum of kinetic and potential energy. Due to a theorem named after Kato, Lion, Lax, Millgram, and Nelson, for which a proof can be found in [114, Theorem 6.29], we know

Theorem 1.2.3 (KLMN Theorem)**.** *Let A be a positive self–adjoint operator with form domain $Q(A)$. Let β be a sesquilinear form with form domain $Q(\beta) \supset Q(A)$ such that there exist $a \in (0, 1)$ and $b \in \mathbb{R}$ with*

$$|\beta(\psi, \psi)| \leq a\langle \psi, A\psi \rangle + b\|\psi\|^2 \tag{1.2.1}$$

for all $\psi \in Q(A)$. Then, the quadratic form

$$\psi \mapsto \langle \psi, A\psi \rangle + \beta(\psi, \psi)$$

defined on $Q(A)$ is the form of a self–adjoint operator, which is bounded from below.

Remark 1.2.4. *Note that we use a slightly sloppy but convenient notation here. If $\psi \in Q(A)$, we also write $\langle \psi, A\psi \rangle = q_A(\psi, \psi)$ where q_A is the quadratic form corresponding to A, even though ψ might not be in the domain of A.*
We call these quadratic forms β form small w.r.t. A. If a can be chosen to be arbitrarily small, more precisely, if for any $a > 0$ there exists $b = b_a$ such that (1.2.1) *holds, we call the form β form tiny w.r.t. A.*

Take for example $A = -\Delta/2 = P^2/2$ with $Q(P^2) = H^1(\mathbb{R}^d)$ such that

$$\langle \psi, P^2 \psi \rangle = \int_{\mathbb{R}^d} |\nabla \psi|^2 dx, \quad \forall \psi \in H^1(\mathbb{R}^d)$$

and $\beta(\psi, \psi) = \langle \psi, V\psi \rangle$ for some potential $V : \mathbb{R}^d \to \mathbb{R}$ such that there are $a \in (0, 1)$ and $b \in \mathbb{R}$ such that

$$\langle \psi, |V|\psi \rangle \leq \frac{a}{2} \int_{\mathbb{R}^d} |\nabla \psi|^2 dx + b \int_{\mathbb{R}^d} |\psi|^2 dx \quad \forall \psi \in H^1(\mathbb{R}^d)$$

then the KLMN theorem (densely) defines a Schrödinger operator as the self–adjoint operator $H = P^2/2 + V$ with form domain $Q(H) = H^1(\mathbb{R}^d)$. In comparison with the condition of the KLMN theorem, it is usual to define the following.

Definition 1.2.5. *Let A be a positive self–adjoint operator and B symmetric. Then B is said to be relatively form bounded with respect to A with relative bound $a > 0$ if $Q(A) \subset Q(B)$ and if there exists $b \in \mathbb{R}$ such that*

$$|(\psi, \psi)_B| \leq a(\psi, \psi)_A + b\|\psi\|^2 \quad , \forall \psi \in \mathcal{H}$$

where $\|\cdot\|$ denotes the norm of the underlying Hilbert space.

Remark 1.2.6. *The definition above can be formulated for general quadratic forms as well.*

To define $H = \frac{1}{2}P^2 + V$ directly as a self–adjoint operator without the usage of quadratic forms, one uses the operator–valued version of the KLMN theorem that was discovered independently by Kato and Rellich and for which a proof can be found, e.g. [114, Theorem 6.4].

Theorem 1.2.7 (Kato–Rellich)**.** *Let $\mathcal{H}$ be a Hilbert space, $A : D(A) \to \mathcal{H}$ be self–adjoint and $B : D(B) \to \mathcal{H}$ symmetric such that B is relatively bounded with respect to A with relative bound less that one. That is $D(A) \subset D(B)$ and there exists some $a < 1$ and $b \in \mathbb{R}$ with*

$$\|B\psi\| \leq a\|A\psi\| + b\|\psi\|, \quad \forall \psi \in D(A) . \tag{1.2.2}$$

Then $A + B : D(A) \to \mathcal{H}$ is self–adjoint.

Summarizing if V is relatively form bounded with respect to $P^2/2$ with relative bound less than one, we can define on $H^1(\mathbb{R}^d)$ the quadratic form

$$q(\psi) = \frac{1}{2} \int_{\mathbb{R}^d} |\nabla \psi|^2 dx + \int_{\mathbb{R}^d} V|\psi|^2 dx \quad \forall \psi \in H^1(\mathbb{R}^d) . \tag{1.2.3}$$

If V is relatively bounded with respect to $\frac{1}{2}P^2$ with relative bound less than one, due to the Kato–Rellich Theorem 1.2.7 the operator $H = \frac{1}{2}P^2 + V$ is self-adjoint with domain

$$D(H) = D(P^2) = H^2(\mathbb{R}^d) .$$

The question for which potentials the Schrödinger operator is self–adjoint is fundamental and has a long story. See for example [54], [64], [102], [111] and [105].
For many applications, it suffices to reduce the discussion to potentials that are infinitesimally form small with respect to P^2, i.e., for any $\varepsilon > 0$, there exists $C(\varepsilon) > 0$ with

$$\langle \psi, |V|\psi \rangle \leq \varepsilon \int_{\mathbb{R}^d} |\nabla \psi|^2 dx + C(\varepsilon) \int_{\mathbb{R}^d} |\psi|^2 dx \quad \forall \psi \in H^1(\mathbb{R}^d) .$$

Following [105] we define the following class of potentials.

Definition 1.2.8 (Kato–class Potentials)**.** *Let $d \geq 2$, then a Borel measurable $V : \mathbb{R}^d \to \overline{\mathbb{R}}$ lies in the Kato–class K_d if*

$$\lim_{\delta \downarrow 0} \sup_{|x| \in \mathbb{R}^d} \int_{|x-y| \leq \delta} g_d(x-y)|V(y)|dy = 0 , \tag{1.2.4}$$

where

$$g_d(x) := \begin{cases} |x|^{2-d} & \text{if} \quad d \geq 3 \\ |\ln|x|| & \text{if} \quad d = 2 \end{cases} , \tag{1.2.5}$$

is, up to a constant, the fundamental solution of the Laplace equation in $\mathbb{R}^d$. In dimension $d = 1$ the Kato class K_1 is the space $L^1_{\text{loc,unif}}(\mathbb{R})$ of uniformly locally L^1-functions.
We say that the potential V is in the local Kato–class $K_{d,\text{loc}}$ if $V\mathbb{1}_K \in K_d$ for all compact sets $K \subset \mathbb{R}^d$.

It is well known (see, e.g. [105, Lemma A.2.2] that

Lemma 1.2.9. *Any potential $V \in K_d$ is infinitesimally form small with respect to P^2.*

Remark 1.2.10. *Recall that $L^p_{\text{loc,unif}}(\mathbb{R}^d)$ is given by Borel measurable functions*

$$f : \mathbb{R}^d \to \overline{\mathbb{R}} := \mathbb{R} \cup \{-\infty, \infty\}$$

for which

$$\|f\|_{p,\text{loc,unif}} := \sup_{x \in \mathbb{R}} \left(\int_{|x-y| \leq 1} |f(y)|^p \, dy \right)^{1/p} < \infty .$$

Due to Hölder's inequality, one sees that $L^p_{\text{loc,unif}}(\mathbb{R}^d) \subset K_d$ for any $p > d/2$, when $d \geq 2$. The inclusion $K_d \subset L^1_{\text{loc,unif}}(\mathbb{R}^d)$ holds in any dimension. Note that the class of potentials $V \in K_d$, include most, if not all, physically relevant potentials, except maybe some highly oscillating potentials.

1.3 IMS Localization

In Chapters 5 and 6, we extensively use the concept of localization. Localization involves partitioning a set $\mathbb{R}^d$ into disjoint regions and expressing the quadratic form of $H = P^2/2 + V$

as a sum of terms, each involving functions localized to these regions. This comes at the expense of an additional correction term known as the localization error. This decomposition is achieved using a well-known result called the IMS localization formula named after Ismagilov [57], Morgan [78], Morgan-Simon [79] and Sigal [99]. Before presenting the IMS localization formula, we first introduce the concept of quadratic partitions of unity. Following [27, Definition 3.1] we define

Definition 1.3.1 (Quadratic Partition of Unity). *A set of smooth functions $\{\chi_k\}_{k\in I}$ where J is some index set is called quadratic partition of unity if*

(i) $0 \leq \chi_k(x) \leq 1$ *and* $\sum_{k\in J} \chi_k^2(x) = 1$ *for all* $x \in \mathbb{R}^d$,

(ii) $\{\chi_k\}_{k\in J}$ *is locally finite, i.e., on any compact set K we have $\chi_k = 0$ for all but finitely many $k \in J$,*

(iii) $\sup_{x\in\mathbb{R}^d} \sum_{k\in J} |\nabla\chi_k(x)|^2 < \infty$.

Following [106, Lemma 3.1] the IMS localization formula can be formulated as

Theorem 1.3.2 (IMS Localization Formula). *Let V be relatively form-bounded with relative bound zero with respect to P^2 and $H = P^2/2 + V$. Let $\{\chi_a\}_{a=0}^k$ be a quadratic partition of unity then*

$$H = \left(\sum_{a=0}^{k} \chi_a H \chi_a\right) - \sum_{a=0}^{k} |\nabla\chi_a|^2. \tag{1.3.1}$$

The IMS localization formula can be formulated for quadratic forms. A proof for that can, for instance, be found in [49, Lemma A.1.]. We include here the following simpler version.

Theorem 1.3.3 (IMS Formula for Quadratic Forms). *Let V be form-bounded with relative bound less than one with respect to $P^2/2$ and $H = P^2/2 + V$. Let $\xi \in W^{1,\infty} \cap C^1$ be real–valued. For all $\psi \in D(P)$ we also have $\xi\psi \in D(P)$, $\xi^2\psi \in D(P)$ and*

$$\mathrm{Re}(\xi^2\psi, \psi)_H = (\xi\psi, \xi\psi)_H - \langle\psi, |\nabla\xi|^2\psi\rangle\,. \tag{1.3.2}$$

Proof. Since ξ is a real–valued multiplication operator, we have

$$\langle\xi^2\psi, V\psi\rangle = \langle\xi\psi, V\xi\psi\rangle\,.$$

We only need to discuss the kinetic part of the quadratic form. Using the identity

$$P(\xi^2\psi) = \xi P(\xi\psi) + (P\xi)\xi\psi,$$

we compute directly:

$$\begin{aligned}\langle P(\xi^2\psi), P\psi\rangle &= \langle P(\xi\psi), P(\xi\psi)\rangle + \langle (P\xi)\psi, P(\xi\psi)\rangle \\ &\quad - \langle P(\xi\psi), (P\xi)\psi\rangle - \langle\psi, |\nabla\xi|^2\psi\rangle.\end{aligned}$$

Taking the real part of the expression above, we obtain

$$\mathrm{Re}\langle P(\xi^2\psi), P\psi\rangle = \langle P(\xi\psi), P(\xi\psi)\rangle - \langle \psi, |\nabla\xi|^2\psi\rangle,$$

which proves (1.3.2). ∎

Using estimates on the localization error, Zhislin formulated in [129] sufficient criteria for the finiteness of $\sigma_{\mathrm{disc}}(H)$. Throughout our discussion of the Efimov effect, we will extensively use these conditions. Here, we demonstrate them as an application of the IMS formula. To this end, we employ the following estimate on the localization error, originally due to Zhislin and Vugalter [120, Lemma 5.1]. A version of this lemma is used in Chapter 6 as Lemma 6.2.5 and the proof is given in Appendix C as Lemma C.1.1; we copy that version here for the convenience of the reader.

Lemma 1.3.4 (see Lemma 6.2.5)**.** *For any $\varepsilon, b > 0$ there exist $0 < a < b$ and continuous functions $u, v : \mathbb{R} \to [0,1]$ with piecewise continuous derivatives, such that $u^2 + v^2 = 1$,*

$$v(x) = \begin{cases} 1, & |x| \geq b \\ 0, & |x| \leq a \end{cases}, \quad u(x) = \begin{cases} 1, & |x| \leq a \\ 0, & |x| \geq b \end{cases},$$

and

$$|u'(x)|^2 + |v'(x)|^2 \leq \frac{\varepsilon}{|x|^2}\mathbb{1}_{\{a\leq|x|\leq b\}}.$$

Moreover, a can be chosen such that

$$e^{-(1+2/\varepsilon)} \leq \frac{a}{b} \leq e^{-2/\varepsilon}.$$

In the following, we denote by $\sigma(H)$ the spectrum of H and by $\sigma_{\mathrm{ess}}(H)$ and $\sigma_{\mathrm{disc}}(H)$ its essential and discrete part, where $\sigma_{\mathrm{disc}}(H)$ consists of all eigenvalues of H having finite multiplicity and being isolated points of the full spectrum and $\sigma_{\mathrm{ess}}(H) = \sigma(H) \setminus \sigma_{\mathrm{disc}}(H)$. The following result was first shown by Zhislin [129] we reproduce it here in a slightly modified form for the convenience of readers. We follow closely [23, Lemma 3.1.3 (ii)]) to find a sufficient criterion for the finiteness of $\sigma_{\mathrm{disc}}(H)$.

Lemma 1.3.5 (Zhislin [129])**.** *Let $d \geq 3$ and V be relatively form-bounded with relative bound zero with respect to P^2 in $L^2(\mathbb{R}^d)$. Consider $H = P^2/2 + V$ on $L^2(\mathbb{R}^d)$ with $\sigma_{\mathrm{ess}}(H) = [0,\infty)$. Assume there exists $\varepsilon > 0$ and some $R > 0$ such, that*

$$L[\psi] := \langle \psi, H\psi\rangle - \varepsilon\langle |x|^{-2}\psi, \psi\rangle \geq 0 \tag{1.3.3}$$

for all $\psi \in H^1(\mathbb{R}^d)$ with $\mathrm{supp}(\psi) \subset \{x \in \mathbb{R}^d : |x| \geq R\}$. Then $\sigma_{\mathrm{disc}}(H)$ is at most finite.

Proof. By the min–max principle, it is sufficient to find a finite–dimensional subspace $\mathcal{M} \subset L^2(\mathbb{R}^d)$ such that for any $\psi \in L^2(\mathbb{R}^3)$ orthogonal to $\mathcal{M}$

$$\langle \psi, H\psi\rangle \geq 0.$$

Note that if Inequality (1.3.3) holds for $\varepsilon, R > 0$ then it also holds for any pair $\tilde{\varepsilon}, R > 0$ with $\tilde{\varepsilon} \in (0, \varepsilon)$. Thus we assume without loss of generality that $\varepsilon, R > 0$ fulfill (1.3.3) and $\frac{1}{2}(1 - \varepsilon - 2c_d\varepsilon) \geq 1/4$ where c_d is the Hardy constant in dimension $d \geq 3$ such that $-\Delta \geq c_d^{-1}|x|^{-2}$.
For this $\varepsilon > 0$ and some fixed $b > 0$ let $0 < a < b$ and $u, v : \mathbb{R} \to [0, 1]$ be a quadratic partition of unity of $\mathbb{R}$ given by Lemma 1.3.4. Let for any $x \in \mathbb{R}^d$

$$\chi_1(x) := u(\beta^{-1}|x|), \quad \chi_2(x) := v(\beta^{-1}|x|) .$$

Then $\{\chi_1, \chi_2\}$ is a quadratic partition of unity of $\mathbb{R}^d$ and by direct computation the localization error fulfills

$$|\nabla\chi_1(x)|^2 + |\nabla\chi_2(x)|^2 \leq \varepsilon|x|^{-2}\mathbb{1}_{\{\beta a \leq |x| \leq \beta b\}}. \tag{1.3.4}$$

Using the IMS formula (1.3.1) together with (1.3.3) and (1.3.4) yields

$$\langle\psi, H\psi\rangle \geq L[\psi\chi_1] + L[\psi\chi_2] .$$

Note that $\mathrm{supp}(\psi\chi_2) \subset \{x \in \mathbb{R}^d : |x| \geq \beta a\}$ and consequently by assumption (1.3.3) we have $L[\psi\chi_2] \geq 0$ for $\beta > 0$ large enough. Next we show that $L[\psi\chi_1] \geq 0$. Since V is relatively form bounded with relative bound zero, there exists $C_\varepsilon > 0$ such that

$$|\langle\psi\chi_1, V\psi\chi_1\rangle| \leq \frac{\varepsilon}{2}\|\nabla(\psi\chi_1)\|^2 + C_\varepsilon\|\psi\chi_1\|^2 \tag{1.3.5}$$

and consequently

$$L[\psi\chi_1] \geq \frac{1}{2}(1 - \varepsilon)\|\nabla(\psi\chi_1)\|^2 - C_\varepsilon\|\psi\chi_1\|^2 - \varepsilon\int_{\mathbb{R}^d}\frac{|\psi\chi_1|^2}{|x|^2}dx . \tag{1.3.6}$$

Using Hardy's Inequality in dimension $d \geq 3$ we find

$$L[\psi\chi_1] \geq \frac{1}{2}(1 - \varepsilon - 2c_d\varepsilon)\|\nabla(\psi\chi_1)\|^2 - C_\varepsilon\|\psi\chi_1\|^2 . \tag{1.3.7}$$

Consequently it suffices to find finite–dimensional $\mathcal{M} \subset L^2(\mathbb{R}^d)$ such that if ψ is orthogonal to $\mathcal{M}$ the following holds

$$\|\nabla(\psi\chi_1)\|^2 - 4C_\varepsilon\|\psi\chi_1\|^2 \geq 0 . \tag{1.3.8}$$

Let $\varphi_1, \varphi_2, \ldots, \varphi_n$ the first n Dirichlet eigenfunctions of the Laplacian on the ball of radius $a\beta$ in $\mathbb{R}^d$. We choose

$$\mathcal{M} = \mathrm{Lin}\{\varphi_1\chi_1, \varphi_2\chi_1, \ldots, \varphi_n\chi_n\} . \tag{1.3.9}$$

Note that if $\psi \perp \mathcal{M}$ then $\psi\chi_1$ is orthogonal to the first n Dirichlet eigenfunctions and consequently (1.3.8) needs to hold for $n \in \mathbb{N}$ large enough. This is due to the well–known fact that the Dirichlet eigenvalues diverge to $+\infty$. ∎

1.4 Virtual Levels

In this section we discuss some spectral properties of the Schrödinger operator $H = P^2/2 + V$ introduced in (1.1.3) with form domain $H^1(\mathbb{R}^d)$ for admissible $V : \mathbb{R}^d \to \overline{\mathbb{R}}$ (infinitesimally form small with respect to P^2) as discussed in Section 1.2 with quadratic form

$$H^1(\mathbb{R}^d) \ni \psi \mapsto \langle \psi, H\psi \rangle = q_H(\psi, \psi) = \frac{1}{2} \int_{\mathbb{R}^d} |\nabla \psi|^2 dx + \int_{\mathbb{R}^d} V|\psi|^2 dx \,.$$

Recall that $\sigma(H)$ denotes the spectrum of H, and by $\sigma_{\text{ess}}(H)$ and $\sigma_{\text{disc}}(H)$, we refer to its essential and discrete part. Let

$$E_0 \coloneqq \inf \sigma(H)$$

be the ground state energy of H. If there exists a minimizer $\varphi_0 \in H^1(\mathbb{R}^d)$ with $\|\varphi_0\| = 1$ of the quadratic form in the sense that

$$\langle \varphi_0, H\varphi_0 \rangle = \inf_{\psi \in H^1(\mathbb{R}^d), \|\psi\|=1} \langle \psi, H\psi \rangle = E_0,$$

then φ_0 is called a ground state of H. Let $\Sigma \coloneqq \inf \sigma_{\text{ess}}(H)$ be the bottom of the essential spectrum. Whenever there exists $\psi \in H^1(\mathbb{R}^d)$ such that

$$\frac{\langle \psi, H\psi \rangle}{\|\psi\|^2} < \Sigma,$$

then $\sigma_{\text{disc}}(H) \neq \emptyset$ and consequently there exists an eigenfunction $\varphi \in H^1$ with $H\varphi = E\varphi$, with $E < \Sigma$. We call such states bound states.
In the following, we restrict our discussion to the case $\Sigma = 0$. Ensuring this requires some decay conditions on the potential V, as explained in [48, Remark 1.6]. We recall the arguments from [48, Remark 1.6] here for completeness. A sufficient condition for $\Sigma = 0$ is that V is relatively form compact with respect to the kinetic energy P^2, a proof for this can be, for instance, found in [114, Lemma 6.2.6]. This condition further implies that V is infinitesimally form bounded with respect to P^2, meaning it is relatively form bounded with relative bound zero. Consequently, this excludes Hardy-type potentials, namely potentials of the form $V(x) = C|x|^{-2}$, $C \in \mathbb{R}$.
A significantly weaker condition for ensuring $\sigma_{\text{ess}}(H) = [0, \infty)$ is that V vanishes asymptotically in comparison to the kinetic energy. More precisely, if

$$|\langle \varphi, V\varphi \rangle| \le a_n \|\nabla \varphi\|^2 + b_n \|\varphi\|^2 \tag{1.4.1}$$

for all $\varphi \in H^1(\mathbb{R}^d)$ supported in $\{|x| \ge R_n\}$, where the sequences $0 \le a_n, b_n \to 0$ and $R_n \to \infty$ as $n \to \infty$, then it follows that $\sigma_{\text{ess}}(H) = [0, \infty)$; see [7, Section 6], [63].
The existence and absence of bound states below the essential spectrum have been studied, e.g., by application of the Birman–Schwinger principle (see [22] and [96]). The famous Cwikel–Lieb–Rozenblum bound (see [26], [70] and [94]) gives for $d \ge 3$ a bound on the

number N of negative eigenvalues of $P^2 + \lambda V$

$$N \leq \lambda^{d/2} L_{0,d} \int_{\mathbb{R}^d} V_-^{d/2} dx \,.$$

Consequently, for $d \geq 3$, weakly negative potentials do not produce bound states. In dimension $d < 3$, the situation is different. Let V be non–positive and strictly negative on an open set, then in dimension, $d < 3$, the operator $P^2 + \lambda V$ has a bound state for arbitrarily small λ (see [107]).
Indeed, the edge $\Sigma = 0$ separates the spectrum of H into two parts with very different behavior. It is well known that the bound states below the essential spectrum decay exponentially at $|x| \to \infty$ (see [2]), whereas for the so–called scattering–states with $\langle \psi, H\psi \rangle > 0$ the decay is much slower.
Whether a zero energy solution is a true eigenfunction, meaning it belongs to $L^2(\mathbb{R}^d)$, or not is generally a very complicated question. A particularly interesting case occurs for critical Schrödinger operators, i.e., Schrödinger operators for which $\sigma_{\text{ess}}(H) = [0, \infty)$ but any negative perturbation creates a negative eigenvalue. See [48, Definition 1.5] for a detailed definition and [48, Appendix A] for explicit examples of critical Schrödinger operators with nonzero potentials in all dimensions. Following [59] we say

Definition 1.4.1. *The operator H has a virtual level at zero if $H \geq 0$ and there exists $\varepsilon_1 \in (0, 1)$ such that for any $\varepsilon \in (0, \varepsilon_1)$*

$$\inf \sigma_{\text{ess}}(H - \varepsilon P^2) = 0 \quad \textit{and} \quad \inf \sigma(H - \varepsilon P^2) < 0\,. \tag{1.4.2}$$

Remark 1.4.2. *The condition* (1.4.2) *ensures the existence of a negative energy ground state φ_ε of $H - \varepsilon P^2$ for any small enough $\varepsilon > 0$. In the limit $\varepsilon \to 0$, this determines a candidate for a zero–energy solution of H, though the family of functions φ_ε does not necessarily converge in $H^1(\mathbb{R}^d)$. But, as explained below, a suitable subsequence will converges in $\dot{H}^1(\mathbb{R}^d)$. The limiting function $\varphi_0 \in \dot{H}^1$ is a zero–energy solution of H but it might not be in $L^2(\mathbb{R}^d)$. If the zero–energy solution is in L^2 it is indeed a true bound state in H^1. In this case, the virtual level is an eigenvalue of H, otherwise the virtual level is called a resonance. If resonances are unique, the whole family ψ_ε will converge.*

Following Remark 1.4.2 it is useful to introduce the homogeneous Sobolev spaces $\dot{H}^1(\mathbb{R}^d)$. To define them one needs to carefully distinguish the cases $d \in \{1, 2\}$ and $d \geq 3$. The easiest definition for $d \geq 3$ is to define $\dot{H}^1(\mathbb{R}^d)$ as the closure of $C_0^\infty(\mathbb{R}^d)$ with respect to the inner product $\langle u, v \rangle_{\dot{H}^1(\mathbb{R}^d)} = \int_{\mathbb{R}^d} (\nabla \overline{u} \cdot \nabla v) \, dx$.
Following [36, Chapter 2.7] this gives the homogeneous Sobolev space for $d \geq 3$ as

$$\dot{H}^1(\mathbb{R}^d) = \{u \in L^2(\mathbb{R}^d, |x|^{-2} dx) : \nabla u \in L^2(\mathbb{R}^d)\},$$

with the norm

$$\|u\|_{\dot{H}^1(\mathbb{R}^d)} := \left(\int_{\mathbb{R}^d} |\nabla u|^2 dx \right)^{1/2} = \langle Pu, Pu \rangle^{1/2}, \; d \geq 3. \tag{1.4.3}$$

The spaces $\dot{H}^1(\mathbb{R}^d)$ are complete and therefore Hilbert spaces and we have the Sobolev embedding $\dot{H}^1(\mathbb{R}^d) \subset L^{2d/(d-2)}$ in dimensions $d \geq 3$.
Following [36, Chapter 2.7] for $d < 3$ the homogeneous Sobolev spaces are

$$\dot{H}^1(\mathbb{R}^d) = \{u \in L^2_{\text{loc}}(\mathbb{R}^d) : \nabla u \in L^2(\mathbb{R}^d)\}, \quad d < 3$$

equipped with the scalar product

$$\langle u, v\rangle_{\dot{H}^1(\mathbb{R}^d)} := \int_{\mathbb{R}^d} (\nabla \overline{u} \cdot \nabla v)\, dx + \int_B \overline{u} v dx, \quad d < 3, \tag{1.4.4}$$

where $B \subset \mathbb{R}^d$ is the ball centered at zero with radius one. Then, the corresponding norm is

$$\|u\|_{\dot{H}^1(\mathbb{R}^d)} := \left(\int_{\mathbb{R}^d} |\nabla u|^2 dx + \|u\|^2_{L^2(B)}\right)^{1/2} = \left(\langle u, P^2 u\rangle + \|u\|_{L^2(B)}\right)^{1/2}, \; d < 3. \tag{1.4.5}$$

For $d < 3$ as well, this space is complete under the norm $\|\cdot\|_{\dot{H}^1(\mathbb{R}^d)}$ and consequently a Hilbert space.
Note, that in dimension $d < 3$ for instance constant functions belong to $\dot{H}^1(\mathbb{R}^d)$. To distinguish functions that differ by a constant the scalar product in (1.4.4) contains an integral over B. As in the case $d \geq 3$ the space $\dot{H}^1(\mathbb{R}^d)$ is the closure of $C_0^\infty(\mathbb{R}^d)$ but now with respect to the modified inner product $\langle u, v\rangle_{\dot{H}^1(\mathbb{R}^d)}$ defined in (1.4.4).

Remark 1.4.3. *The spaces $\dot{H}^1(\mathbb{R}^d)$ for $d < 3$ are sometimes denoted by $\widetilde{H}^1(\mathbb{R}^d)$ to emphasize their different definitions. Throughout this document the symbol $\dot{H}^1(\mathbb{R}^d)$ is used for any $d > 0$.*

In the case, $d = 3$ Yafaev did study Schrödinger operators $H = P^2/2 + V$ with short–range interactions that have a virtual level.

Definition 1.4.4 (Short–Range Potentials)**.** *A potential $V : \mathbb{R}^d \to \mathbb{R}$ is called short–range if there exist constants $C, \delta > 0$ and $A > 0$ such that*

$$|V(x)| \leq C(1 + |x|)^{-2-\delta}, \quad |x| \geq A\,.$$

Remark 1.4.5. *Potentials V defined according to Definition 1.4.4 are not allowed to have singularities outside of a compact set. In many cases one can instead assume that there exists $W \in K_d$ a Kato–class potential and $\theta > 0$ such that*

$$V(x) = (1 + |x|)^{-2-\theta} W(x) \tag{1.4.6}$$

for $x \in \mathbb{R}^d$.

Yafaev found for short–range potentials as defined in Definition 1.4.4, the virtual level is indeed a resonance in the sense explained in Remark 1.4.2. In Chapter 4 we discuss a three–particle system that consists of one and two dimensional two–particle subsystems. We use the following Theorem for which a proof can be found in [13, Theorem 2.2]. We repeat that theorem here.

Theorem 1.4.6. *Let $d < 3$. Consider $H = P^2/2 + V$ with V relatively form bounded with respect to $P^2/2$ with relative bound zero and short–range. If H has a virtual level at zero, then the following assertions hold:*

a) *There exists a solution $\varphi_0 \in \dot{H}^1(\mathbb{R}^d)$, $\varphi_0 \neq 0$, of the equation $(P^2/2)\varphi_0 + V\varphi_0 = 0$, i.e., for all $\psi \in \dot{H}^1(\mathbb{R}^d)$*

$$\frac{1}{2}\langle P\varphi_0, P\psi\rangle + \langle \varphi_0, V\psi\rangle = 0. \tag{1.4.7}$$

b) *If in addition the potential V is relatively $-\Delta$-bounded, i.e., there exists a constant $C > 0$, such that*

$$\|V\psi\|^2 \leq C\left(\|\Delta\psi\|^2 + \|\psi\|^2\right) \tag{1.4.8}$$

holds for all functions $\psi \in H^2(\mathbb{R}^d)$, then there exists a constant $\mu > 0$, such that for any function $\psi \in H^1(\mathbb{R}^d)$ satisfying $\langle P\psi, P\varphi_0\rangle = 0$

$$\langle \psi, H\psi\rangle \geq \mu\|P\psi\|^2. \tag{1.4.9}$$

Remark 1.4.7. *If* (1.4.7) *or* (1.4.11) *holds, then φ_0 is a weak local zero–energy solution, meaning that $\varphi_0 \in H^1_{\text{loc}}$ and that* (1.4.7) *or* (1.4.11) *holds for all $\psi \in C_0^\infty(\mathbb{R}^d)$, and even for all $\psi \in H^1(\mathbb{R}^d)$ with compact support.*
However, functions in H^1_{loc} have virtually no growth restrictions at infinity. Any resonance function φ_0, in addition to being a weak local zero–energy solution of H, does also have finite kinetic energy.

In dimension $d \geq 3$ a theorem similar to Theorem 1.4.6 under slightly different assumptions on V was proven in [23, Chapter 3]. We repeat a version of that theorem here.

Theorem 1.4.8. *Let $d \geq 3$. Consider $H = P^2/2 + V$ with V relatively form bounded with respect to $P^2/2$ with relative bound zero and short–range. Moreover, assume that there exists $C > 0$ with*

$$\langle \psi, |V|\psi\rangle \leq C\|P\psi\|, \quad \forall\psi \in \dot{H}^1(\mathbb{R}^d)\,. \tag{1.4.10}$$

Then,

a) *there exists a non–vanishing $\varphi_0 \in \dot{H}^1(\mathbb{R}^d)$ with $\|\varphi_0\|_{\dot{H}^1(\mathbb{R}^d)} = 1$ such that for any $\psi \in \dot{H}^1(\mathbb{R}^d)$*

$$\frac{1}{2}\langle P\psi, P\varphi_0\rangle + \langle \psi, V\varphi_0\rangle = 0\,. \tag{1.4.11}$$

b) *If in addition the potential V is P^2 bounded, i.e. there exists $C > 0$ with*

$$\|V\psi\|^2 \leq C\langle(\|P\psi\|^2 + \|\psi\|^2), \quad \forall\psi \in C_0^\infty(\mathbb{R}^d) \tag{1.4.12}$$

then the solution $\varphi_0 \in \dot{H}^1(\mathbb{R}^d)$ is unique and there exists a constant $\mu > 0$ such that for any $\psi \in H^1(\mathbb{R}^2)$ with $\langle P\psi, P\varphi_0\rangle = 0$

$$\langle \psi, H\psi\rangle \geq \mu\|P\psi\|^2\,. \tag{1.4.13}$$

Remark 1.4.9. *Note that for short–range potentials condition (3.1.6) in [23] is fulfilled by suitably adjusting the relevant parameters. The result for an energy gap in Theorem 1.4.8 needs that, in addition, V^2 is relatively form bounded w.r.t. P^2.*

Remark 1.4.10. *Recall that the spectrum of H on $L^2(\mathbb{R}^d)$ is purely essential with*

$$\sigma(H) = \sigma_{ess}(H) = [0, \infty) .$$

The existence of a spectral gap *for H on the homogenous Sobolev space $\dot{H}^1$ shows that the spectral properties of H on $\dot{H}^1$ are very different from its properties on $L^2(\mathbb{R}^d)$.*

The assumptions on the positive part of the potential in Theorem 1.4.8 can be relaxed. In Theorem 1.4.11 we prove an alternative version of Theorem 1.4.8, concerning the existence of resonances in dimension $d \geq 3$. It considerably relaxes the condition on the positive part of V, but imposes a (weak) short range condition on the negative part of the potential V.
Theorem 1.4.12 below provides a uniqueness result for the resonance and a spectral gap, under slightly stronger assumptions than the ones made in Theorem 1.4.8.
Similarly to the form domain $Q(V_+)$, which is the space of all functions $f \in L^2(\mathbb{R}^d)$ for which $\langle f, V_+ f\rangle = \|V_+^{1/2} f\|^2 < \infty$, we define $\dot{Q}(V_+)$ as the space of all functions $\psi \in \dot{H}^1(\mathbb{R}^d)$ for which $\langle \psi, V_+\psi\rangle < \infty$.

Theorem 1.4.11 (Existence of Resonances = Theorem D.1.2)**.** *Let $d \geq 3$, consider the potential $V : \mathbb{R}^d \to \mathbb{R}$ and define $V_+ = \max(0, V)$ and $V_- = \min(0, V)$. Suppose that the operator $H = P^2/2 + V$ (considered as a quadratic form) has a virtual level at zero. Assume the following conditions:*

a) $V_+ \in L^1_{\text{loc}}(\mathbb{R}^d)$,
b) *V_- is infinitesimally form-bounded w.r.t. P^2,*
c) *There exists $\theta > 0$ such that the weighted potential $\widetilde{V}_- := (1 + |\cdot|)^{2+2\theta} V_-$ is form bounded w.r.t. P^2.*

Then there exists a non–vanishing function $\varphi_0 \in \dot{H}^1(\mathbb{R}^d) \cap \dot{Q}(V_+)$ satisfying

$$\frac{1}{2}\langle P\psi, P\varphi_0\rangle + \langle \psi, V\varphi_0\rangle = 0, \quad \forall \psi \in \dot{H}^1(\mathbb{R}^d \cap \dot{Q}(V_+)). \tag{1.4.14}$$

In particular,

$$\frac{1}{2}\langle P\varphi_0, P\varphi_0\rangle + \langle \varphi_0, V\varphi_0\rangle = 0 . \tag{1.4.15}$$

In addition, compared to Theorem 1.4.8, we do not need much more regularity of the potential to have a uniqueness result for resonances and an energy gap.

Theorem 1.4.12 (Uniqueness and Energy Gap = Theorem D.2.1)**.** *We consider dimension $d \geq 3$. In addition to the short–range condition from Theorem 1.4.11 we assume that the potential $V \in L^{d/2}_{\text{loc}}$ as well as $V_+ \in K_{d,\text{loc}}$ and $V_- \in K_d$.*
Then the resonance solution φ_0 from Theorem 1.4.11 is unique and can be chosen to be strictly positive. Moreover, there exists a constant $\mu > 0$ such that, as quadratic forms,

$$\langle \psi, H\psi\rangle \geq \mu \|P\psi\|^2 \tag{1.4.16}$$

for all $\psi \in \dot{H}^1(\mathbb{R}^d) \cap \dot{Q}(V_+)$ *orthogonal to the resonance* φ_0 *in* $H^1(\mathbb{R}^d)$*, i.e.,* $\langle P\psi, P\varphi_0\rangle = 0$.

Remark 1.4.13. *The conditions on* V *in Theorem 1.4.11 are for instance fulfilled if* V *is short range in the sense that* $V = (1 + |\cdot|)^{-2-\theta} W$ *for some* $\theta > 0$ *and with* $W \in K_d$ *a Kato potential. The conditions of Theorem 1.4.12 are satisfied if, in addition to being in the Kato–class, we also have* $W \in L^{d/2}_{\mathrm{loc}}$ *such that* $W \in L^{d/2}_{\mathrm{loc}} \cap K_d$.

We give the proof of Theorem 1.4.11, respectively Theorem 1.4.12, in the Appendix, see Theorem D.1.2, respectively Theorem D.2.1.

1.5 Many Particle Operator

The approach explained in Sections 1.1 and 1.2 does generalize for many–particle systems without difficulties. In contrary to the units chosen in Section 1.1 we may not set all the (possibly different) masses m_k, $k \in \mathbb{N}$ to a fixed value. Given N particles of masses $m_1, m_2, \dots m_N > 0$ at the positions $x = (x_1, x_2, \dots, x_N) \in \mathbb{R}^{dN}$ the kinetic energy of the system can be described by

$$\mathcal{T} = \sum_{k=1}^{N} \frac{P_k^2}{2m_k}, \quad P_k = -i\nabla_k \,.$$

Here ∇_k denotes the gradient with respect to the coordinate $x_k \in \mathbb{R}^d$. For the potential energy of this system, we consider the potential $V_{ij} : \mathbb{R}^d \to \mathbb{R}$ which describes the interactions between particles at positions $x_i, x_j \in \mathbb{R}^d$. The Schrödinger operator of the system is then

$$H^{(n)} := \sum_{k=1}^{n} T_k + \sum_{1 \le i < j \le n} V_{ij}(x_i - x_j) \,. \tag{1.5.1}$$

The operators above can be densely defined in the appropriate Hilbert spaces by similar approaches as outlined in Section 1.2. The Hilbert space of the N–particle system is the N-fold tensor product of the Hilbert space for a single particle with the usual inner product for the tensor product. When considering particles with spin $S \in \mathbb{N}_0/2 = \{0, 1/2, 1, 3/2 \dots\}$ the allowed values s for the spin are in $\{-S, -S+1, \dots, S-1, S\}$ and consequently the Hilbert space for a single particle is

$$\mathcal{H}_1 = L^2(\mathbb{R}^3) \otimes \mathbb{C}^{2S+1} \cong L^2(\mathbb{R}^3; \mathbb{C}^{2S+1}) \cong L^2(\mathbb{R}^3 \times \{-S, -S+1, \dots, S-1, S\})$$

Therefore we can think of $\psi \in L^2(\mathbb{R}^3; \mathbb{C}^{2S+1})$ as a spinor, that is a vector with $2S+1$ components

$$\psi(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \\ \vdots \\ \psi_{2S+1}(x) \end{pmatrix}$$

with $\psi_{s+S+1}(x) = \psi(x, s)$ with $s \in \{-S, \dots, S\}$. In this case, the full Hilbert space for N-particles each with spin S is

$$\mathcal{H}_N \coloneqq \bigotimes_{i=1}^{N} L^2(\mathbb{R}^3; \mathbb{C}^{2S+1}) \,. \tag{1.5.2}$$

When considering identical particles we have to distinguish between fermions or bosons. Let $z_1, \dots z_N$ be the combined position–spin coordinate of a single particle, $z_j = (x_j, s_j)$. Considering identical particles we only consider states $\psi \in \mathcal{H}_N$ such that

$$\left|\psi(\dots z_i, \dots, z_j, \dots)\right|^2 = \left|\psi(\dots z_j, \dots, z_i, \dots)\right|^2. \tag{1.5.3}$$

We distinguish between fermions or bosons. For fermions, the state space is the subspace of totally antisymmetric functions $\mathcal{H}_N^f$. We call $\psi \in \mathcal{H}_N$ totally antisymmetric if

$$\psi(\dots z_i, \dots, z_j, \dots) = -\psi(\dots z_j, \dots, z_i, \dots) \quad \text{for all } i \neq j \in \{1, \dots, N\} \,.$$

For bosons, we consider the subspace of totally symmetric functions denoted by $\mathcal{H}_N^b$. We call $\psi \in \mathcal{H}_N$ totally symmetric if

$$\psi(\dots z_i, \dots, z_j, \dots) = \psi(\dots z_j, \dots, z_i, \dots) \quad \text{for all } i \neq j \in \{1, \dots, N\} \,.$$

With regards to real atoms, the particles of interest are electrons and thus the fermionic case with spin $S = 1/2$ is the natural one.

1.5.1 Internal Schrödinger Operator

Given n particles with positions $x_1, x_2, \dots, x_n \in \mathbb{R}^d$ and masses $m_1, m_2, \dots m_n$ be the operator $H^{(n)}$ in (1.5.1) is invariant under simultaneous translation of all particles and thus we can separate the center of mass motion. Let $M = \sum_{i=1}^n m_i$ the total mass of the system. Following [100] this separation can be understood by introducing the following spaces

$$R_0 \coloneqq \left\{ (x_1, x_2, \dots, x_n) \in \mathbb{R}^{nd} : \sum_{i=1}^{n} m_i x_i = 0 \right\}$$
$$R_c \coloneqq \left\{ (x_1, x_2, \dots, x_n) \in \mathbb{R}^{nd} : x_k = \frac{\sum_{j=1}^n m_j x_j}{M},\ k \in \{1, 2, \dots n\} \right\}$$

and the scalar product

$$\langle \cdot, \cdot \rangle_1 : \mathbb{R}^{nd} \times \mathbb{R}^{nd} \to \mathbb{R},\ \langle x, y \rangle \mapsto \sum_{i=1}^{n} m_i (x_i, y_i) \tag{1.5.4}$$

where $(\cdot,\cdot)$ denotes the usual scalar product in $\mathbb{R}^d$. We define the norm $|\cdot|_1^2 := \langle\cdot,\cdot\rangle_1$ corresponding to this new scalar product. We have $R_0 \perp R_c$ in the sense of the product $\langle\cdot,\cdot\rangle_1$ and hence $\mathbb{R}^{nd} = R_0 \oplus R_c$. Consequently

$$L^2(\mathbb{R}^{nd}) \cong L^2(R_0) \otimes L^2(R_c)\,. \tag{1.5.5}$$

The space R_0 is a $(n-1)d$-dimensional subspace of $\mathbb{R}^{nd}$. Let $-P_0^2$ be the corresponding Laplace-Beltrami operator on $C_0^2(R_0)$ which can be extended to a self-adjoint operator on $L^2(R_0)$. Then in the center of mass frame the relevant operator is

$$H_0 := \frac{P_0^2}{2} + \sum_{i<j} V_{ij}(x_i - x_j) \tag{1.5.6}$$

on $L^2(R_0)$. The operator H_0 is called the internal Schrödinger operator. The remaining degrees of freedom correspond to the motion of the center of mass which corresponds to a particle moving freely. To study the spectrum of the internal Schrödinger operator we can neglect the motion of the center of mass.
For an arbitrary number of particles $n \in \mathbb{N}$, it is convenient to introduce coordinates within subsystems by the help of orthogonal projections onto these subsystems, to obtain an explicit representation of the operator P_0^2. Since Chapters 5 and 6 focus exclusively on the case $n = 3$, we will now examine this scenario in more detail. For three-particle systems, it is a common practice to use Jacobi coordinates. We use the common aberration for labeling pairs of particles as $\alpha = (ij) \in I$, where $I := \{(12),(13),(23)\}$. The remaining particle is then labeled by $k \in \{1,2,3\} \setminus \{i,j\}$. The Jacobi coordinates $(\tilde{q}_\alpha, \tilde{\xi}_\alpha)$ for the three–particle system are

$$\tilde{q}_{ij} := x_i - x_j, \quad \tilde{\xi}_{ij} := \underbrace{\frac{m_i x_i + m_j x_j}{m_i + m_j}}_{=\text{ COM of pair (ij)}} - x_k\,.$$

In Figure 1.1 we give the sketch of this specific choice of coordinates. One can express P_0^2 in this new set of coordinates. For simplicity we drop here the indices (ij) so that $\tilde{q}_{(ij)} = \tilde{q}$ and $\tilde{\xi}_{(ij)} = \tilde{\xi}$ and denote by $P_{\tilde{q}}$ and $P_{\tilde{\xi}}$ the momentum operator with respect to $\tilde{q}$ and $\tilde{\xi}$. Then by direct calculations

$$\frac{P_0^2}{2} = \frac{P_{\tilde{q}}^2}{2\mu_{ij}} + \frac{P_{\tilde{\xi}}^2}{2\nu_{ij}}, \quad \mu_{ij} := \frac{m_i m_j}{m_i + m_j}, \quad \nu_{ij} := \frac{(m_i + m_j)m_k}{(m_i + m_j) + m_k} \tag{1.5.7}$$

and

$$x_i - x_k = \tilde{\xi} + \frac{m_j}{m_i + m_j}\tilde{q}, \quad x_j - x_k = \tilde{\xi} - \frac{m_i}{m_i + m_j}\tilde{q}\,.$$

The number μ_{ij} is the reduced mass of particles with masses m_i and m_j whereas ν_{ij} is the reduced mass of particles with masses $m_i + m_j$ and m_k. The operator $H_0 = P_0^2/2 + \sum_{\alpha\in I} V_\alpha$ in

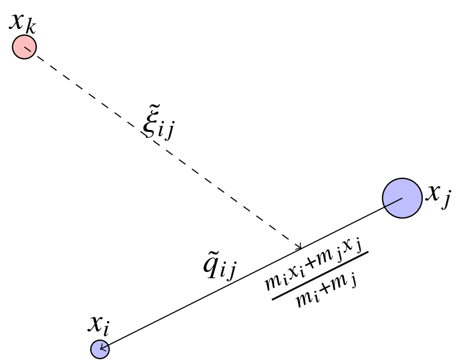

FIGURE 1.1: Jacobi coordinates for the choice of a two–particle subsystem $(ij) \in \{(12), (13), (23)\}$ (colored blue) of the three–particle system with particles at positions $x_1, x_2, x_3 \in \mathbb{R}^d$ and masses $m_1, m_2, m_3 > 0$.

this set of coordinates reads

$$H_0 = \frac{P_{\tilde{q}}^2}{2\mu_{ij}} + \frac{P_{\tilde{\xi}}^2}{2\nu_{ij}} + V_{ij}(\tilde{q}) + V_{ik}\left(\tilde{\xi} + \frac{m_j}{m_i + m_j}\tilde{q}\right) + V_{jk}\left(\tilde{\xi} - \frac{m_i}{m_i + m_j}\tilde{q}\right). \tag{1.5.8}$$

Sometimes it is more convenient to avoid the prefactors of the Laplace operators in (1.5.8). We introduce the rescaled Jacobi coordinates (q_α, ξ_α) with

$$q_{ij} \coloneqq \left(2\mu_{ij}\right)^{1/2} \tilde{q}_{ij}, \quad \xi_{ij} \coloneqq \left(2\nu_{ij}\right)^{1/2} \tilde{\xi}_{ij}, \tag{1.5.9}$$

Then a direct computation shows

$$\langle (x_1, x_2, x_3), (x_1, x_2, x_3) \rangle_1 = \sum_{i=1}^{3} m_i |x_i|^2 = |q_\alpha|^2 + |\xi_\alpha|^2, \quad \forall \alpha \in I\,. \tag{1.5.10}$$

The coordinates in (1.5.9) are chosen such that the kinetic energy operator is independent of the masses and in particular it takes the form

$$\frac{P_0^2}{2} = P_{q_\alpha}^2 + P_{\xi_\alpha}^2 \qquad \text{on } L^2(\mathbb{R}^{2d})\,. \tag{1.5.11}$$

Any system of three particles can be decomposed in three different two–particle subsystems labeled with $\alpha \in I$. In the set of coordinates chosen above each of these two–particle subsystems is then described by the Schrödinger operator

$$h_{ij} \coloneqq \frac{P_{x_i}^2}{2m_i} + \frac{P_{x_j}^2}{2m_j} + V_{ij}(x_i - x_j)\,.$$

The famous HVZ theorem, proved by Zhislin [127], van Winter [123] and Hunziker [53], says that the bottom of the essential spectrum of an N-particle Schrödinger operator (after separating off the free center of mass motion) is given by the lowest possible energy which two independent subsystems can have. By direct application of the HVZ theorem we can therefore locate the essential spectrum of the internal Hamiltonian H_0 and in particular

Proposition 1.5.1 (HVZ theorem for three particle operators)**.** *Let $V_{ij} \in L^p_{\mathrm{loc}}(\mathbb{R}^d)$ with $p = 2$ for $d = 4$ and $p = d/2$ for $d \geq 3$, $d \neq 4$ be short–range in the sense of Definition 1.4.4. Then*

$$\sigma_{\mathrm{ess}}\left(\frac{P_0^2}{2} + \sum_{\alpha\in I} V_\alpha\right) = [\Sigma, \infty), \text{ where } \Sigma := \min_{\alpha\in I} \sigma\left(h_\alpha\right) .$$

1.5.2 Conspiracy of Potential Wells and Proto–Efimov effect

Equipped with the representation of H_0 in (1.5.8) we give here a brief argument why the double well operator studied in Chapter 6 is relevant for the discussion of the discrete spectrum of H_0 and the Efimov effect (see Chapter 3 for an Overview on the Efimov effect).
In the case of equal masses $m_i = m_j = m$ and $m_k = \omega$ the situation simplifies and the operator in (1.5.8) then reads

$$H_0 = \frac{P_{\tilde{q}}^2}{m} + \frac{2m+\omega}{4m\omega} P_{\tilde{\xi}}^2 + V_{ij}(\tilde{q}) + V_{ik}\left(\tilde{\xi} + \frac{1}{2}\tilde{q}\right) + V_{jk}\left(\tilde{\xi} - \frac{1}{2}\tilde{q}\right) . \tag{1.5.12}$$

It is well known that the Efimov effect can only occur if at least two of the two–particle subsystems have a virtual level, see [60], [118]. Assume that the particle pairs (ij) and (ik) have a virtual level. For (ik) for instance that is that the operator

$$h_{ik} = \frac{P_{x_i}^2}{2m} + \frac{P_{x_k}^2}{2\omega} + V_{ik}(x_i - x_k) \tag{1.5.13}$$

has a virtual level. As for the many particle operator we can change to the internal operator of the two–particle operator. Let $s = x_i - x_k$ and $\rho = (m_i x_i + \omega x_k)/(m_i + \omega)$ then the operator in (1.5.13) reads

$$h_{ik} = \left[\frac{m+\omega}{2m\omega} P_s^2 + V_{ik}(s)\right] \otimes \mathbb{1} + \mathbb{1} \otimes \frac{P_\rho^2}{2(m+\omega)} .$$

Note that since the operator h_{ik} has a virtual level, the internal operator

$$h_{ik,0} = \frac{m+\omega}{2m\omega} P_s^2 + V_{ik}(s) \quad \text{ on } L^2(\mathbb{R}^d), \tag{1.5.14}$$

has a virtual level as well. By construction $s = \tilde{\xi} + \tilde{q}/2$ and for fixed $\tilde{q} \in \mathbb{R}^d$ we have $P_s = P_{\tilde{\xi}}$ due to the translation invariance of derivatives. Comparing the prefactor of P_s^2 in (1.5.14) with the prefactor of $P_{\tilde{\xi}}^2$ in (1.5.12) one directly notes that a direct application of the existence of virtual levels is not possible. We therefore note

$$H_0 = \frac{P_{\tilde{q}}^2}{m} + V_{ij}(\tilde{q}) + \frac{1}{4m}P_{\tilde{\xi}}^2 - \frac{m+\omega}{2m\omega}P_{\tilde{\xi}}^2 + V_{ik}\left(\tilde{\xi} + \frac{1}{2}\tilde{q}\right) + V_{jk}\left(\tilde{\xi} - \frac{1}{2}\tilde{q}\right)$$

and define for fixed $\tilde{q}$ the double well operator

$$\mathcal{H}[\tilde{q}] \coloneqq -\frac{m+\omega}{2m\omega}P_{\tilde{\xi}}^2 + V_{ik}\left(\tilde{\xi} + \frac{1}{2}\tilde{q}\right) + V_{jk}\left(\tilde{\xi} - \frac{1}{2}\tilde{q}\right) . \tag{1.5.15}$$

We explain now how to find a bound state of H_0 by usage of the ground state $E[\tilde{q}]$ of the operator $\mathcal{H}[\tilde{q}]$ at large $|\tilde{q}|$. Assume that V_{ik} and V_{jk} are short–range then for large $|\tilde{q}|$ the parameter $|\tilde{q}|$ separates the potentials V_{ik} and V_{jk} in two regions for which either V_{ik} or V_{jk} is small (if the potentials are compactly supported they even vanish in those regions). Given the shift in the potentials it is expected that for any fixed $\tilde{q}$ such that $|\tilde{q}|$ is large enough the ground state $\Phi : \mathbb{R}^d \to \mathbb{C}$ of $\mathcal{H}[\tilde{q}]$ does approximately behave as $\Phi(\tilde{\xi} \pm \frac{1}{2}\tilde{q})$. Let $u \in L^2(\mathbb{R}^d)$ with $\|u\|_2 = 1$ then we make the ansatz $\psi(\tilde{q}, \tilde{\xi}) = u(\tilde{q})\Phi(\tilde{q}, \tilde{\xi})$. By direct computations

$$\begin{aligned} \langle \psi, P_{\tilde{q}}^2 \psi \rangle_{L^2(d\tilde{q}, d\tilde{\xi})} &= \langle u, P_{\tilde{q}}^2 u \rangle_{L^2(d\tilde{q})} - \left\langle u, \left(\int_{\mathbb{R}^d} \left|\nabla_{\tilde{q}} \Phi\right|^2 d\tilde{\xi} \right) u \right\rangle_{L^2(d\tilde{q})} \\ &\approx \langle u, P_{\tilde{q}}^2 u \rangle_{L^2(d\tilde{q})} + \frac{1}{4} \langle \psi, P_{\tilde{\xi}}^2 \psi \rangle_{L^2(d\tilde{q}, d\tilde{\xi})} . \end{aligned} \tag{1.5.16}$$

Consequently, by combining (1.5.16) with (1.5.12) one expects

$$\langle \psi, H_0 \psi \rangle_{L^2(d\tilde{q}, d\tilde{\xi})} \approx \left\langle u, \left(\frac{P_{\tilde{q}}^2}{m} + V_{ij}(\tilde{q}) + E[\tilde{q}] \right) u \right\rangle_{L^2(d\tilde{q})} . \tag{1.5.17}$$

As a consequence, the ground state $E[\tilde{q}]$ of the operator $\mathcal{H}[\tilde{q}]$ takes the role of an effective potential. Whenever the operator

$$\frac{P_{\tilde{q}}^2}{m} + V_{ij}(\tilde{q}) + E[\tilde{q}] \tag{1.5.18}$$

has infinitely many bound states we also expect H_0 to have infinitely many bound states. If the ground state energy $E[\tilde{q}]$ is strong enough to produce infinitely many bound states this is called the *Baby–Efimov* or *Proto–Efimov effect*.

Ovchinnikov and Sigal [89] used that approach to give a variational proof of the Efimov effect. Later Tamura [113] improved that result by constructing good approximations to the ground state Φ. In dimension $d = 3$ and $m = \omega = 1$ the Proto–Efimov effect was already shown by Klaus and Simon in [66]. In particular they show that $E[\tilde{q}] \sim -c|\tilde{q}|^{-2}$ for $c = 0.321651512\ldots$ whenever $|\tilde{q}|$ is large, which is enough for binding as the Hardy constant in dimension $d = 3$ is $1/4$. This phenomenon is called conspiracy of potential wells.

In higher dimensions there is also a conspiracy of potential wells, but it is not strong enough to produce the Proto–Efimov effect. Under some additional assumptions on the potentials it was shown in [91][Theorem 4.3] by Pinchover, that if $d \geq 5$ there exists $C \geq 0$ with

$$-C|\tilde{q}|^{2-d} \leq E[\tilde{q}] \leq -C^{-1}|\tilde{q}|^{2-d}$$

for $|\tilde{q}|$ large. In dimension $d = 4$ we prove that

$$-C|\tilde{q}|^{-2}\log(|\tilde{q}|)^{-1} \leq E[\tilde{q}]$$

for some $C > 0$ in Theorem 6.2.4. There exists a matching upper bound in dimension $d = 4$ by Pinchover [90][Theorem 2.3] under additional assumptions on the involved potentials.

1.5.3 Constrained Three Particle System

In Chapter 5 we study a system of three geometrically constrained bosons. In particular, we study a system of three bosons with short-range interactions, each confined to a separate line in $\mathbb{R}^3$. Two of these lines are parallel within a plane P. The third line intersects P at a nonzero angle and lies in a plane perpendicular to P which intersects P in a line parallel to the first two lines. See Figure 1.2. In contrary to the unconstrained operator $H^{(3)}$ in (1.5.1) the system

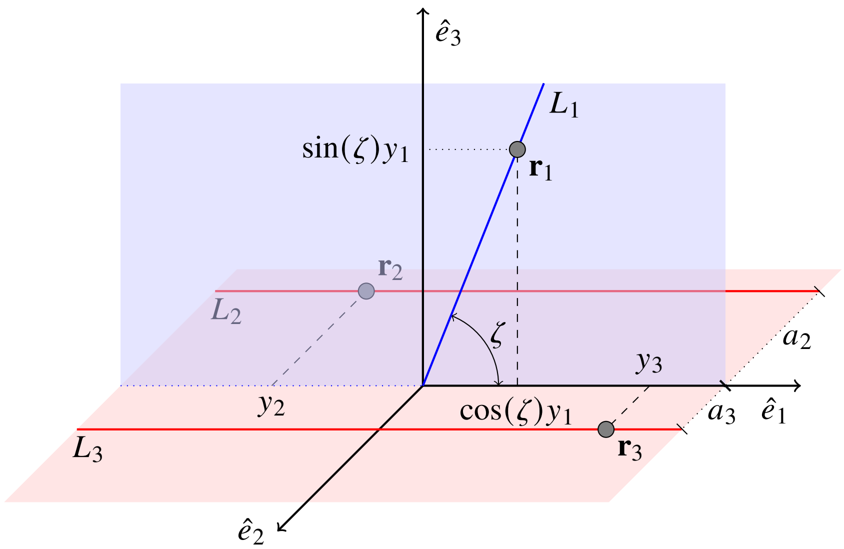

FIGURE 1.2: Geometrically constrained configuration space of particles.

in Figure 1.2 is not invariant under translations. Still we can find a Schrödinger operator that describes this configuration of particles. Let $y_i \in \mathbb{R}$ be the distance of the i-th particle from the origin along the line L_i, and let $\mathbf{r}_i \in \mathbb{R}^3$ be the three–dimensional position vector of this particle. Then

$$\mathbf{r}_1 = \begin{pmatrix} y_1\cos(\zeta) \\ 0 \\ y_1\sin(\zeta) \end{pmatrix}, \mathbf{r}_2 = \begin{pmatrix} y_2 \\ a_2 \\ 0 \end{pmatrix}, \mathbf{r}_3 = \begin{pmatrix} y_3 \\ a_3 \\ 0 \end{pmatrix},$$

where $a_j \in \mathbb{R}$ with $j \in \{2, 3\}$ denotes the distance between the line L_j and the $\hat{e}_1$–axis as indicated in Figure 1.2.
By the usual quantum mechanic correspondence principle we find the kinetic energy by writing down the classical kinetic energy of the system supposing the particles move freely on the Lines L_1, L_2 and L_3. This energy is given by

$$\sum_{k=1}^{3} \frac{|\partial_t \mathbf{r}_k|^2}{2m_k} = \sum_{k=1}^{3} \frac{|\partial_t y_k|^2}{2m_k}, \tag{1.5.19}$$

where ∂_t denotes the derivative with respect to time. Given the energy in (1.5.19) we can interpret the particles at $\mathbf{r}_k$ as one–dimensional particles and replace $\partial_t y_k/(2m_k)$ by the quantum-mechanical momentum operator $P_k \coloneqq -i\partial_{y_k}$ and arrive at

$$\mathcal{T} = \sum_{k=1}^{3} \frac{P_{y_k}^2}{2m_k} .$$

Denote by $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ the distance between the particles i and j. We assume that the particles interact pairwise by three-dimensional forces, therefore we assume that the potentials depend on the distances $\mathbf{r}_\alpha$ with $\alpha \in I$ only. The Schrödinger operator of the system, expressed in this coordinate system, is given by

$$H = \sum_{k=1}^{3} \frac{P_{y_k}^2}{2m_k} + \sum_{\alpha \in I} V_\alpha(|\mathbf{r}_\alpha|) \quad \text{on } L^2(\mathbb{R}^3) \tag{1.5.20}$$

where $V_\alpha : \mathbb{R} \longrightarrow \mathbb{R}$ is the interaction potential between the particle pairs, indexed by $\alpha \in I$, with $I \coloneqq \{(12), (13), (23)\}$ and $m_1, m_2, m_3 > 0$ are the masses of the particles. Regarding the potentials we assume that $V_{1j} \in L^2_{\text{loc}}(\mathbb{R}^2)$ and $V_{23} \in L^2_{\text{loc}}(\mathbb{R})$ and V_α short–range for any $\alpha \in I$. The operator H is not of the same form as the n–particle operator in (1.5.1) and looks more like an internal Hamiltonian as it is not invariant under translations.
Similarly as in Section 1.4.4, we want to pass to a mass–invariant description and consequently it is convenient to introduce the scaling $y_k = \sqrt{2m_k} x_k$. Then $P_{y_k}^2 = 2m_k P_{x_k}^2$ and in abuse of notation, we denote the transformed operator by the same letter such that

$$H = -\sum_{k=1}^{3} P_{x_k}^2 + \sum_{\alpha \in I} V_\alpha(|\mathbf{r}_\alpha|) \quad \text{on } L^2(\mathbb{R}^3) . \tag{1.5.21}$$

In this new set of coordinates the distances $|\mathbf{r}_\alpha|$ are

$$\begin{aligned}\left|\mathbf{r}_{1j}\right| &= \left(\frac{x_1^2}{2m_1} + \frac{x_j^2}{2m_j} - \frac{\cos(\zeta)}{\sqrt{m_1 m_j}} x_1 x_j + a_j^2\right)^{1/2}, \\ |\mathbf{r}_{23}| &= \left(\left(\frac{x_2}{\sqrt{2m_2}} - \frac{x_3}{\sqrt{2m_3}}\right)^2 + (a_2 - a_3)^2\right)^{1/2}.\end{aligned} \tag{1.5.22}$$

The decay properties of zero–energy solutions in the two–particle subsystems do depend on given symmetries. Contrary to the case of unconstrained particles the potentials V_α are not invariant under simultaneous translation or rotation of particle pairs. Still the subsystem (23) is invariant under translations $(x_2, x_3) \mapsto (x_2, x_3) + (s, s)$, $s \in \mathbb{R}$ and in the corresponding center of mass coordinates the Schrödinger operator of this system will be one–dimensional. The subsystems $(1j)$ for $j \in \{2, 3\}$ lack this translation invariance. The corresponding two–particle subsystems are therefore two–dimensional. The subsystems (12) and (13) do have a mirror–symmetry under the transformation $(x_1, x_j) \mapsto (-x_1, -x_j)$, $j \in \{2, 3\}$ as this transformation keeps the distance $\left|\mathbf{r}_{1j}\right|$ invariant. The subsystems are described by the Schrödinger operators

$$h_{1j} = P_{x_1}^2 + P_{x_j}^2 + V_{1j}(\left|\mathbf{r}_{1j}\right|),\ j \in \{2, 3\}\,.$$

Similarly to the HVZ theorem stated in Proposition 1.5.1, we can determine the essential spectrum of the operator H. However, Proposition 1.5.1 cannot be applied directly. Unlike the case of unconstrained particles, where each two-particle system is three-dimensional in its center-of-mass frame, the confined system is more complicated (as discussed above). We give here the corresponding version of the HVZ theorem and give the proof following closely a proof of the HVZ theorem by Enss in [30].

Proposition 1.5.2 (HVZ Theorem for Geometrically Constrained Particles)**.** *Let* $\Sigma_{ij} := \inf \sigma(h_{ij})$ *be the bottom of the spectrum of* h_{ij} *and let* $\Sigma := \min\{\Sigma_\alpha : \alpha \in I\}$. *Then* $\sigma_{\text{ess}}(H) = [\Sigma, \infty)$.

Proof. There exists a technically simple proof of the HVZ theorem by Enss in [30]. In the statement by Enss the assumptions are given in terms of the Schrödinger operator alone without reference to potentials which is beneficial to our situation. The inequality

$$\inf \sigma_{ess}(H) \geq \Sigma \tag{1.5.23}$$

follows directly by application of his proof [30, Theorem 1 and Theorem 2]. We show that the criteria in [30] are fulfilled. These criteria are:

a) The operator H is bounded from below and (essentially) self–adjoint on $\mathcal{H}$.

b) There exists a core $D \subset \mathcal{H}$ of H that is invariant under multiplication with bounded C^∞ functions with bounded derivatives. Moreover, for every bounded $f, g \in C^\infty$ with bounded derivatives

$$\langle\psi, \big[f(x/d), \big[H, g(x/d)\big]\big]\psi\rangle \leq h_d(f,g)\|(\mathbb{1} + |H|)\psi\|^2$$

for some $h_d(f,g) > 0$ with $\lim_{d\to\infty} h_d(f,g) = 0$. Here $x = (x_1, x_2, x_3)$ are the rescaled positions of the particles as discussed above.

c) Let F_R be the multiplication with the characteristic function on the set such that $|\mathbf{r}_\alpha| < R$ for any $\alpha \in I$. The operator $F_R(i\mathbb{1} + H)^{-1}$ is compact for all $R > 0$.

By the assumptions on V_α the operator H is (essentially) self adjoint on $\mathcal{H}$ with form core $C_0^\infty(\mathbb{R}^3)$ and bounded from below. Hence, the first criterion is fulfilled. Considering $D = C_0^\infty(\mathbb{R}^3)$ multiplication by f, g leaves this space invariant, and consequently the following is well–defined

$$\begin{aligned}\langle\psi, \big[f(x/d), \big[H, g(x/d)\big]\big]\psi\rangle \leq &\langle\psi, \big[f(x/d), \big[\sum_{k=1}^{3} P_{x_k}^2, g(x/d)\big]\big]\psi\rangle \\ &+ \langle\psi, \big[f(x/d), \big[\sum_{\alpha} |V_\alpha|, g(x/d)\big]\big]\psi\rangle\end{aligned} \tag{1.5.24}$$

The second term on the right–hand side of (1.5.24) vanishes as V_α is a multiplication operator for $\alpha \in I$. For the first term on the right–hand side of (1.5.24) using that f, g have bounded derivatives it follows from direct computations that there exists $c > 0$ with

$$\left\langle\psi, \left[f(x/d), \big[\sum_{k=1}^{3} P_{x_k}^2, g(x/d)\big]\right]\psi\right\rangle \leq \frac{c}{d^2} \to 0$$

as $d \to \infty$. Consequently, the second criterion of Enss is also fulfilled. The compactness in the third condition follows from the fact that $\sum_{k=1}^{3} P_{x_k}^2$ is form bounded with respect to H. A proof of the compactness condition can be found in [5, Appendix I].

Due to (1.5.23), it suffices to show

$$[\Sigma_\alpha, \infty) \subset \sigma_{ess}(H) \quad \text{for } \alpha \in I\,. \tag{1.5.25}$$

We follow the proof in [114, 11.2. The HVZ theorem]. To this end, we show that for arbitrary $\lambda > 0$ we have $\Sigma_\alpha + \lambda \in \sigma(H)$. We only consider the case $\alpha = (12)$ the case $\alpha = (13)$ is similar. Since the spectrum is closed $\Sigma_{12} \in \sigma(h_{12})$ and consequently for given $\varepsilon > 0$ there exists $\psi_{12} \in L^2(\mathbb{R}^2)$ depending on the internal coordinates $x_1, x_2 \in \mathbb{R}$ with $\|\psi_{12}\| = 1$ and $\|(h_{12} - \Sigma_{12})\psi_{12}\| < \varepsilon$. Since $\sigma_{\mathrm{ess}}(P_{x_3}^2) = [0,\infty)$ there also exists $u \in L^2(\mathbb{R})$ with $\|u\| = 1$ and $\big\|(P_{x_3}^2 - \lambda)u\big\| < \varepsilon$. Consider for $r \in \mathbb{R}$ the function

$$\psi_r(x_1, x_2, x_3) = \psi_{12}(x_1, x_2)u_r(x_3) = \psi_{12}(x_1, x_2)u(x_3 - r)$$

then

$$\|(H-\lambda-\Sigma_{12})\psi_r\| \leq \|(h_{12}-\Sigma_{12})\,\psi_{12}\| + \left\|(P_{x_3}^2-\lambda)u_r\right\| + \|(V_{13}+V_{23})u_r\| \,. \tag{1.5.26}$$

Using that $P_{x_3}^2$ is translation invariant the first two terms in the right–hand side of (1.5.26) are each smaller than ε. Since $C_0^\infty(\mathbb{R})$ is a form core of $P_{x_3}^2$ we can assume $u_r \in C_0^\infty(\mathbb{R})$ and consequently it vanishes pointwise as $r \to \infty$. The potential $V_{13}+V_{23}$ vanishes asymptotically. Since the distances $|\mathbf{r}_{13}|$ and $|\mathbf{r}_{23}|$ tend to infinity by replacing x_3 with x_3-r in the limit $r \to \infty$, we also have

$$(V_{13}+V_{23})u_r \to 0 \quad \text{as } r \to \infty \,.$$

Consequently, for $r > 0$ large enough we arrive at

$$\|(H-\lambda-\Sigma_{12})\psi_r\| \leq 3\varepsilon \,.$$

In the case $\alpha = (23)$ the Schrödinger operator h_{23} is invariant under translations and the internal Hamiltonian of the subsystem (23) is one–dimensional and $\sigma(h_{23}) = \sigma_{\mathrm{ess}}(h_{23}) = [\Sigma_{23}, \infty)$. A similar construction as in the case $\alpha = (23)$ does work with the obvious changes giving (1.5.25). Combining (1.5.23) and (1.5.25) completes the proof of Proposition 1.5.2. ∎

1.5.4 Atomic Schrödinger Operator

In [50] we study the spectrum of the atomic Schrödinger operator in dimension $d = 3$. We assume that the nucleus is a pointlike particle of elementary charge Z at position $x_{N+1} = r \in \mathbb{R}^3$ with mass $M > 0$ interacting with N electrons at positions $(x_1, x_2, \ldots x_N) \in \mathbb{R}^{3N}$ of mass $m_e = 1$. This means, that we consider the operator $H^{(n)}$ for $n = N+1$ with the choices

$$V_{ij}(x_i - x_j) = \frac{\alpha}{\left|x_i - x_j\right|}, \quad 1 \leq i < j \leq N$$
$$V_{i(N+1)}(x_i - r) = \frac{-Z\alpha}{|x_i - r|}, \quad i \leq N$$

i.e. the operator

$$\mathcal{H}_{N,Z} = \frac{1}{2M}P_r^2 + \sum_{k=1}^{N}\frac{1}{2}P_k^2 - \sum_{i=1}^{N}\frac{Z\alpha}{|x_i - r|} + \sum_{1\leq i<j\leq N}\frac{\alpha}{\left|x_i - x_j\right|}, \quad P_r = -i\nabla_r \,.$$

The operator $\mathcal{H}_{N,Z}$ is invariant under combined translation of all particles and consequently $\sigma(\mathcal{H}_{N,Z}) = \sigma_{\mathrm{ess}}(\mathcal{H}_{N,Z})$. To study the inner degrees of freedom of this system, one needs to use a non–translationally invariant operator. In the infinite mass approximation, that is $M \to \infty$ we assume that the nucleus is fixed at $r = 0$ so that we can ignore the kinetic energy of the nucleus. We arrive at the internal Hamiltonian

$$H_{N,Z} \coloneqq \frac{1}{2}\sum_{k=1}^{N} P_k^2 - \sum_{i=1}^{N}\frac{Z\alpha}{|x_i|} + \sum_{1\leq i<j\leq N}\frac{\alpha}{\left|x_i - x_j\right|} \,. \tag{1.5.27}$$

This operator then describes a fixed nucleus surrounded by N identical particles. The operator $H_{N,Z}$ is bounded from below and the bottom of the spectrum of $H_{N,Z}$ is called ground state energy

$$E_{N,Z} \coloneqq \inf \sigma(H_{N,Z}) \,. \tag{1.5.28}$$

As for the many–particle operators in the previous sections, one can formulate the HVZ theorem for this operator. Following [114, Theorem 11.2] we have

Theorem 1.5.3 (HVZ theorem for atomic Schrödinger operator)**.** *The operator $H_{N,Z}$ is bounded from below and*

$$\sigma_{\text{ess}}(H_{N,Z}) = [E_{N-1,Z}, \infty) \,.$$

For large atoms $Z \gg 1$, the particles should be considered to be relativistic. To include a simple pseudorelativistic case, we will study in Section 2 the N-particle Chandrashekar operator

$$C_{N,Z} \coloneqq \sum_{k=1}^{N} \left(\sqrt{\alpha^{-2} P_k^2 + \alpha^{-4}} - \alpha^{-2} \right) - \sum_{i=1}^{N} \frac{Z}{|x_i|} + \sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|} \,. \tag{1.5.29}$$

We apply our results from [50] and prove new bounds on the maximal allowed excess charge in the psuedorelativistic case. The operator $C_{N,Z}$ is bounded from below if and only if $Z\alpha < 2/\pi$ (See [65, Chapter 5, (5.33) and (5.34)], [45, Theorem 2.5] and [121] for reference). Since $\alpha = e^2/(\hbar c) \approx 1/137$ we have $Z < 87.22$ in the pseudorelativistic case. Then, if $Z\alpha < 2/\pi$ and all of the involved particles have spin S, the operator $C_{N,Z}$ can be defined on $\mathcal{H}_N$ defined in (1.5.2) as the Friedrichs extension of the corresponding quadratic form with form domain $H^{1/2}(\mathbb{R}^{3N} : \mathbb{C}^{2S+1}) \cap \mathcal{H}_N$.

Chapter 2

The Excess Charge Problem

2.1 Overview

The question of maximal negative ionization of atoms is a widely studied but still unresolved fundamental problem in quantum mechanics. We refer, for instance, to Barry Simon's Fifteen Problems in Mathematical Physics [103]. For a comprehensive review, see [37, pp. 99-130] and references therein. To the best of our knowledge, there is no experimental evidence that a single neutral atom in a vacuum can bind more than one, or at most two, additional electrons. Considering an (ionized) atom with Z protons and N electrons, the excess charge is $Q = N - Z$. The case $Q = 0$ is then the atomic case. The ionization conjecture on the maximal number of electrons an atom with nuclear charge Z can bind is $Q \leq Q_{\max}$ for a constant $Q_{\max} > 0$ independent of Z and probably $Q_{\max} = 1$ or $Q_{\max} = 2$. Up to now, there is no proof that $Q_{\max}$ is uniformly bounded in Z.
Considering the many-particle Schrödinger operator $H_{N,Z}$ on $\mathcal{H}_N^f$ introduced in Section 1.5 the bottom of the spectrum of $H_{N,Z}$ is called ground state energy

$$E_{N,Z} \coloneqq \inf \sigma(H_{N,Z}) = \inf_{\psi \in \mathcal{H}_N^f} \frac{\langle \psi, H_{N,Z}\psi \rangle}{\|\psi\|^2} . \tag{2.1.1}$$

Since $H_{N,Z}$ is bounded from below on $\mathcal{H}_N^f$, the value $E_{N,Z}$ is finite for any values of N and Z. To answer the Ionization conjecture it suffices to show that in the case $N \geq Z + 2$ the right–hand side of (2.1.1) is not a minimum in $\mathcal{H}_N^f$. Due to an early work of Zhislin [128], we know that there is a minimizer in the case $N < Z + 1$, which proves that atoms and positively charged ions do indeed exist.
We define the critical number of electrons that a nucleus with Z particles can bind as the largest number $N_c = N_c(Z)$ such that $E_{N_c,Z}$ is a minimum (that is, $E_{N_c,Z} = \inf \sigma(H_{N,Z})$ is an eigenvalue of $H_{N,Z}$ in $\mathcal{H}_N$). Note that it is also an open question whether $E_{N,Z}$ not being a minimum also implies that $E_{n,Z}$ is not a minimum for all $n > N$. Due to the famous HVZ we know $\sigma_{\text{ess}}(H_{N,Z}) = [E_{N-1,Z}, \infty)$ and consequently the binding inequality

$$E_{N,Z} = \inf \sigma(H_{N,Z}) \leq E_{N-1,Z}$$

does hold for all $N \in \mathbb{N}$.

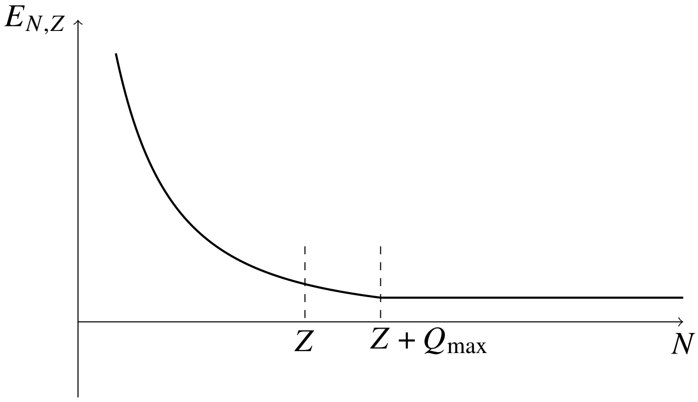

FIGURE 2.1: Sketch of the predicted behavior of the ground state energy $E_{N,Z}$ for fixed $Z > 1$. The prediction suggests that configurations with more particles (e.g., electrons) are preferred, as they lower the energy $E_{N,Z}$ up to a critical number of particles $N_c(Z) = Z + Q_{\max}$. The graph of $E_{N,Z}$ is expected to be convex, reflecting the fact that the ionization energies are growing. Specifically, $|E_{N,Z} - E_{N-1,Z}|$ decreases as N increases until it vanishes for $N > N_c(Z)$.

Remark 2.1.1. *If $E_{N,Z} < E_{N-1,Z}$ then $E_{N,Z} \in \sigma_{\text{disc}}(H_{N,Z})$. In particular, there exists an eigenfunction $\psi_{N,Z} \in \mathcal{H}_N$ with $H_{N,Z}\psi_{N,Z} = E_{N,Z}\psi_{N,Z}$*

Regarding the excess charge problem, the following results are known. As discussed above, due to the early work of Zhislin [128]

$$\liminf_{Z\to\infty} \frac{N_c(Z)}{Z} \geq 1$$

was known for a long time already. That there is a critical number $N_c(Z) < \infty$ that an atom of charge Z can bind was first shown independently by Ruskai [95] and Sigal [99]. Later, Lieb, Sigal, Simon, and Thirring [77] proved

$$\lim_{Z\to\infty} \frac{N_c(Z)}{Z} = 1 \, .$$

In fact, they proved the result with lim replaced by lim sup. The result by Lieb, Sigal, Simon, and Thirring uses a compactness argument and does not provide any quantitative bounds on how big $N_c(Z)$ is for finite nuclear charge Z.
If the particles are bosons, it is known from the work of Benguria and Lieb [17] that the asymptotic neutrality does not hold and, in particular,

$$\lim_{Z\to\infty} \frac{N_c(Z)}{Z} = t_c > 1 \, . \tag{2.1.2}$$

Later Baumgartner [15] determined computationally $t_c \approx 1.21$.

Considering finite values of Z Fefferman and Seco [32] and Seco, Sigal and Solovej [97] proved in 1990

$$N_c(Z) - Z \leq CZ^{5/7} \tag{2.1.3}$$

for some $C > 0$. Non–asymptotic bounds are rare. For a long time, the only non-asymptotic bound was due to Lieb [71], who proved his famous bound

$$N_c(Z) < 2Z + 1 \quad \text{for all } Z \geq 1\,. \tag{2.1.4}$$

Lieb's result is independent of the statistics of the particles, i.e., independent of whether they are fermions of bosons, and it also holds, suitably modified, for systems of atoms, i.e., molecules. While Lieb's bound certainly overcounts $N_c(Z)$, it shows that Hydrogen ($Z = 1$) can bind at most two electrons, which is observed in nature.
It took 28 years until Nam's breakthrough result [81] could significantly improve Lieb's longstanding bound. Nam showed, for a single atom with fermionic statistics, that

$$N_c(Z) < 1.22Z + 3Z^{1/3} \quad \text{for all } Z \geq 1\,. \tag{2.1.5}$$

In this work, we provide even tighter bounds on N_c. In particular, we prove in Proposition 4.2.5

$$N_c(Z) < 1.1185Z + 3.90Z^{1/3} + 0.0134 + 0.184Z^{-1/3} + 0.0196Z^{-2/3}, \quad \text{for all } Z \geq 4\,.$$

Rounding numbers up this shows $N < 1.12\,Z + 4Z^{1/3}$ for all $Z \geq 4$. We want to stress that this shows that for large nuclear charges Z, fermionic atoms do indeed behave much differently from bosonic atoms. Bosonic atoms are known to allow for a surcharge of 21 %, i.e., large bosonic atoms can bind roughly $N \sim 1.21Z$ bosonic particles for large Z. The leading order coefficient in Nam's bound is just above 1.21, whereas in our bound, it is lower, with a good safety margin.
To achieve our improvements, we significantly extend Nam's approach and, in addition, prove some of his conjectures made in [81].
For bosonic atoms, we have utilized approaches by Benguria et al. [19] involving the *Hartree Model* to prove new bounds on the ground state energy of bosonic ions. Specifically, we show in Corollary 4.8.6

$$E_{N,Z} \geq -\frac{2t_c}{9}Z^3 + O(Z^{7/3})\,.$$

Interestingly, this bound involves the parameter t_c from (2.1.2). By combining the new techniques developed for the fermionic case with the new bounds on the ground state energy, we have derived in Theorem 4.2.7

$$N_c(Z) \leq \frac{t_c}{x_0^2}Z + O(Z^{1/2})$$

where $x_0 > 0$ is the unique positive solution of:

$$0.782\, t_c = (1 + 0.1463 x_0)\, x_0^2 \,.$$

With $t_c \approx 1.21$, we find $t_c x_0^{-2} \approx 1.45$. To the best of our knowledge, this is the first improvement over Lieb's result of $2Z + 1$ in the bosonic case.

Remark 2.1.2. *The best analytic bound on t_c was for a long time due to Lieb's result given by $t_c \leq 2$. Benguria and Tubino showed in [14] $t_c < 1.5211$ together with our improvements we are able to improve upon their result and show $t_c < 1.47$ see Lemma A.7.1 and the Remark thereafter.*

2.2 The Excess Charge Problem for the Pseudorelativistic Operator

In [50], we did not discuss relativistic models. Our improvements generalize for these cases and can also give refined bounds on $N_c(Z)$ in these cases. We will cover here the pseudorelativistic case given by the operator

$$C_{N,Z} := \sum_{k=1}^{N} \left(\sqrt{\alpha^{-2} P_k^2 + \alpha^{-4}} - \alpha^{-2} \right) - \sum_{l=1}^{N} \frac{Z}{|x_l|} + \sum_{1 \leq l < m \leq N} \frac{1}{|x_l - x_m|} \,. \tag{2.2.1}$$

which was defined in (1.5.29). In particular, we prove the following Theorems in Section 2.2.1

Theorem 2.2.1. *Let $\lambda > 1$ and let $E_{N,Z}^{\mathrm{rel}} := \inf \sigma(C_{N,Z})$ be an eigenvalue of $C_{N,Z}$ on $L^2(\mathbb{R}^3)$ in $\mathcal{H}_N^f$ then there exists $c_\lambda > 0$ with*

$$N < \frac{1}{2}\left(\sqrt{2} + 1\right) Z + c_\lambda Z^{1/3}, \quad \textit{for } Z > 0 \textit{ with } \lambda Z \alpha < 2/\pi \,.$$

Remark 2.2.2. *Theorem 2.2.1 refines the inequality by Nam in [84, Thoerem 3].*

To prove this results we apply the so–called Benguria-Lieb-Nam argument (see Section 4.3), that is to multiply the Schrödinger equation from the left by $|x_k|^2 \overline{\psi_{N,Z}}$, where $\psi_{N,Z}$ is a ground state corresponding to $E_{N,Z}$ then, in the quadratic form sense,

$$0 = \langle |x_k|^2 \psi_{N,Z}, (C_{N,Z} - E_{N,Z}) \psi_{N,Z} \rangle = \mathrm{Re} \langle |x_k|^2 \psi_{N,Z}, (C_{N,Z} - E_{N,Z}) \psi_{N,Z} \rangle \,. \tag{2.2.2}$$

As in the non–relativistic case we have $C_{N-1,Z} \geq E_{N-1} \geq E_N$ using the HVZ theorem for pseudorelativistic operators from [69] which holds for $Z \in (0, 2/(\pi\alpha)]$. Applying the symmetry of $\psi_{N,Z} \in \mathcal{H}_N^f$ and defining

$$\alpha_{N,2} := \inf \left\{ \frac{\sum_{1 \leq j < k \leq N} \frac{|x_k|^2 + |x_i|^2}{|x_i - x_k|}}{(N-1) \sum_{k=1}^{N} |x_k|} : x_k \in \mathbb{R}^3 \text{ for } k = 1, \dots, N \right\} \tag{2.2.3}$$

this yields, as explained in Section 4.3, the inequality

$$\alpha_{N,2}(N-1) < Z - \frac{1}{2}\frac{\mathrm{Re}\left\langle |x_1|^2\psi_{N,Z}, T_1^{\mathrm{rel}}\psi_{N,Z}\right\rangle}{\left\langle |x_1|\psi_{N,Z}, \psi_{N,Z}\right\rangle}. \tag{2.2.4}$$

Here T_1^{rel} is the pseudorelativistic operator acting on $x_1 \in \mathbb{R}^3$ and is defined by

$$T_1^{\mathrm{rel}} = \sqrt{\alpha^{-2}P_1^2 + \alpha^{-4}} - \alpha^{-2}, \quad P_1 = -i\nabla_{x_1}.$$

We need two ingredients to prove Theorem 2.2.1. The first one is an estimate for the expression $\alpha_{N,2}$ and the second one is a lower bound for the weighted kinetic energy in the right–hand side of (2.2.4). To estimate $\alpha_{N,2}$ one can apply Nam's mean field type argument and our improvements in Section 4.4 to find

Lemma 2.2.3. *Let $\alpha_{N,2}$ be defined as in* (2.2.3) *then for every $N \geq 2$, $r > 0$*

$$\frac{(1+r)^3 - (|1-r|)^3}{6r} N\beta_2 \leq \frac{(1+r)^4 - (|1-r|)^4}{8r}\left(\alpha_{N,2}(N-1) + \frac{1}{r}\right),$$

where

$$\beta_2^{-1} \leq \frac{1}{2}\left(\sqrt{2}+1\right).$$

Proof. The first inequality follows directly from Lemma 4.5.9 and Remark 4.4.6. For the estimate on β_2^{-1} see Section 4.4. ∎

In dimension $d = 3$ in the non-relativistic case $T = P^2$ by application of the IMS localization formula, we obtain

$$\frac{\varphi(x)^2 T + T\varphi(x)^2}{2} = \frac{1}{2}\left(\varphi(x)T\varphi(x) - |P\varphi(x)|^2\right) \tag{2.2.5}$$

and for $\varphi(x) = |x|$ this yields together with the Hardy inequality

$$\frac{|x|^2 T + T|x|^2}{2} = \frac{1}{2}\left(|x|T|x| - |P|x||^2\right) \geq -\frac{3}{8} \tag{2.2.6}$$

as an operator on $L^2(\mathbb{R}^3)$. Chen and Siedentop proved in [24] the generalization that if $a + b \leq d$ with $\min\{a, b\} \in [0, 2]$ with $d > 0$ the underlying spatial dimension, then

$$|P|^a|x|^b + |x|^b|P|^a \geq 0 \text{ on } L^2(\mathbb{R}^d). \tag{2.2.7}$$

They remarked the importance of this inequality in the excess charge problem and Handrek and Siedentop [44] applied the inequality to the ultrarelativistic operator

$$D_{N,Z} := \sum_{k=1}^{N} |P_k + A(x_k)| + \sqrt{\alpha}\sigma_k \cdot \mathcal{A}(x_i) - \sum_{i=1}^{N}\frac{Z\alpha}{|x_i|} + \sum_{1\leq i<j\leq N}\frac{\alpha}{|x_i - x_j|}. \tag{2.2.8}$$

with $A \in L^2_{\text{loc}}(\mathbb{R}^2, \mathbb{R}^2)$ and $|\mathcal{A}(x)| \leq \delta |x|^{-1}$ for some $\delta > 0$, which is a simplified model describing particles interacting with a graphene quantum dot. They showed

$$N_c(Z) < 2(\delta + Z) + 1 \tag{2.2.9}$$

by application of the Benguria–Lieb argument.

Remark 2.2.4. *For $d = 3$, the ultrarelativistic case $a = 1$ and $b = 2$ is covered in [24]. The case $a = 2$ and $b = 1$ was discussed by Lieb in [71]. In dimension $d = 2$, one can reproduce Lieb's result with this inequality, but $a = b = 1$ is the borderline case for positivity. In [81], Nam did discuss the case $b = 2$ for pseudorelativistic operators.*

The following inequalities hold

Lemma 2.2.5. *Let $d = 3$, then on $C_0^\infty(\mathbb{R}^d)$*

$$\frac{|x|^2 T^{\text{rel}} + T^{\text{rel}} |x|^2}{2} \geq -\frac{3}{8}, \quad \frac{|x|^2 |P| + |P||x|^2}{2} \geq 0 \tag{2.2.10}$$

and for $d = 2$

$$\frac{|x|^2 |P| + |P||x|^2}{2} \geq -\frac{\Gamma^2(1/4)}{4\pi^2} |x| \,. \tag{2.2.11}$$

Remark 2.2.6. *We will use the first inequality* (2.2.10) *to establish bounds on the excess charge for the operator $C_{N,Z}$. The other two inequalities apply to the ultrarelativistic case. In particular,* (2.2.11) *can be used in the discussion of the operator $D_{N,Z}$ defined in* (2.2.8).

Proof. The second inequality in (2.2.10) is covered by the result of Chen and Siedentop (see (2.2.7)). The first inequality in (2.2.10) was proven by Nam in [81, eq. (24)]). We give a different proof of this inequality. Since T^{rel} is (essentially) self adjoint on $C_0^\infty(\mathbb{R}^d)$ we find that

$$\left\langle \psi, \frac{|x|^2 T^{\text{rel}} + T^{\text{rel}} |x|^2}{2} \psi \right\rangle = \text{Re}\langle |x|^2 \psi, T^{\text{rel}} \psi \rangle$$

Consider $t : k \in \mathbb{R}^d \mapsto \sqrt{\alpha^{-2}|k|^2 + \alpha^{-4}} - \alpha^{-2}$, which is the Fourier multiplier of T^{rel} then due to the Plancherel theorem

$$\text{Re}\langle |x|^2 \psi, T^{\text{rel}} \psi \rangle = \text{Re}\langle (-\Delta_k) \hat{\psi}, t \hat{\psi} \rangle \,. \tag{2.2.12}$$

The expectation on the right–hand side is real (apply the IMS formula and use $t(k)$ is positive). Following [8, p. 420 ff] we can define fractional powers of any closed operator A as

$$A^\kappa = \frac{\sin(\kappa\pi)}{\pi} \int_0^\infty \frac{A}{A + r} \frac{dr}{r^{1-\kappa}} \,. \tag{2.2.13}$$

By direct calculations and (2.2.13) with $\kappa = 1/2$, we find the representation

$$T^{rel} = \sqrt{\alpha^{-2} P^2 + \alpha^{-4}} - \alpha^{-2} = \frac{\alpha^{-1} P^2}{\pi} \int_{\alpha^{-2}}^\infty \frac{\sqrt{r - \alpha^{-2}}}{r + P^2} \frac{dr}{r} \,.$$

For the Fourier multiplier, this is indeed a pointwise identity such that

$$t(k) = \frac{\alpha^{-1}|k|^2}{\pi} \int_{\alpha^{-2}}^{\infty} \frac{\sqrt{r-\alpha^{-2}}}{r+|k|^2} \frac{dr}{r} \quad \forall k \in \mathbb{R}^d \,. \tag{2.2.14}$$

Inserting (2.2.14) into the right hand side of (2.2.12) yields

$$\langle |x|^2\psi, T^{\mathrm{rel}}\psi\rangle = \frac{\alpha^{-1}}{\pi} \int_{\alpha^{-2}}^{\infty} \sqrt{r-\alpha^{-2}} \left\langle (-\Delta_k)\hat{\psi}, |k|^2(r+|k|^2)^{-1}\hat{\psi}\right\rangle \frac{dr}{r} \,. \tag{2.2.15}$$

Define $\hat{u} \coloneqq (r+|k|^2)^{-1}\hat{\psi}$, then the weighted kinetic energy under the integral can be written as

$$\left\langle (-\Delta_k)\hat{\psi}, |k|^2(r+|k|^2)^{-1}\hat{\psi}\right\rangle = r\langle (-\Delta_k)\hat{u}, |k|^2\hat{u}\rangle + \langle (-\Delta_k)(|k|^2\hat{u}), |k|^2\hat{u}\rangle \,. \tag{2.2.16}$$

By the same arguments as in the non–relativistic case (see Lemma 4.6.2) it follows for the first term in the right–hand side of (2.2.16) that

$$r\langle (-\Delta_k)\hat{u}, |k|^2\hat{u}\rangle \geq -\frac{3r}{4}\langle \hat{u}, \hat{u}\rangle = -\frac{3r}{4}\langle \hat{\psi}, (r+|k|^2)^{-2}\hat{\psi}\rangle \,. \tag{2.2.17}$$

By Hardy's inequality, we can estimate the second term on the right–hand side of (2.2.16) to find

$$\langle (-\Delta_k)(|k|^2\hat{u}), |k|^2\hat{u}\rangle \geq \left(\frac{d-2}{2}\right)^2 \langle \hat{u}, |k|^2\hat{u}\rangle \geq 0 \,. \tag{2.2.18}$$

Note that one could keep this positive contribution and try to prove a better inequality after solving the integral over dr by optimizing in $|k|$. However, we could not obtain enough information on $\hat{\psi}$ for an improvement.
Consequently by inserting (2.2.17) and (2.2.18) into (2.2.16) we arrive at

$$\left\langle (-\Delta_k)\hat{\psi}, |k|^2(r+|k|^2)^{-1}\hat{\psi}\right\rangle \geq \left\langle \hat{\psi}, \frac{-3r}{4}(r+|k|^2)^{-2}\hat{\psi}\right\rangle \,. \tag{2.2.19}$$

Combining (2.2.15) and (2.2.19) we find

$$\langle |x|^2\psi, T^{\mathrm{rel}}\psi\rangle \geq \frac{-3}{4}\frac{\alpha^{-1}}{\pi} \int_{\alpha^{-2}}^{\infty} \sqrt{r-\alpha^{-2}} \left\langle \hat{\psi}, (r+|k|^2)^{-2}\hat{\psi}\right\rangle dr \,.$$

By direct calculations, one finds

$$-\frac{3}{4}\frac{\alpha^{-1}}{\pi} \int_{\alpha^{-2}}^{\infty} \sqrt{r-\alpha^{-2}}(r+|k|^2)^{-2} dr \geq -\frac{3}{8} \,,$$

where we used

$$\frac{\alpha^{-1}}{\pi}\int_{\alpha^{-2}}^{\infty}\frac{\sqrt{r-\alpha^{-2}}}{(r+|k|^2)^2}dr \le \frac{\alpha^{-1}}{\pi}\int_{\alpha^{-2}}^{\infty}\frac{\sqrt{r-\alpha^{-2}}}{r^2}dr = \frac{1}{2}\,.$$

Consequently, the first inequality in (2.2.10) follows immediately.
Similarly, we now prove the inequality on the ultrarelativistic kinetic energy in dimension $d=2$. Let $\tau : k \in \mathbb{R}^2 \mapsto |k|$, then by the Plancherel theorem

$$\langle |x|^2\psi, |P|\psi\rangle = \langle(-\Delta_k)\hat{\psi}, \tau\hat{\psi}\rangle \tag{2.2.20}$$

and using (2.2.13) we find

$$\tau(k) = \frac{1}{\pi}\int_0^{\infty}\frac{|k|^2}{|k|^2+r}\frac{dr}{r^{1/2}}\,. \tag{2.2.21}$$

Define $\hat{u} := (r+|k|^2)^{-1}\hat{\psi}$ then by inserting (2.2.21) into (2.2.20) we arrive at

$$\begin{aligned}\langle |x|^2\psi, |P|\psi\rangle &= \frac{1}{\pi}\int_0^{\infty}\langle(-\Delta_k)(|k|^2+r)\hat{u}, |k|^2\hat{u}\rangle\frac{dr}{r^{1/2}}\\ &\ge \frac{1}{\pi}\int_0^{\infty}\langle(-\Delta_k)\hat{u}, |k|^2\hat{u}\rangle r^{1/2}dr\,.\end{aligned} \tag{2.2.22}$$

By application of the IMS localization formula in (2.2.5) with $\varphi(k) : k \in \mathbb{R}^2 \mapsto |k|^2$ we find

$$\langle(-\Delta_k)\hat{u}, |k|^2\hat{u}\rangle = \langle\hat{u}, (|k|(-\Delta_k)|k|-1)\,\hat{u}\rangle \ge -\langle\hat{u},\hat{u}\rangle\,. \tag{2.2.23}$$

Note that contrary to dimension three, we cannot apply Hardy's inequality to the equation above. Inserting (2.2.23) into the right–hand side of (2.2.22) yields

$$\langle |x|^2\psi, |P|\psi\rangle \ge -\left\langle\hat{\psi}, \int_0^{\infty}\frac{r^{1/2}}{(r+|k|^2)^2}dr\hat{\psi}\right\rangle = -\left\langle\hat{\psi}, |k|^{-1}\hat{\psi}\right\rangle\,. \tag{2.2.24}$$

We apply the following Hardy-type inequality (see [38])

$$\int_{\mathbb{R}^d}|x|^{-2s}|f(x)|^2\,dx \le C_{s,d}^{-1}\int_{\mathbb{R}^d}|\xi|^{2s}|\hat{f}(\xi)|^2\,d\xi, \qquad f \in C_0^{\infty}(\mathbb{R}^d), \tag{2.2.25}$$

which is valid for $0 < 2s < d$. The sharp constant in (2.2.25),

$$K_{s,d} := 2^{2s}\frac{\Gamma^2((d+2s)/4)}{\Gamma^2((d-2s)/4)}\,, \tag{2.2.26}$$

has been found independently by Herbst [45] and Yafaev [125]. In our case $s=1/2$ and $d=2$ with

$$K_{1/2,2}^{-1} = \Gamma^2(1/4)/(4\pi^2)$$

and consequently by combining (2.2.25) and (2.2.24), we arrive at

$$\langle |x|^2\psi, |P|\psi\rangle \geq -K_{1/2,2}^{-1}\langle \psi, |x|\psi\rangle \,.$$

∎

2.2.1 Critical Number of Electrons

Equipped with the inequality (2.2.4) and the Lemmas 2.2.3 and 2.2.5 we prove now Theorem 2.2.1.

Proof of Theorem 2.2.1. Combining (2.2.4) and the first inequality in (2.2.10) yields

$$\alpha_{N,2}(N-1) \leq Z + \frac{3}{8}\left\langle |x_1|\psi_{N,Z}, \psi_{N,Z}\right\rangle^{-1} \,. \tag{2.2.27}$$

To estimate the right–hand side above, we first note that by application of Jensen's inequality

$$\left\langle |x_1|\psi_{N,Z}, \psi_{N,Z}\right\rangle^{-1} \leq \left\langle |x_1|^{-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle = \left\langle \psi_{N,Z}, |x_1|^{-1}\psi_{N,Z}\right\rangle \,.$$

Recall that $C_{N,Z}$ is the many–particle Chandrashekar operator defined in (1.5.29). Let $\lambda > 0$ then due to the symmetry of $\psi_{N,Z}$

$$(\lambda-1)NZ\left\langle \psi_{N,Z}, |x_1|^{-1}\psi_{N,Z}\right\rangle = \langle \psi_{N,Z}, (C_{N,Z} - C_{N,\lambda Z})\psi_{N,Z}\rangle \leq E_{N,Z} - E_{N,\lambda Z} \,.$$

Assume $\lambda > 1$ then Dividing by $\lambda - 1$ yields

$$\left\langle \psi_{N,Z}, |x_1|^{-1}\psi_{N,Z}\right\rangle \leq \frac{E_{N,Z} - E_{N,\lambda Z}}{(\lambda-1)NZ} \leq \frac{-E_{N,\lambda Z}}{(\lambda-1)NZ} \,.$$

Using that there exists $C_\lambda > 0$ with $-C_\lambda Z^{7/3} < E_{N,\lambda Z} < 0$ for any $Z > 0$ with $\lambda Z\alpha < 2/\pi$ and consequently for $N > Z$

$$\left\langle \psi_{N,Z}, |x_1|^{-1}\psi_{N,Z}\right\rangle \leq \frac{C_\lambda}{\lambda-1}Z^{1/3}, \quad \text{for } \lambda Z\alpha < 2/\pi \,. \tag{2.2.28}$$

For fixed ratio N/Z in the large Z limit it was shown by Sorensen [88], that $E_{N,Z}$ in leading order in Z is the same as in the non-relativistic case, given by (non-relativistic) Thomas-Fermi theory. Define $\hat{C}(\lambda) := \frac{3}{8}C_\lambda(\lambda-1)^{-1}$ then with (2.2.27) and (2.2.28) we arrive at

$$\alpha_{N,2}(N-1) \leq Z + \hat{C}(\lambda)Z^{1/3}, \quad \text{for } \lambda Z\alpha < 2/\pi \,.$$

Applying Lemma 2.2.3 yields for any $r \in (0,1)$

$$\frac{(1+r)^3 - (1-r)^3}{6r}N\beta_2 \leq \frac{(1+r)^4 - (1-r)^4}{8r}\left(Z + \hat{C}(\lambda)Z^{1/3} + \frac{1}{r}\right) \,. \tag{2.2.29}$$

In Appendix A as Lemma A.5.1 we have shown

$$\frac{(1+r)^3-(1-r)^3}{3} \geq \left(1-\frac{2}{3}r^2\right)\frac{(1+r)^4-(1-r)^4}{4}\,. \tag{2.2.30}$$

Combining (2.2.29) and (2.2.30) yields

$$N\beta_2 \leq Z + \hat{C}(\lambda)Z^{1/3} + \frac{1}{r} + N\beta_2\frac{2}{3}r^2\,.$$

Choose $r = \mu Z^{-1/3}$ for some $\mu > 0$ such that $r \in (0,1)$ then for $N \leq 3Z$ (which we can always assume due to $N_c(Z) < 2Z + 1$)

$$N \leq \beta_2^{-1}Z + \beta_2^{-1}\left(\hat{C}(\lambda) + \mu^{-1} + 2\beta_2\mu^{2/3}\right)Z^{1/3}$$

which proves the statement of Theorem 2.2.1 since

$$\beta_2^{-1} \leq \frac{1}{2}\left(\sqrt{2}+1\right)$$

by Lemma 2.2.3. ∎

Chapter 3

The Efimov Effect

3.1 Overview

Consider a Schrödinger operator $H = P^2/2 + V$ with $\sigma_{\text{ess}} = [0, \infty)$ which is, for instance, fulfilled if the potential vanishes at infinity in the sense of (1.4.1). It is well known that if V is a short–range potential, then there are always at most finitely many bound states. For many–particle operators, the spectrum is more complicated. Due to the famous HVZ theorem (see Proposition 1.5.1), the essential spectrum of a many-particle operator is $[\Sigma, \infty)$ where $\Sigma \in \mathbb{R}$ is the bottom of the spectra of the Schrödinger operators with one particle less. In the corresponding center of mass frame, the n-particle Operator can have bound states that correspond to isolated eigenvalues of finite multiplicity below the essential spectrum. In the case of short–range potentials and $\Sigma < 0$, which is the same as saying that one of the sub–systems does already have a bound state, independently Zhislin [129] and Yafaev [58] found that the negative spectrum is at most finite. The case $\Sigma = 0$ is much more complicated. Indeed, it was predicted in the 1960s by Efimov [28] that there are situations in which the three–particle systems with short–range interactions can have an infinite number of bound states. To be precise, the effect can be described in the following way:

The Efimov effect is a phenomenon where three particles in three-dimensional space that interact with short–range potentials form an infinite number of bound states even if none of the two-particle subsystems are bound. This effect can only occur if at least two of the two–particle subsystems possess a virtual level (see Definition 1.4.1).

That the effect can only occur if at least two subsystems possess a virtual level was already proven in [60], and for a fully variational proof of this, see [118].
The Efimov effect is surprising for several reasons. An infinite number of bound states is usually seen in systems with long–range interactions and is not to be expected for short–range potentials as described above. Another important feature of the Efimov effect is its universality. In physics, a property is said to be universal if it does not depend on the specific microscopic details of the interactions and appears in the same way in any system that exhibits the effect. In particular, for the Efimov effect, the number of bound states $N(E)$ below $E < 0$ satisfies

$$\lim_{E \to 0^-} \frac{N(E)}{|\ln(|E|)|} = C_0 \tag{3.1.1}$$

for some constant $C_0 > 0$, which depends solely on the particle masses and not on the interaction potentials. Importantly, the universality of Efimov physics does not mean it happens in every system. It means that any system that meets the conditions for it will show the same universal features. In fact, the restriction to systems with virtual levels is a highly significant limitation on the possible potentials.
After the first description by Efimov, it took several years to find the first rigorous mathematical description of the effect and much longer to confirm the effect experimentally. Yafaev gave the first mathematical proof [59]. The proof of Yafaev is based on so–called Faddeev equations for three-body systems. Later, Sobolev [108] did add to the proof of Yafaev and, in addition, showed the asymptotic behavior in (3.1.1). Utilizing the ideas of the Born–Oppenheimer approximation, Ovchinikov and Sigal [89] gave a fully variational proof of the Efimov effect under some restrictions on the involved particle masses. Later, the proof was improved and generalized to arbitrary particle masses by Tamura [113]. In the proof of Tamura [113], well–believed explicit bounds on the decay properties of zero–energy solutions [113, Proposition 3.1] have been used without explicit proof. Since these bounds are relevant for many applications and in particular concerning the Efimov effect, we discuss and prove these estimates in Sections 3.2 and 3.3 below.
It took until 2006 for the first definitive experimental confirmation of the Efimov effect in an ultracold gas of cesium atoms [67]. See [33] and the references therein for an extensive review of the experimental findings and advancements concerning the Efimov effect. Beyond the case of three particles in dimension three, it is an interesting question whether or not an Efimov-type effect can exist for different numbers of particles or different spatial dimensions. We refer to the introduction Chapter 5 for a review of several of these cases and the dissertation of Andreas Bitter in [23].

In Chapter 5, we discuss the absence of the Efimov effect in a system of geometrically constrained particles. Recent advancements in experiments with ultracold gases and magnetic traps have increased interest in exploring the potential existence of the Efimov effect in systems with mixed dimensions (see [84],[85],[86]). This phenomenon, sometimes called the *Confinement Induced Efimov Effect* [85], has been predicted in various scenarios, as shown in Figure 5.1. We have studied several of these configurations. In some of these cases, the existence of the Efimov effect can be confirmed by extending the ideas in [113]. For this, the explicit bounds on the decay of the zero–energy solution in Theorem 3.2.2 are necessary.
Through a detailed analysis of the properties of *zero–energy resonances* in two-dimensional Schrödinger operators, we have *disproved* the existence of the Confinement Induced Efimov Effect in the system illustrated in Figure 5.2. This result is notable as it is one of the rare cases where predictions in the physics literature do not hold up to a rigorous mathematical analysis. To achieve this result, we applied the criterion of Zhislin [129] for the finiteness of the discrete spectrum (see Lemma 1.3.5) and build on methods and techniques as, for example, in [120],[117] and [13].
The method we developed to disprove the Confinement Induced Efimov Effect has proven to be robust and is also relevant for unconfined three-particle configurations in $d = 4$ dimensions. In dimensions $d \geq 5$, zero–energy solutions for the two-particle subsystems are square-integrable.

Thus, zero is an eigenvalue of the corresponding Hamiltonian, with the absence of the Efimov effect demonstrated in [11]. In dimension $d = 4$, the situation is considerably more complex because the zero–energy solutions for particle pairs interacting with short–range potentials are not square-integrable. Thus, zero is a resonance rather than an eigenvalue of the two-particle operator. Using our study of two-dimensional Schrödinger operators, we prove the absence of the Efimov effect for three particles in dimension $d = 4$ under minimal assumptions on the interaction potentials using a fully variational proof.

3.2 On the Decay of Resonance Functions

For many applications, and in particular, for the description of the Efimov effect, it is useful to have some knowledge of the explicit properties of the decay of resonances and their corresponding zero–energy solutions. Given that the potential is short–range it is expected that such a solution $\varphi_0 \in \dot{H}^1(\mathbb{R}^d)$ has the asymptotics

$$|\varphi_0(x)| \sim |x|^{2-d}, \quad |\nabla\varphi_0(x)| \sim |x|^{1-d}, \quad d \geq 3\,. \tag{3.2.1}$$

This behavior is well-believed, and under additional assumptions besides the short–range property of the potential, it can be proven by elementary steps directly from the Schrödinger equation. It is not trivial how to deduce the decay properties of φ_0 under minimal assumptions on the potential from works such as [59].

Throughout this section we consider the Schrödinger operator $H = P^2/2 + V \geq 0$ on $L^2(\mathbb{R}^d)$ with potential $V : \mathbb{R}^d \to \mathbb{R}$ such that there exists $W \in K_d$ and $\theta > 0$ such that

$$V(x) = (1 + |x|)^{-2-\theta} W(x) \tag{3.2.2}$$

for $x \in \mathbb{R}^d$ and we assume H has a virtual level at zero as defined in Definition 1.4.1 with corresponding zero–energy solution denoted by $\varphi_0 \in \dot{H}^1(\mathbb{R}^d)$.

Remark 3.2.1. *Note that any short–range potential $V \in K_d$ satisfies condition* (1.4.6)*. However, condition* (1.4.6) *also permits potentials that have singularities outside of compact sets.*

To prove the sharp asymptotics of the distributional gradient $\nabla\varphi_0$ we define for $d \geq 2$ the set $K_{d,1} \subset K_d$ as any real–valued potential V such that

$$\lim_{\delta\downarrow 0} \sup_{|x|\in\mathbb{R}^d} \int_{|x-y|\leq\delta} |x-y|^{1-d} |V(y)| dy = 0\,. \tag{3.2.3}$$

For convenience, we write

$$\langle V, \varphi_0 \rangle = \int_{\mathbb{R}^d} V(y)\varphi_0(y) dy\,.$$

The next theorem shows that $V\varphi_0 \in L^1(\mathbb{R}^d)$ under condition (1.4.6), i.e., $\langle V, \varphi_0 \rangle$ is well defined. In Section 3.3 we prove

Theorem 3.2.2 (Precise asymptotic of virtual levels)**.** *Let $d \geq 3$. Under the short–range assumption* (1.4.6) φ_0 *is (globally) bounded. Moreover,* φ_0 *has a continuous version,* $V\varphi_0 \in L^1$*, and* φ_0 *has the asymptotics*

$$\varphi_0(x) = -2c_d \frac{\langle V, \varphi_0 \rangle}{|x|^{d-2}} + E_1(x) \quad \textit{for } x \to \infty\,, \tag{3.2.4}$$

where $c_d = (d-2)^{-1}\left|\mathbb{S}^{d-1}\right|^{-1}$ *and, for any* $0 < \kappa < 1$ *there exists a constant* $C_\kappa < \infty$ *and* $R > 0$ *such that the error is bounded by*

$$|E_1(x)| \leq C_\kappa |x|^{2-d-\kappa\theta} \quad \textit{for } |x| \geq R\,. \tag{3.2.5}$$

Moreover, if the function W *in the definition* (1.4.6) *of the potential* V *is in* $K_{d,1}$*, then the distributional gradient of* φ_0 *has a continuous version and*

$$\nabla\varphi_0(x) = 2(d-2)c_d \langle V, \varphi_0 \rangle x|x|^{-d} + E_2(x), \quad \textit{for } x \to \infty \tag{3.2.6}$$

where for any $0 < \kappa < 1$ *there exists* $c_\kappa > 0$ *and* $R > 0$ *with*

$$|E_2(x)| \leq c_\kappa |x|^{1-d-\kappa\theta} \quad \textit{for } |x| \geq R\,. \tag{3.2.7}$$

We prove Theorem 3.2.2 in Section 3.3 and start the discussion of the results of Theorem 3.2.2 with some remarks.

Remark 3.2.3. *In [113, Proposition 3.1], where the three dimensional case is considered under a global uniform short–range condition*

$$|V(x)| \leq C(1+|x|)^{-2-\theta_0} \quad \textit{for all } x \in \mathbb{R}^d$$

it is claimed that one can use $\kappa = 1$ *in the bounds* (3.2.5)*, respectively* (3.2.7)*, for the errors. However, no proof of this claim is given in [113].*
Our Theorem 3.2.2 requires $\kappa < 1$ *since the constants* c_κ *and* C_κ *diverge in the limit* $\kappa \to 1$*. So up to an epsilon loss in the exponent, the asymptotic for the virtual level* φ_0 *claimed in [113, Proposition 3.1] is correct, even for a much larger class of potentials.*
Fortunately, for the results in [113] concerning the existence of the Efimov effect for three particles in three dimensions, our estimates are sufficient since $0 < \kappa < 1$ *can be chosen arbitrarily close to one. Furthermore, our result requires minimal regularity and decay of the potential* V*.*

Remark 3.2.4. *Since* φ_0 *is bounded, we also have*

$$\varphi_0(x) = -2c_d \frac{\langle V, \varphi_0 \rangle}{1+|x|^{d-2}} + \tilde{E}_1(x) \quad \forall x \in \mathbb{R}^d,$$

where for any $0 < \kappa < 1$ *there exists* $c_\kappa > 0$ *with*

$$\left|\tilde{E}_1(x)\right| \leq c_\kappa (1+|x|)^{2-d-\kappa\theta} \quad \forall x \in \mathbb{R}^d\,.$$

Since $\kappa \in (0,1)$ *we have*

$$\tilde{E}_1 \in L^p(\mathbb{R}^d) \quad \text{if } p > \frac{d}{d+\theta-2}$$

which generalizes and confirms the results in [11] and [23, Theorem 3.3.1]. This also shows directly that $\varphi_0 \in L^p(\mathbb{R}^d)$ *for all* $p > \frac{d}{d-2}$. *Consequently for* $d \geq 5$ *we have* $\varphi_0 \in L^2(\mathbb{R}^d)$. *This confirms the common knowledge that for dimension* $d \geq 5$, *virtual levels are eigenfunctions instead of resonances.*
Similarly if $V(x) = (1+|x|)^{-2-\theta}W(x)$ *with* $W \in K_{d,1}$, *the distributional gradient has a continuous representation, which is therefore locally bounded, so the asymptotics* (3.2.6) *implies that*

$$\nabla\varphi_0(x) = 2(d-2)c_d \frac{x\langle V, \varphi_0\rangle}{1+|x|^d} + \tilde{E}_2(x) \quad \text{for } x \in \mathbb{R}^d,$$

where for any $0 < \kappa < 1$

$$\left|\tilde{E}_2(x)\right| \lesssim (1+|x|)^{1-d-\kappa\theta} \quad \text{for } x \in \mathbb{R}^d\,.$$

Thus $\tilde{E}_2 \in L^p(\mathbb{R}^d)$ *if* $p > \frac{d}{d+\theta-1}$, *and*

$$\nabla\varphi_0 \in L^p(\mathbb{R}^d) \quad \text{for } p > \frac{d}{d-1}\,.$$

Note that $1 < \frac{d}{d-1} < 2$ *for all* $d \geq 3$.

Our proof is based on integral representations of the zero–energy solution φ_0. In the proof of Theorem 3.2.2 we will use the following integral representations of φ_0 and its weak gradient, see also Theorem D.5.2 in Appendix D.

Theorem 3.2.5 (= Theorem D.5.2)**.** *Let* $d \geq 3$ *and assume that* V *satisfies the short–range condition* (1.4.6). *Then the zero–energy solution* φ_0 *has a continuous version, it is bounded with* $V\varphi \in L^1(\mathbb{R}^d)$, *and satisfies the integral equation*

$$\varphi_0(x) = -2c_d \int_{\mathbb{R}^d} |x-y|^{-(d-2)} V(y)\varphi_0(y)dy, \quad \forall x \in \mathbb{R}^d, \tag{3.2.8}$$

with $c_d = (d-2)^{-1}\left|\mathbb{S}^{d-1}\right|^{-1}$, *where* $\left|\mathbb{S}^{d-1}\right| = d\left|B_1^d\right|$ *is the surface area of the unit sphere in* $\mathbb{R}^d$ *and* $\left|B_1^d\right|$ *the volume of the unit ball in* $\mathbb{R}^d$. *If additionally the function* W *in the short–range condition* (1.4.6) *for* V *satisfies* $W \in K_{d,1}$, *then the distributional gradient* $\nabla\varphi_0$ *has a continuous version and satisfies the integral equation*

$$\nabla\varphi_0(x) = 2(d-2)c_d \int_{\mathbb{R}^d} \frac{x-y}{|x-y|^d} V(y)\varphi_0(y)dy \quad \forall x \in \mathbb{R}^d\,. \tag{3.2.9}$$

Remark 3.2.6. *The conclusion that the zero–energy solution* φ_0 *is globally bounded, derived from subsolution estimates as in ([3] and [101]), appears to be new.*

We will give the proof of Theorem 3.2.5 in Appendix D, see Theorem D.5.2. Before we prove Theorem 3.2.2, together with the explicit error bounds, we prove an important a–priori bound on φ_0, which has the correct order of decay.

Proposition 3.2.7 (A–priori decay bound)**.** *Let $d \geq 3$ then there exists a constant $c > 0$ such that*

$$|\varphi_0(x)| \leq c(1+|x|)^{2-d} \quad \textit{for all } x \in \mathbb{R}^d .$$

Proof. Following Theorem 3.2.5 the zero–energy solution φ_0 is bounded and since V is short–range in the sense of (1.4.6) there exists $W \in K_d$ and $\theta > 0$ such that for any $\delta \in (0, \theta]$

$$|V(x)\varphi_0(x)| \leq |W(x)|(1+|x|)^{-2-\delta} \quad \forall x \in \mathbb{R}^d . \tag{3.2.10}$$

Using the integral representation in (3.2.8) we arrive at

$$|\varphi_0(x)| \lesssim \int_{\mathbb{R}^d} |x-y|^{-(d-2)}(1+|y|)^{-2-\delta}|W(y)|dy . \tag{3.2.11}$$

Note that for $|x-y| \leq 1$ we have

$$(1+|y|)^{-(2+\delta)} \lesssim (1+|x|)^{-(2+\delta)} \tag{3.2.12}$$

and for $|x-y| \geq 1$ we have

$$|x-y|^{-(d-2)} \lesssim (1+|x-y|)^{-(d-2)} . \tag{3.2.13}$$

Splitting the domain of integration in the right–hand side of (3.2.11) into the sets $|x-y| \leq 1$ and $|x-y| \geq 1$ and inserting (3.2.12) and (3.2.13) we arrive at

$$\begin{aligned} |\varphi_0(x)| \lesssim & (1+|x|)^{-(2+\delta)} \int\limits_{|x-y|\leq 1} |x-y|^{-(d-2)}|W(y)|dy \\ & + \int\limits_{|x-y|\geq 1} (1+|x-y|)^{-(d-2)}(1+|y|)^{-(2+\delta)}|W(y)|dy . \end{aligned} \tag{3.2.14}$$

Let

$$h_{\alpha,\beta}(x) := \int_{\mathbb{R}^d} (1+|x-y|)^{-\beta}(1+|y|)^{-\alpha}W(y)dy \tag{3.2.15}$$

with $\alpha = 2+\delta$ and $\beta = d-2$. Since $W \in K_d$ we conclude from (3.2.14) we find

$$|\varphi_0(x)| \lesssim (1+|x|)^{-\alpha} + h_{\alpha,\beta}(x) .$$

In the Appendix D we have shown as Lemma D.6.1 that if $\alpha < d$, $\beta < d$ and $\alpha + \beta > d$, then

$$h_{\alpha,\beta}(x) \lesssim (1+|x|)^{d-(\alpha+\beta)} = (1+|x|)^{-\delta}$$

and consequently

$$|\varphi_0(x)| \le (1+|x|)^{-\delta}\,.$$

With this estimate, we can repeat the argument by replacing (3.2.10) with

$$|V(x)\varphi_0(x)| \le |W(x)|(1+|x|)^{-2-2\delta} \quad \forall x \in \mathbb{R}^d$$

to find

$$|\varphi_0(x)| \lesssim (1+|x|)^{-\alpha_2} + h_{\alpha_2,\beta}(x)$$

with $\alpha_2 = 2+2\delta$ and $\beta = d-2$. If $2+2\delta < d$ this proves

$$|\varphi_0(x)| \lesssim (1+|x|)^{-2\delta}\,.$$

Define $\alpha_n \coloneqq 2+n\delta$ for all $n \in \mathbb{N}$. Let $n_0 \in \mathbb{N}$ satisfy

$$\alpha_{n_0} = 2+n_0\delta < d \quad \text{and} \quad \alpha_{n_0+1} = 2+(n_0+1)\delta > d\,.$$

Note that such an $n_0 \in \mathbb{N}$ may not exist for every $\delta \in (0,\theta]$, but it is always possible to shrink $\delta \in (0,\theta]$ to ensure the existence of such an $n_0 \in \mathbb{N}$. Iterating the initial argument n_0-times, we arrive at

$$|\varphi_0(x)| \lesssim (1+|x|)^{-\alpha_{n_0}} + h_{\alpha_{n_0},\beta}(x) \lesssim (1+|x|)^{-n_0\delta}\,.$$

We can apply the same argument one more time, then

$$|\varphi_0(x)| \lesssim (1+|x|)^{-\alpha_{n_0+1}} + h_{\alpha_{n_0+1},\beta}(x)\,.$$

Since $\alpha_{n_0+1} > d > \beta$ it follows from Lemma D.6.1 that

$$h_{\alpha_{n_0+1},\beta}(x) \lesssim (1+|x|)^{\beta} = (1+|x|)^{2-d}\,.$$

Since $\beta < \alpha_{n_0+1}$ this proves

$$|\varphi_0(x)| \lesssim (1+|x|)^{d-2}\,.$$

∎

3.3 Proof of the Decay Properties of Resonance Functions

Using the a priori estimates from Proposition 3.2.7 and the integral representation of zero–energy solutions from Theorem 3.2.5, we can now prove Theorem 3.2.2, which establishes the sharp asymptotic behavior of the resonance function for critical Schrödinger operators and provides estimates for the lower-order terms. We give this proof now.

Proof of Theorem 3.2.2. We will use the integral representations from Theorem 3.2.5 together with the a–priori bound from Proposition 3.2.7 for the proof of the error bounds in Theorem 3.2.2. We begin with E_1. Note that due to the a–priori bound on φ_0 from Proposition 3.2.7

and the decay assumption on the potential V we have

$$|V(y)\varphi_0(y)| \lesssim (1+|y|)^{-(d+\theta)}|W(y)|\,, \tag{3.3.1}$$

for some $\theta > 0$ and $W \in K_d \subset L^1_{\mathrm{loc,unif}}(\mathbb{R}^d)$. Hence the bound (D.4.5) from Lemma D.4.1 shows that $V\varphi_0 \in L^1(\mathbb{R}^d)$. Thus, we can rewrite the integral representation from Theorem 3.2.5 as follows,

$$\begin{aligned}\varphi_0(x) &= -2c_d \int_{\mathbb{R}^d} |x-y|^{-(d-2)} V(y)\varphi_0(y)dy \\ &= -2c_d \int_{\mathbb{R}^d} \left(|x-y|^{-(d-2)} - |x|^{-(d-2)}\right) V(y)\varphi_0(y)dy \\ &\quad - 2c_d |x|^{-(d-2)} \underbrace{\int_{\mathbb{R}^d} V(y)\varphi_0(y)dy}_{=\langle V,\varphi_0\rangle}\,.\end{aligned} \tag{3.3.2}$$

Fix $L(x) > 0$ and split the domain of integration of the first integral in the second line of (3.3.2) of into the sets $A(x) := \{y \in \mathbb{R}^d : |y| > L(x)\}$ and $B(x) := \{y \in \mathbb{R}^d : |y| \le L(x)\}$ to find

$$\begin{aligned}\varphi_0(x) = -2c_d|x|^{-(d-2)}\langle V,\varphi_0\rangle &+ 2c_d|x|^{-(d-2)} \int_{A(x)} V(y)\varphi_0(y)dy \\ &- 2c_d \int_{B(x)} \left(|x-y|^{-(d-2)} - |x|^{-(d-2)}\right) V(y)\varphi_0(y)dy \\ &- 2c_d \int_{A(x)} |x-y|^{-(d-2)} V(y)\varphi_0(y)dy\,.\end{aligned} \tag{3.3.3}$$

We define

$$\begin{aligned} g_1(x) &:= -2c_d \int_{A(x)} V(y)\varphi_0(y)dy, \\ g_2(x) &:= -2c_d \int_{B(x)} \left(|x-y|^{-(d-2)} - |x|^{-(d-2)}\right) V(y)\varphi_0(y)dy, \\ g_3(x) &:= -2c_d \int_{A(x)} |x-y|^{-(d-2)} V(y)\varphi_0(y)dy\,. \end{aligned} \tag{3.3.4}$$

Comparing (3.3.3) with (3.2.4) we find

$$E_1(x) = |x|^{-(d-2)} g_1(x) + g_2(x) + g_3(x), \quad \forall x \in \mathbb{R}^d\,. \tag{3.3.5}$$

Using again (3.3.1) in (3.3.4) we arrive at

$$\begin{aligned}
|g_1(x)| &\lesssim \int_{A(x)} (1+|y|)^{-(d+\theta)}|W(y)|dy,\\
|g_2(x)| &\lesssim \int_{B(x)} \Big||x-y|^{-(d-2)} - |x|^{-(d-2)}\Big|(1+|y|)^{-(d+\theta)}|W(y)|dy,\\
|g_3(x)| &\lesssim \int_{A(x)} |x-y|^{-(d-2)}(1+|y|)^{-(d+\theta)}|W(y)|)dy\,.
\end{aligned}$$

where $\lesssim$ means that the inequality holds up to a constant $c > 0$ independent of $x \in \mathbb{R}^d$. In Lemma D.6.3 from Appendix D we prove the following estimates under the assumption $L(x) < |x|/2$ for $|x| > 1$ large enough,

$$\begin{aligned}
g_1(x) &\lesssim (1+L(x))^{-\theta},\\
g_2(x) &\lesssim (1+L(x))^{1-\theta}(|x|-L(x))^{1-d},\\
g_3(x) &\lesssim (1+L(x))^{1-\theta}(1+|x|)^{1-d}\,.
\end{aligned}$$

Let $\kappa \in (0,1)$ and choose $L(x) = |x|^\kappa$ then for any $|x| > 1$ large enough

$$\begin{aligned}
|x|^{-(d-2)}g_1(x) &\lesssim |x|^{-(d-2)-\theta\kappa},\\
g_2(x) &\lesssim |x|^{1-d+\kappa(1-\theta)},\\
g_3(x) &\lesssim |x|^{1-d+\kappa(1-\theta)}\,.
\end{aligned} \tag{3.3.6}$$

Note that

$$-(d-2) - \theta\kappa > 1 - d + \kappa(1-\theta)\,,$$

consequently (3.3.5) and (3.3.6) yields

$$|E_1(x)| \lesssim |x|^{-(d-2)-\kappa\theta}$$

for any $\kappa \in (0,1)$ and $|x| > 1$ large enough.
The proof of the estimates on the lower order terms of $\nabla\varphi_0$ are similar, and we give them now. Using a again Theorem 3.2.5 and $V\varphi_0 \in L^1$ we rewrite

$$\begin{aligned}
\nabla\varphi_0(x) &= 2(d-2)c_d \int_{\mathbb{R}^d} \frac{x-y}{|x-y|^d} V(y)\varphi_0(y)dy\\
&= 2(d-2)c_d \int_{\mathbb{R}^d} \frac{x-y}{|x-y|^d} - \frac{x}{|x|^d} V(y)\varphi_0(y)dy + 2(d-2)c_p \frac{x}{|x|^d}\int_{\mathbb{R}^d} V(y)\varphi_0(y)dy\,.
\end{aligned}$$

As in the previous case, we split the domain of integration into the sets

$$A(x) = \{y \in \mathbb{R}^d : |y| > L(x)\} \quad \text{and} \quad B(x) = \{y \in \mathbb{R}^d : |y| \le L(x)\}\,.$$

Then

$$\begin{aligned}\nabla\varphi_0(x) = \; & 2(d-2)c_d\frac{x}{|x|^d}\langle V,\varphi_0\rangle \\ & - 2(d-2)c_d\frac{x}{|x|^d}\int_{A(x)} V(y)\varphi_0(y)dy \\ & + 2(d-2)c_d\int_{B(x)}\left(\frac{x-y}{|x-y|^d}-\frac{x}{|x|^d}\right)V(y)\varphi_0(y)dy \\ & + 2(d-2)c_d\int_{A(x)}\frac{x-y}{|x-y|^d}V(y)\varphi_0(y)dy\,.\end{aligned} \tag{3.3.7}$$

Comparing (3.3.7) with (3.2.6) we find

$$|E_2(x)| \lesssim |x|^{-(d-1)}|g_1(x)| + |f_2(x)| + |f_3(x)|, \quad \forall x\in\mathbb{R}^d, \tag{3.3.8}$$

where

$$\begin{aligned} f_2(x) &\coloneqq \int_{B(x)}\left(\frac{x-y}{|x-y|^d}-\frac{x}{|x|^d}\right)V(y)\varphi_0(y)dy, \\ f_3(x) &\coloneqq \int_{A(x)}\frac{x-y}{|x-y|^d}V(y)\varphi_0(y)dy\,.\end{aligned}$$

As in the previous case, we can use the bound (3.3.1) and Lemma D.6.3 to see that

$$\begin{aligned}|f_3(x)| &\lesssim \int_{A(x)}|x-y|^{-(d-1)}(1+|y|)^{-(d+\theta)}|W(y)|)dy \\ &\leq (1+L(x))^{-\theta}\,(1+|x|)^{-(d-1)}\;.\end{aligned} \tag{3.3.9}$$

In Lemma D.6.3 we also show that

$$\begin{aligned}|f_2(x)| &\lesssim \int_{B(x)}\left|\frac{x-y}{|x-y|^d}-\frac{x}{|x|^d}\right|(1+|y|)^{-(d+\theta)}|W(y)|dy \\ &\lesssim (1+L(x))^{1-\theta}|x|(|x|-L(x))^{-(d+1)}\end{aligned} \tag{3.3.10}$$

and

$$|x|^{-(d-1)}|g_1(x)| \lesssim |x|^{-(d-1)}(1+L(x))^{-\theta}\,. \tag{3.3.11}$$

Combining (3.3.11), (3.3.10) and (3.3.9) with (3.3.8) we arrive at

$$|E_2(x)| \lesssim (1+L(x))^{-\theta}\left(|x|^{-(d-1)} + (1+L(x))|x|(|x|-L(x))^{-(d+1)} + (1+|x|)^{-(d-1)}\right)$$

for $|x|>1$ large enough. Choose $L(x)=|x|^\kappa$ for $\kappa\in(0,1)$ then for $|x|>1$ large enough

$$|E_2(x)| \lesssim |x|^{-\kappa\theta}\left(|x|^{-(d-1)} + |x|^{\kappa-d} + |x|^{-(d-1)}\right) \lesssim |x|^{-(d-1)-\kappa\theta}$$

which completes the proof of Theorem 3.2.2. ∎

Chapter 4

On the Excess Charge Problem of Atoms

4.1 Introduction

It is widely accepted that a single atom in a vacuum can bind at most one or two additional electrons. From a heuristic perspective, this is evident: atoms are electrically neutral, and while an additional electron may coexist with the atom, adding more electrons becomes challenging due to Coulomb repulsion caused by the net-negative charge of the resulting configuration. Deriving this behavior from the many–body Schrödinger equation remains a challenging open question for many decades.

An atom of nuclear charge Z should be able to bind at least $N < Z + 1$ electrons since the farthest out electron will experience a net Coulomb attraction to the nucleus. The remaining $N - 1$ electrons cannot fully screen the charge of the nucleus when $N - 1 < Z$. This was made rigorous in the early work of Zhislin [128], so $\liminf_{Z\to\infty} \frac{N_c(Z)}{Z} \geq 1$ was known for a long time, already. That there is a critical number $N_c(Z) < \infty$ that an atom of charge Z can bind was first shown independently by Ruskai [95] and Sigal [99]. Later, Lieb, Sigal, Simon, and Thirring [77] proved

$$\lim_{Z\to\infty} \frac{N_c(Z)}{Z} = 1 .$$

In fact, they proved the result with lim replaced by lim sup. The result by Lieb, Sigal, Simon, and Thirring uses a compactness argument and does not provide any quantitative bounds on how big $N_c(Z)$ is for finite nuclear charge Z. Fefferman and Seco [32] and Seco, Sigal and Solovej [97] proved in 1990

$$N_c(Z) \leq Z + O(Z^{5/7}) \quad \text{as } Z \to \infty .$$

Non–asymptotic bounds are rare. For a long time, the only non-asymptotic bound was due to Lieb [71], who proved his famous bound

$$N_c(Z) < 2Z + 1 \quad \text{for all } Z \geq 1 .$$

Lieb's result is independent of the statistic of the particles, i.e., independent of whether they are fermions of bosons, and it also holds, suitably modified, for systems of atoms, i.e., molecules.

While Lieb's bound certainly overcounts $N_c(Z)$, it shows that Hydrogen ($Z = 1$) can bind only two electrons, which is observed in nature.
It took 28 years until Nam's breakthrough result [81] could significantly improve Lieb's longstanding bound. Nam showed, for a single atom with fermionic statistics, that

$$N_c(Z) < 1.22Z + 3Z^{1/3} \quad \text{for all } Z \geq 1 \,.$$

In this work, we provide even tighter bounds on N_c. In particular, we prove

$$N_c(Z) \leq 1.12Z + 4Z^{1/3} \quad \text{for all } Z \geq 4 \,.$$

We would like to stress that this shows that for large nuclear charges Z, fermionic atoms do indeed behave much differently from bosonic atoms. Bosonic atoms are known to allow for a surcharge of 21 %, i.e., large bosonic atoms can bind roughly $N \sim 1.21Z$ bosonic particles for large Z. The leading order coefficient in Nam's bound is just above 1.21, whereas in our bound, it is lower, with a good safety margin.
To achieve our improvements, we significantly extend Nam's approach and, in addition, prove some of the conjectures made in [81].

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4.2 Basic Notation and Main Result

We consider a nucleus of charge Z placed at the origin and N particles located at positions $x_1, \ldots x_N \in \mathbb{R}^3$. In the limit of infinite nuclear mass and after appropriate rescaling (see Section 1.1), the Schrödinger operator of a single atom is given by

$$H_{N,Z} \coloneqq \frac{1}{2}\sum_{k=1}^{N} P_k^2 - \sum_{i=1}^{N} \frac{Z\alpha}{|x_i|} + \sum_{1\leq i<j\leq N} \frac{\alpha}{|x_i - x_j|} \,. \tag{4.2.1}$$

Here $\alpha = e^2/(\hbar c)$ is the fine structure constant, and $P_j = -i\hbar\nabla_j$ denotes the usual three-dimensional momentum operator with respect to the variable x_j.

Remark 4.2.1. *We choose atomic units, that is $\hbar = m_e = c = e = 1$ and consequently $\alpha = 1$. Another usual choice of units is setting the electron mass $m_e = 1/2$ as, for example, in [72], such that the factor in the kinetic energy vanishes. The question on the maximal excess charge is independent of the choice of these units.*

Following Section 1.5 the Hilbert space of N particles of spin $S \in \mathbb{N}_0/2$ is the N–fold tensor product

$$\mathcal{H}_N := \bigotimes_{i=1}^{N} L^2(\mathbb{R}^3; \mathbb{C}^{2S+1}) . \tag{4.2.2}$$

Let $z_1, \dots z_N$ be the combined position–spin coordinate of a single particle, $z_j = (x_j, s_j)$. Considering identical particles we only consider stats $\psi \in \mathcal{H}_N$ such that

$$\left|\psi(\dots z_i, \dots, z_j, \dots)\right|^2 = \left|\psi(\dots z_j, \dots, z_i, \dots)\right|^2. \tag{4.2.3}$$

We distinguish between fermions and bosons. For fermions, the state space is the subspace of totally antisymmetric functions $\mathcal{H}_N^f$. We call $\psi \in \mathcal{H}_N$ totally antisymmetric if

$$\psi(\dots z_i, \dots, z_j, \dots) = -\psi(\dots z_j, \dots, z_i, \dots) \quad \text{for all } i \neq j \in \{1, \dots, N\} .$$

For bosons, we consider the subspace of totally symmetric functions denoted by $\mathcal{H}_N^b$. We call $\psi \in \mathcal{H}_N$ totally symmetric if

$$\psi(\dots z_i, \dots, z_j, \dots) = \psi(\dots z_j, \dots, z_i, \dots) \quad \text{for all } i \neq j \in \{1, \dots, N\} .$$

Regarding real atoms, the particles of interest are electrons. Thus, the fermionic case with spin $S = 1/2$ is the natural one. Thus we discuss $H_{N,Z}$ on $\mathcal{H}_N^f$ first and discuss the case of bosons later. The bottom of the spectrum of $H_{N,Z}$ is called ground state energy

$$E_{N,Z} := \inf \sigma(H_{N,Z}) . \tag{4.2.4}$$

At first, $E_{N,Z}$ does not need to be an eigenvalue of $H_{N,Z}$. The HVZ theorem (see Theorem 1.5.3) shows that the essential spectrum of $H_{N,Z}$ is given by $\sigma_{\text{ess}}\left(H_{N,Z}\right) = [E_{N-1,Z}, \infty)$. Thus the *binding condition*

$$E_{N,Z} < E_{N-1,Z} \tag{4.2.5}$$

ensures that there is some discrete spectrum below the essential spectrum. Hence, the atom can bind N electrons. In particular, (4.2.5) ensures that $E_{N,Z}$ is an eigenvalue of $H_{N,Z}$, i.e., there exists a function $\psi_{N,Z}$ such that

$$H_{N,Z}\psi_{N,Z} = E_{N,Z}\psi_{N,Z} . \tag{4.2.6}$$

Thus, it is natural to call

$$N_c(Z) := \max\{N \in \mathbb{N} : E_{N,Z} < E_{N-1,Z}\}$$

the critical number of particles that an atom of charge Z can bind.
In this paper, we derive new bounds on $N_c(Z)$. The strategy of our proof is inspired by [72] and, in particular, [81]. One assumes (4.2.6) with $E_{N,Z} < E_{N-1,Z}$ for fixed nuclear charge $Z > 0$ (not necessarily an integer) which will then lead to a contradiction if N is too large. We sketch the original Bunguria–Lieb argument together with Nam's improvement in Section 4.3.

Our main result is

Theorem 4.2.2. *Let $s \in (1,3]$ then there exists $c(s) > 0$ such that*

$$N_c(Z) < b(s)\,Z + c(s)Z^{1/3},$$

where

$$b(s) := \frac{s-1}{st_0} \tag{4.2.7}$$

with t_0 the unique solution of $t^s + st + 1 - s = 0$ in $(0,1)$.

Remark 4.2.3. *We conjecture that Theorem 4.2.2 holds for any $s \geq 1$ with the same $b(s)$ and some $c(s) < \infty$ with $c(s) \to \infty$ as $s \to \infty$.*

We prove Theorem 4.2.2 in Section 4.7. Finding good bounds on $c(s)$ is technical. We study the cases $s = 2$ and $s = 3$ in greater detail. In particular, for $s = 2$ we show

Proposition 4.2.4. *For any $Z \geq 2$*

$$N_c(Z) < \frac{1}{2}(\sqrt{2}+1)\,Z + 2.96Z^{1/3}\,. \tag{4.2.8}$$

where $1.2071 < \frac{1}{2}(\sqrt{2}+1) < 1.2072$.

For $s = 3$ we show

Proposition 4.2.5. *For any $Z \geq 4$*

$$N \leq b(3)Z + 3.90Z^{1/3} + 0.0134 + 0.184Z^{-1/3} + 0.0196Z^{-2/3}, \tag{4.2.9}$$

with

$$1.1184 < b(3) = \frac{2}{3}\frac{\sqrt[3]{1+\sqrt{2}}}{(1+\sqrt{2})^{2/3} - 1} < 1.1185\,.$$

Remark 4.2.6. *Proposition 4.2.4 is better than the estimate of $N_c(Z) < 2Z + 1$ in [71] for $Z > 5.3$. Since the constant $(\sqrt{2}+1)/2$ is slightly better than the one in [81] it improves the result of [81] for all $Z \geq 2$. For $Z \geq 35.8$ the bound in (4.2.9) is better than (4.2.8). In particular Proposition 4.2.4 proves*

$$N \leq 1.12Z + 4Z^{1/3}, \quad Z \geq 4\,.$$

We prove the Propositions 4.2.4 and 4.2.5 in Section 4.7.
Proposition 4.2.5 significantly improves upon the results of [81] for large Z. More importantly, while it falls short of proving the asymptotic neutrality of fermionic atoms, it provides the first quantitative result showing that, for atoms, the distinction between fermions and bosons is crucial. In [17], Benguria and Lieb showed that in contrary to fermions for bosonic atoms

$$\lim_{Z\to\infty} \frac{N_c(Z)}{Z} = t_c > 1\,.$$

Numerically one finds $t_c \approx 1.21$ (see [15]). Thus, large bosonic atoms can have an excess charge of 21 %. On the other hand, as proven in [77], fermionic atoms are asymptotically neutral. Our bound (4.2.9) shows that fermionic atoms are very much different from bosonic atoms not only in the limit of infinite nuclear charge Z but also, quantitatively, for a large but finite nuclear charge. The constant $\frac{1}{2}(\sqrt{2}+1) < 1.2072$ in our bound (4.2.8) is just a bit smaller than $t_c \approx 1.21$, and thus, this conclusion is not allowed if one also allows for possible numerical uncertainties in the calculation of the precise value of t_c. However, the constant $b(3) < 1.1185$ in the leading order term of (4.2.9) is certainly much smaller than t_c, including possible numerical errors.
Thus our results, in particular Proposition 4.2.5, show that fermionic atoms are quantitatively quite different from bosonic atoms, not only in the limit of large nuclear charges but already for medium values of Z.
For bosonic atoms, i.e., considering totally symmetric functions as explained above, we have

Theorem 4.2.7. *The critical number of bosonic particles that an atom can bind is at most*

$$N_c(Z) < \frac{t_c}{x_0^2} Z + \theta_1 Z^{1/2} + \theta_2 Z^{1/3} + \theta_3 Z^{-4/3}$$

where $x_0 > 0$ *is the unique positive solution of*

$$0.782\, t_c = (1 + 0.1463 x_0)\, x_0^2$$

and

$$\theta_1 \leq 6.52, \quad \theta_2 \leq 0.361, \quad \theta_3 \leq 0.378\,.$$

We prove Theorem 4.2.7 in Section 4.8.6.

Remark 4.2.8. *With* $t_c \approx 1.21$ *one finds* $t_c x_0^{-2} \approx 1.45$. *Using the analytic bound* $t_c \leq 1.47$ *in Lemma A.7.1 one can prove*

$$N_c(Z) < 1.47 Z + O(Z^{1/2}) \tag{4.2.10}$$

with minimal changes in our proof.

4.3 The Benguria–Lieb–Nam Argument: Playing With Weights

Based on an idea by Benguria, Lieb showed $N_c < 2Z + 1$ for any $Z \geq 1$ in [71]. One starts by taking the scalar product of the solution of the Schrödinger equation

$$H_{N,Z}\psi_{N,Z} = E_{N,Z}\psi_{N,Z} \tag{4.3.1}$$

with $|x_k|\psi_{N,Z}$ where x_k is the position of the k^{th} electron. Using an idea from Benguria allows us to control the terms involving electron-electron repulsion, which, together with the crucial positivity of the weighted kinetic energy term $\mathrm{Re}\langle |x_k|\psi, P^2\psi\rangle$, leads to the bound $N < 2Z + 1$

under the binding condition (4.2.5). This led to the first non–asymptotic quantitative bound for the number of particles an atom can bind for arbitrary $Z > 0$ We sketch more of the main ideas shortly.
In [81], Nam used a similar approach but changed the weight from $|x_k|$ to $|x_k|^2$. This change in weight complicated the analysis considerably. Mainly because $\mathrm{Re}\langle |x_k|\psi, P^2\psi\rangle$ is no longer positive anymore. With Nam's choice of weight, the analysis of the terms, including the electron–electron repulsion, gets considerably more involved. Nevertheless, Nam was able to prove $N_c(Z) < 1.22Z + 3Z^{1/3}$ with the help of his new choice of weight, a breakthrough compared to the bound of Benguria–Lieb.
We refer to [82] for a recent and comprehensive review, which includes a discussion of what we would call the *Benguria-Lieb-Nam Argument*. In this work, we follow the same argument but modify the power in the ansatz to a general power $|x|^s$ with $s \in (1, 3]$. The case $s = 1$ is the case treated by Lieb in [71]. The strategy is the following. Assume (4.3.1). Let $k \in \{1, 2, \dots, N\}$ and multiply the Schrödinger equation from the left by $|x_k|^s\overline{\psi_{N,Z}}$ then, in the quadratic form sense,

$$0 = \langle |x_k|^s\psi_{N,Z}, (H_{N,Z} - E_{N,Z})\psi_{N,Z}\rangle = \mathrm{Re}\langle |x_k|^s\psi_{N,Z}, (H_{N,Z} - E_{N,Z})\psi_{N,Z}\rangle\,. \qquad (4.3.2)$$

Note that $\psi_{N,Z}$ is a many–particle function, and the inner product above is the inner product of $\mathcal{H}_N$ defined in equation (4.2.2). For an introductory explanation, see [76, Chapter 3]. We ignore the spin for now since it is irrelevant to the argument.
We want to single out the k^{th} particle. Let $N(k) := \{1, 2, 3, \dots N\} \setminus \{k\}$. Then the atomic operator $H_{N,Z}$ for N particles, defined (4.2.1), can be written as

$$H_{N,Z} = \frac{1}{2}P_k^2 - \frac{Z}{|x_k|} + \sum_{i\in N(k)} \frac{1}{|x_i - x_k|} + H^{(k)}_{N-1,Z}\,. \qquad (4.3.3)$$

with

$$H^{(k)}_{N-1,Z} = \sum_{\substack{i=1\\ i\neq k}}^{N} \left(\frac{1}{2}P_i^2 - \frac{Z}{|x_i|}\right) + \sum_{\substack{i,j\in N(k)\\ i<j}} \frac{1}{|x_i - x_j|}\,.$$

the operator of an $N - 1$ particle system where the k^{th} particle is removed. Combining (4.3.2) and (4.3.3) we find

$$\begin{aligned} 0 = \mathrm{Re}&\left\langle |x_k|^s\psi_{N,Z}, \left[\frac{1}{2}P_k^2 - \frac{Z}{|x_k|} + \sum_{i\in N(k)} \frac{1}{|x_i - x_k|}\right]\psi_{N,Z}\right\rangle \\ &+ \mathrm{Re}\langle |x_k|^s\psi_{N,Z}, (H^{(k)}_{N-1,Z} - E_{N,Z})\psi_{N,Z}\rangle\,. \end{aligned} \qquad (4.3.4)$$

From (4.2.5) we have $H^{(k)}_{N-1,Z} \geq E_{N-1}$. Since $H^{(k)}_{N-1,Z}$ commutes with $|x_k|^s$ and for fixed x_k the function $|x_k|^s\psi$ has the same symmetry as ψ in the other $N-1$ variables, we have

$$\begin{aligned}&\operatorname{Re}\langle |x_k|^s\psi_{N,Z}, (H^{(k)}_{N-1,Z} - E_{N,Z})\psi_{N,Z}\rangle \\ &\quad = \langle |x_k|^{s/2}\psi_{N,Z}, (H^{(k)}_{N-1,Z} - E_{N,Z})|x_k|^{s/2}\psi_{N,Z}\rangle \geq 0\,.\end{aligned} \tag{4.3.5}$$

Combining (4.3.4) and (4.3.5) we arrive at

$$\begin{aligned}0 \geq\ & \frac{1}{2}\operatorname{Re}\left\langle |x_k|^s\psi_{N,Z}, P_k^2\psi_{N,Z}\right\rangle - Z\left\langle \psi_{N,Z}, |x_k|^{s-1}\psi_{N,Z}\right\rangle \\ &+ \sum_{i\in N(k)}\left\langle \psi_{N,Z}, \frac{|x_k|^s}{|x_i - x_k|}\psi_{N,Z}\right\rangle\,.\end{aligned} \tag{4.3.6}$$

Of course, $\left\langle |x_k|^s\psi_{N,Z}, P_k^2\psi_{N,Z}\right\rangle = \left\langle \nabla_k(|x_k|^s\psi_{N,Z}), \nabla_k\psi_{N,Z}\right\rangle$ in the quadratic form sense, where ∇_k is the gradient with respect to the position of the k^{th} particle.
Due to the symmetry of the ground state, see (4.2.3), the first two terms of (4.3.6) do not depend on k. Consequently, by summing over $k \in \{1, 2, \dots, N\}$ we arrive at

$$\begin{aligned}0 \geq\ & \frac{1}{2}\operatorname{Re}\left\langle \nabla_1(|x_1|^s\psi_{N,Z}), \nabla_1\psi_{N,Z}\right\rangle - Z\left\langle |x_1|^{s-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle \\ &+ \frac{1}{N}\sum_{k=1}^N\sum_{j\in N(k)}\left\langle \psi_{N,Z}, \frac{|x_k|^s}{|x_j - x_k|}\psi_{N,Z}\right\rangle\,.\end{aligned} \tag{4.3.7}$$

Symmetrizing the double sum above yields

$$\begin{aligned}\frac{1}{N}\sum_{k=1}^N\sum_{i\in N(k)}\left\langle \psi_{N,Z}, \frac{|x_k|^s}{|x_i - x_k|}\psi_{N,Z}\right\rangle &= \frac{1}{2N}\sum_{k=1}^N\sum_{j\in N(k)}\left\langle \psi_{N,Z}, \frac{|x_j|^s + |x_k|^s}{|x_j - x_k|}\psi_{N,Z}\right\rangle \\ &= \frac{1}{N}\sum_{\substack{j,k=1\\ j<k}}^N\left\langle \psi_{N,Z}, \frac{|x_j|^s + |x_k|^s}{|x_j - x_k|}\psi_{N,Z}\right\rangle\,.\end{aligned} \tag{4.3.8}$$

For $N \in \mathbb{N}$ with $N \geq 2$ we define

$$\alpha_{N,s} := \inf\left\{\frac{\sum_{1\leq j<k\leq N}\frac{|x_j|^s + |x_k|^s}{|x_j - x_k|}}{(N-1)\sum_{k=1}^N |x_k|^{s-1}} : x_k \in \mathbb{R}^3 \text{ for } k = 1, \dots, N\right\} \tag{4.3.9}$$

which for $s = 2$ was introduced by Nam in [81, Equation (1)]. Combining (4.3.7) and (4.3.8) and using the definition of $\alpha_{N,s}$ yields

$$\alpha_{N,s}(N-1) < Z - \frac{1}{2}\frac{\operatorname{Re}\left\langle \nabla_1(|x_1|^s\psi_{N,Z}), \nabla_1\psi_{N,Z}\right\rangle}{\left\langle |x_1|^{s-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle}\,. \tag{4.3.10}$$

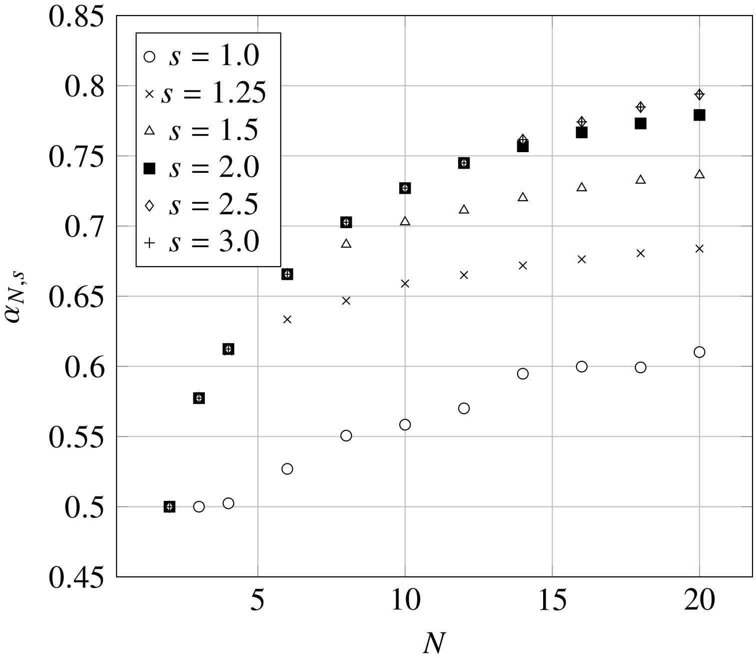

FIGURE 4.1: Numerical approximation of the values of $\alpha_{N,s}$ for various s and N. Starting from an initial sample set of vectors, the values of $\alpha_{N,s}$ have been obtained using a Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm implemented in Python. For $s = 2.5$ and $s = 3.0$, the values of $\alpha_{N,s}$ seem to be almost identical for $N \leq 20$. In the plot $\alpha_{16,1} > \alpha_{18,1}$ which is contrary to Lemma 4.3.2 and due to the fact that numerical approximation is difficult for small $s \geq 1$.

Remark 4.3.1. *Note that this inequality is central to the analysis. The problem is now reduced to find good estimates for $\alpha_{N,s}$ and the fraction on the right–hand side of* (4.3.10).

When $s = 1$ we have $\alpha_{N,s} \geq 1/2$ since $|x| + |y| \geq |x - y|$ by the triangle inequality. Also, for $s = 1$ we have $\operatorname{Re}\left\langle \nabla_1(|x_1|^s \psi_{N,Z}), \nabla_1 \psi_{N,Z} \right\rangle > 0$, using the IMS localization formula and Hardy's inequality. Thus, one directly recovers Lieb's result in the case of a single atom.
It is not hard to see that for all $s \geq 1$, one has $\alpha_{2,s} = 1/2$ as well. Besides these two cases, finding good lower bounds for $\alpha_{N,s}$ is nontrivial. In [81], Nam showed a way how to derive bounds for $\alpha_{N,2}$. He also showed that $\alpha_{N,2}$ is monotone increasing in N. This also holds for general $s \geq 1$.

Lemma 4.3.2. *$\alpha_{N,s}$ is increasing in $N \in \mathbb{N}$ for all $s \geq 1$.*

Proof. In fact, Nam's original proof carries over with minor changes in notation. For the convenience of the reader, we give the short argument. Singling out the particle m, we have

$$\sum_{1 \leq j < k \leq N} \frac{|x_j|^s + |x_k|^s}{|x_j - x_k|} = \sum_{m=1}^{N} \left(\frac{1}{N-2} \sum_{\substack{1 \leq j < k \leq N \\ j \neq m, k \neq m}} \frac{|x_j|^s + |x_k|^s}{|x_j - x_k|} \right)$$

$$\geq \sum_{m=1}^{N} \left(\alpha_{N-1,s} \sum_{\substack{k=1 \\ k \neq m}}^{N} |x_k|^s \right) = \alpha_{N-1,s}(N-1) \sum_{k=1}^{N} |x_k|^s$$

using the definition of $\alpha_{N-1,s}$. This shows that $\alpha_{N,s} \leq \alpha_{N+1,s}$ for all $N \in \mathbb{N}$. ∎

Lemma 4.3.2 shows that $\alpha_{N,s}$ is increasing in N, so once it is bounded, it has a limit. Similar as in [81] we will use a mean-field type approximation for $\alpha_{N,s}$ given by

$$\beta_s := \inf \left\{ \frac{\iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|x|^s + |y|^s}{2|x-y|} d\mu(x) d\mu(y)}{\int_{\mathbb{R}^3} |x|^{s-1} d\mu(x)} : \mu \in P\left(\mathbb{R}^3\right) \right\}. \tag{4.3.11}$$

where $P(\mathbb{R}^3)$ is the set of probability measures on $\mathbb{R}^3$. In fact, for technical reasons, we will additionally assume further regularity of the probability measures μ in the definition of β_s, see (4.4.1) below.

Lemma 4.3.3. *For all $N \in \mathbb{N}$ and $s \geq 1$ we have $\alpha_{N,s} \leq \beta_s$.*

Proof. Again, the proof follows the argument in [81]. By symmetry,

$$\iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|x|^s + |y|^s}{2|x-y|} d\mu(x) d\mu(y) = \frac{1}{N} \int_{\mathbb{R}^{3N}} \frac{1}{N-1} \sum_{1 \leq j < k \leq N} \frac{|x_j|^s + |x_k|^s}{2|x_j - x_k|} d\mu(x_1) \ldots d\mu(x_N)$$

$$\geq \frac{\alpha_{N,s}}{N} \int_{\mathbb{R}^{3N}} \sum_{k=1}^{N} |x_k|^{s-1} d\mu(x_1) \ldots d\mu(x_N) = \alpha_{N,s} \int_{\mathbb{R}^3} |x|^{s-1} d\mu(x)\,.$$

Thus $\alpha_{N,s} \leq \beta_s$ for all $N \in \mathbb{N}$ and $s \geq 1$. ∎

Remark 4.3.4. *Given the monotonicity of $\alpha_{N,s}$ in N and the fact that mean-field expressions such as* (4.3.11) *often are an excellent approximation for many–particle expression such as the one for $\alpha_{N,s}$, one expects that $\alpha_{N,s}$ converges to β_s in the limit of large N. This is indeed the case. Lemma 4.5.5 shows that* $\lim_{N\to\infty} \alpha_{N,s} = \beta_s$ *for all $s \geq 2$, see Remark 4.5.6.*

That leaves us with the task of finding the value of β_s or, at least, good lower bounds. Nam conjectured in [81] that the infimum in the definition of β_2 is achieved by radially symmetric probability measures μ. If this is the case, one can easily find excellent lower bounds for β_2 and β_s. In the next section, we show that this is indeed true, not only for $s = 2$ but even in the range $2 \leq s \leq 3$. This allows us to tighten the lower bound for β_2 and it also yields excellent lower bounds for β_s in the range $2 \leq s \leq 3$.
In Section 4.5 we then show how to derive lower bounds for $\alpha_{N,s}$ in terms of β_s. This works for all $s \geq 2$, but using the lower bounds for β_s derived in Section 4.4 requires to restrict our studies to $2 \leq s \leq 3$. In the limit $s \to 1$, our estimate reduces to the estimate found by Lieb, and in the case $s = 2$, we find a new improved estimate, sharpening the results in [81]. We further improve the results by choosing $s \in (1, 3]$ optimally.
In Section 4.6, we derive upper bounds for the right–hand side of (4.3.10). In Section 4.7, we prove the main Theorem 4.2.2 along with Propositions 4.2.4 and 4.2.5.

4.4 On the Symmetry of Relevant Minimizers

First, we give a more careful definition of β_s. From now on, we set, for $s \geq 1$,

$$\beta_s := \inf \left\{ \frac{\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s+|y|^s}{2|x-y|} d\mu(x)d\mu(y)}{\int_{\mathbb{R}^3} |x|^{s-1} d\mu(x)} : \mu \in D_s(\mathbb{R}^3) \right\} \tag{4.4.1}$$

where $D_s(\mathbb{R}^3) = P(\mathbb{R}^3) \cap H^{-1}(\mathbb{R}^3) \cap L_{s-1}(\mathbb{R}^3)$. Here $P(\mathbb{R}^3)$ is the set of all probability measures in $\mathbb{R}^3$, H^{-1} is the usual Sobolev space of negative order

$$H^{-1}(\mathbb{R}^d) = \left\{ f \in \mathcal{S}^*(\mathbb{R}^d) : \|f\|_{H^{-1}} = \left(\int_{\mathbb{R}^d} \frac{|\widehat{f}(k)|^2}{1+|k|^2} dk \right)^{1/2} < \infty \right\}$$

where $\mathcal{S}^*(\mathbb{R}^d)$ is the space of tempered distributions, $\widehat{f}$ the Fourier transform of a tempered distribution f, and $L_t(\mathbb{R}^3)$ the set of all finite signed or complex–valued measures for which $\int_{\mathbb{R}^3} |x|^t d|\mu|(x) < \infty$, where $|\mu|$ is the modulus of μ.
First, we show that for $1 \leq s \leq 3$, the infimum in (4.4.1) can be computed using only radially symmetric probability measures.

Definition 4.4.1. *Let $\rho \in P(\mathbb{R}^3)$. The radial part of ρ is the measure $\overline{\rho}$ given by*

$$\int_{\mathbb{R}^3} f(x) d\overline{\rho}(x) := \int_{\mathbb{R}^3} \int_{SO(3)} f(U^{-1}x)\, dU d\rho(x), \tag{4.4.2}$$

for any bounded measurable function f where dU is the normalized Haar measure on $SO(3)$. We say that a probability measure ρ is radial if $\rho = \overline{\rho}$. The set of radial probability measures on $\mathbb{R}^3$ is given by

$$P_{rad}(\mathbb{R}^3) := \left\{ \rho \in P(\mathbb{R}^3) : \rho = \overline{\rho} \right\} .$$

With this definition, we have

Theorem 4.4.2. *For all $1 \leq s \leq 3$ we have*

$$\beta_s = \beta_s^{rad} := \inf \left\{ \frac{\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s+|y|^s}{2|x-y|} d\mu(x)d\mu(y)}{\int_{\mathbb{R}^3} |x|^{s-1} d\mu(x)} : \mu \in D_{s,rad}(\mathbb{R}^3) \right\} \tag{4.4.3}$$

where $D_{s,rad}(\mathbb{R}^3) = P_{rad}(\mathbb{R}^3) \cap H^{-1}(\mathbb{R}^3) \cap L_{s-1}(\mathbb{R}^3)$.

The proof of this theorem is based on

Lemma 4.4.3. *Let $\rho \in P(\mathbb{R}^3) \cap H^{-1}(\mathbb{R}^3)$ and*

$$I_s(\rho) := \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s + |y|^s}{2|x-y|} d\rho(x)d\rho(y) . \tag{4.4.4}$$

Then for any $s \in (1,3]$

$$I_s(\rho) \geq I_s(\overline{\rho})$$

where $\overline{\rho}$ is the radial part of ρ.

Remark 4.4.4. *I_0 is the Coulomb energy, which is known to be positive definite, that is, $I_0(\rho) \geq 0$ for all signed and even complex–valued measures (see [41], or [76, Theorem 5.1]). From this the bound $I_0(\rho) \geq I_0(\overline{\rho})$ follows easily. Indeed let $\nu = \rho - \overline{\rho}$ be the non–radial part of ρ and also define the bilinear version $I_0(\rho_1, \rho_2) = \iint \frac{1}{|x-y|} d\rho_1(x) d\rho_2(y)$. Then*

$$I_0(\rho) = I_0(\overline{\rho} + \nu, \overline{\rho} + \nu) = I_0(\overline{\rho}, \overline{\rho}) + 2I_0(\overline{\rho}, \nu) + I_0(\nu, \nu)$$

Since $\overline{\rho}$ is a radial measure, Newtons theorem shows that its potential, given by $V_{\overline{\rho}}(y) = \int \frac{1}{|x-y|} d\overline{\rho}(x) = \int \frac{1}{\max(|x|,|y|)} d\overline{\rho}(x) = V_{\overline{\rho}}(|y|)$ is also radial, hence

$$I_0(\overline{\rho}, \nu) = \frac{1}{2} \int V_{\overline{\rho}}(|y|) d\nu(y) = 0$$

since the non–radial part ν is orthogonal to radial functions. Hence

$$I_0(\rho) = I_0(\overline{\rho}) + I_0(\nu) \geq I_0(\overline{\rho}) \,.$$

Unfortunately, we don't know of any such simple argument based on positive definiteness for I_s when $s > 0$.
Since the proof of Lemma 4.4.3 is a bit lengthy, we postpone it to the end of this section and will first show how it implies Theorem 4.4.2 and discuss its consequences. We will always assume $s \geq 1$ in the following.

Proof of Theorem 4.4.2. In the definition of β_s, the infimum is taken over quotients of the form $I_s(\rho)/(\int |x|^{s-1} d\rho(x))$. The denominator does not change under radial symmetrization, i.e., we have

$$\int |x|^{s-1} d\rho(x) = \int |x|^{s-1} d\overline{\rho}(x)$$

where $\overline{\rho}$ is the radial part of ρ. Note that $\overline{\rho}$ is again a probability measure and it is also in H^{-1}. By Lemma 4.4.3 we have $I_s(\rho) \geq I_s(\overline{\rho})$ when $1 \leq s \leq 3$. So for this range of parameters s we have

$$\frac{I_s(\rho)}{\int |x|^{s-1} d\rho(x)} \geq \frac{I_s(\overline{\rho})}{\int |x|^{s-1} d\overline{\rho}(x)},$$

which implies (4.4.3). ∎

Equipped with Theorem 4.4.2, we can compute a lower bound to β_s when $1 < s \leq 3$.

Proposition 4.4.5. *Let $s \in (1,3]$ and let β_s be defined as in* (4.4.1) *then*

$$\beta_s \geq \min_{t\in[0,1]} \frac{1+t^s}{1+t^{s-1}} = \frac{s}{s-1} t_0 =: b(s)^{-1}$$

where $t_0 \in (0,1)$ is the unique root of $t \mapsto t^s + st + 1 - s$ in $(0,1)$.

Proof. By definition and Lemma 4.4.3 we have for any $s \in [1,3]$

$$\beta_s \geq \inf \left\{ \frac{\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s+|y|^s}{2|x-y|} (d\overline{\rho}(x) d\overline{\rho}(y)}{\int_{\mathbb{R}^3} |x|^{s-1} d\overline{\rho}(x)} : \overline{\rho} \in P_{\text{rad}}(\mathbb{R}^3) \cap H^{-1}(\mathbb{R}^3) \right\}$$

where the infimum is taken only over radial probability measures $\overline{\rho}$. Using Newtons Theorem [76, Theorem 5.2] for fixed $\overline{\rho}$ yields

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s+|y|^s}{2|x-y|} d\overline{\rho}(x) d\overline{\rho}(y) = \frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s+|y|^s}{\max(|x|,|y|)} d\overline{\rho}(x) d\overline{\rho}(y) .$$

Therefore, with $t(x,y) = \frac{\min(|x|,|y|)}{\max(|x|,|y|)}$,

$$\begin{aligned}
&\frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s+|y|^s}{|x-y|} d\overline{\rho}(x) d\overline{\rho}(y) \\
&= \frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s+|y|^s}{\max(|x|,|y|)(|x|^{s-1}+|y|^{s-1})} (|x|^{s-1}+|y|^{s-1}) d\overline{\rho}(x) d\overline{\rho}(y) \\
&= \frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{1+t(x,y)^s}{1+t(x,y)^{s-1}} (|x|^{s-1}+|y|^{s-1}) d\overline{\rho}(x) d\overline{\rho}(y) \\
&\geq \min_{0\leq t\leq 1} \frac{1+t^s}{1+t^{s-1}} \int_{\mathbb{R}^3} |x|^{s-1} d\overline{\rho}(x) .
\end{aligned}$$

Consequently,

$$\beta_s \geq \min_{t\in[0,1]} \frac{1+t^s}{1+t^{s-1}}. \tag{4.4.5}$$

While this minimum can easily be computed for $s = 2$ and $s = 3$, it cannot be computed in a closed form for arbitrary $2 < s < 3$. The minimum is obviously not attained at the boundary $t \in \{0,1\}$ since

$$\frac{1+\left(\frac{1}{2}\right)^s}{1+\left(\frac{1}{2}\right)^{s-1}} = \frac{2^s+1}{2^s+2} < 1.$$

We locate the position of the minimum by differentiating

$$\left(\frac{1+t^s}{1+t^{s-1}}\right)' = \frac{t^s(t^s+s(t-1)+1)}{(t^s+t)^2}$$

which vanishes for $t_0 \in (0,1)$ iff

$$t_0^s + st_0 + 1 - s = 0\,. \tag{4.4.6}$$

The minimum in equation (4.4.5) is therefore attained at $t_0 \in (0,1)$. Combining the equation (4.4.6) and (4.4.5) shows

$$\beta_s \geq \min_{t\in[0,1]} \frac{1+t^s}{1+t^{s-1}} = \frac{s}{s-1} t_0 = b(s)^{-1}\,.$$

∎

Remark 4.4.6. *Nam conjectured in [81] that β_2 could be calculated using only radial probability measures. Theorem 4.4.2 shows that this is indeed correct. Because of this, our lower bound for β_2 is slightly better than the one in [81]. More importantly, the main improvement in our analysis of the ionization problem comes from the fact that the lower bound for β_s is increasing in $s \in [2,3]$ and substantially bigger than β_2 when s is close to 3. We would like to take s much larger than 2. However, we do not know whether the lower bound of Proposition 4.4.5 extends to $s > 3$.*
For $s = 2$ and $s = 3$, one can compute the value of β_s explicitly. One finds

$$\beta_2 = 2(\sqrt{2}-1) \Rightarrow b(2) = \frac{1}{2}(\sqrt{2}+1) \leq 1.2072,$$
$$\beta_3 = \frac{3}{2}\frac{(1+\sqrt{2})^{2/3}-1}{\sqrt[3]{1+\sqrt{2}}} \Rightarrow b(3) = \frac{2}{3}\frac{\sqrt[3]{1+\sqrt{2}}}{(1+\sqrt{2})^{2/3}-1} \leq 1.1185\,.$$

To find upper bounds on β_s, respectively lower bounds on $b(s)$, one can choose an explicit measure in (4.4.3). To produce Figure 4.2 we have chosen

$$\overline{\rho}_{num}(x) = \begin{cases} A|x|^{-p}, & |x| \in [1,n] \\ 0, & |x| \notin [1,n] \end{cases}\,.$$

and have optimized numerically in the parameters p and n and chose $A > 0$ such that $\overline{\rho}_{num}$ is the density of a probability measure. The results of this study are plotted in Figure 4.2 where $b_{num}(s)$ are the numerically obtained lower bounds on β_s^{-1} after the optimization explained above. Next, we give the

Proof of Lemma 4.4.3. Before we give a detailed proof, let us clarify the strategy. We want to mimic the strategy for the Coulomb potential I_0 outlined in Remark 4.4.4, but the weight $|x|^s$ seems to spoil the argument and, as far we know, no arguments using positive definiteness, as for I_0, or conditional positive definiteness, i.e., $I_s(\nu) \geq 0$ for all (suitable) signed measures ν with total mass $\nu(\mathbb{R}^3) = 0$, seem to be available. So we have to use a different route. We introduce the bilinear version

$$I_s(\rho_1, \rho_2) = \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s + |y|^s}{2|x-y|} d\rho_1(x) d\rho_2(y)\,. \tag{4.4.7}$$

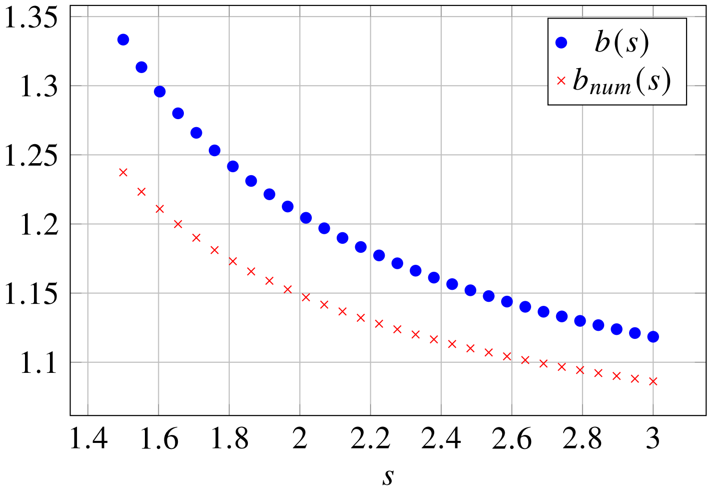

FIGURE 4.2: Values of $b(s)$ according to Proposition 4.4.5, where t_0 was computed numerically. The lower bounds $b_{num}(s)$ on β_s^{-1} have been found by choosing explicit measures in (4.4.3) and numerical optimization. The exact value of β_s^{-1} has to be between both lines. The values $b(3)$ and $b_{num}(3)$ differ by approximately 3 %.

Then, as for I_0, we have

$$I_s(\rho) = I_s(\overline{\rho}) + 2I_s(\overline{\rho}, \nu) + I_s(\nu)$$

where $\nu = \rho - \overline{\rho}$ is the non–radial part of ρ. Since $\overline{\rho}$ is a radial measure, Newton's theorem shows again that the functions

$$\int \frac{|x|^s}{|x-y|} d\overline{\rho}(x) = \int \frac{|x|^s}{\max(|x|,|y|)} d\overline{\rho}(x) =: V_1(|y|)\,,$$
$$\int \frac{1}{|x-y|} d\overline{\rho}(x) = \int \frac{1}{\max(|x|,|y|)} d\overline{\rho}(x) =: V_2(|y|)$$

are radial. Thus

$$2I_s(\overline{\rho}, \nu) = \int_{\mathbb{R}^3} V_1(|y|) d\nu(y) + \int_{\mathbb{R}^3} V_2(|y|)|y|^s d\nu(y) = 0 \tag{4.4.8}$$

since the measure ν is orthogonal to radial functions. Thus, it is enough to show that $I_s(\nu) \geq 0$ for measures ν, which are orthogonal to radial functions. Note that the potential $V_\mu = \int \frac{1}{|x-y|} d\mu(y)$ solves the equation

$$-\Delta V_\mu = 4\pi\mu$$

in the sense of distributions. Hence, at least informally,

$$\begin{aligned} I_s(\mu) &= \int_{\mathbb{R}^3} |x|^s \int_{\mathbb{R}^3} \frac{1}{|x-y|} d\mu(x) d\mu(y) = \int_{\mathbb{R}^3} |x|^s V_\mu(x) d\mu(x) \\ &= \frac{1}{4\pi} \int |x|^s V_\mu(x)(-\Delta V_\mu(x)) dx = \frac{1}{4\pi} \left\langle |x|^s V_\mu, -\Delta V_\mu \right\rangle \end{aligned}$$

where $\langle \cdot, \cdot \rangle$ is the usual scalar product on $L^2(\mathbb{R}^3)$ and we used symmetry for the first equality. Since μ is real-valued, so is its potential V_μ, hence using the IMS formula and Hardy's inequality, there exists a $c_H > 0$ such that

$$\begin{aligned} 4\pi I_s(\mu) &= \mathrm{Re}\langle |x|^s V_\mu, -\Delta V_\mu \rangle = \langle |x|^{s/2} V_\mu, -\Delta(|x|^{s/2} V_\mu) \rangle - \langle V_\mu, \frac{s^2}{4} |x|^{s-2} V_\mu \rangle \\ &= \left\langle |x|^{s/2} V_\mu, \left[-\Delta - \frac{s^2}{4|x|^2} \right] (|x|^{s/2} V_\mu) \right\rangle \geq \left(c_H - \frac{s^2}{4} \right) \langle V_\mu, |\cdot|^{s-2} V_\mu \rangle . \end{aligned}$$

Using $\mu = \nu = \rho - \overline{\rho}$ above and noting that ν is orthogonal to radial functions, one sees that also its potential V_ν is orthogonal to radial functions. Hence

$$4\pi I_s(\nu) \geq \left(c_H - \frac{s^2}{4} \right) \langle V_\nu, |\cdot|^{s-2} V_\nu \rangle$$

with the improved Hardy constant $c_H = d^2/4$ in dimension $d \geq 2$, (see [29, Lemma 2.4]), since the potential V is orthogonal to radial symmetric functions in the L^2-sense. Hence $I_s(\nu) = I_s(\rho - \overline{\rho}) \geq 0$ whenever $s \leq d = 3$. Of course, this is not yet a rigorous proof. The weight $|x|^s$ is not bounded, so the application of the IMS localization formula is not clear. In addition, it is not clear that the potential V_ν is well–defined.

To make this argument rigorous, one has to be a bit more careful. For any $x \in \mathbb{R}^3$, $\varepsilon, \lambda > 0$ and $\mu \in H^{-1}(\mathbb{R}^3)$ we define

$$\varphi_{\varepsilon,s}(x) := \frac{|x|^s}{1 + \varepsilon |x|^s}, \quad V_{\mu,\lambda}(x) := \int_{\mathbb{R}^3} \frac{e^{-\lambda|x-y|}}{4\pi|x-y|} d\mu(y), \tag{4.4.9}$$

These are regularized versions of the weight $|x|^s$ and the potential V_ν, respectively. Let us collect some properties of $\varphi_{\varepsilon,s}$, $V_{\lambda,\mu}$ and $u[\mu]$ before we continue. Note that $V_{\mu,\lambda}$ is the solution to the differential equation

$$(-\Delta + \lambda^2) V_{\mu,\lambda} = \mu. \tag{4.4.10}$$

in the sense of distributions. It is elementary to verify that $\varphi_{\varepsilon,s} \in W^{1,\infty}$ since $x \mapsto |x|^s$ is weakly differentiable and $\varphi_{\varepsilon,s}$ is bounded by construction. In the definition of β_s in (4.4.1) we also assumed that $\mu \in H^{-1}(\mathbb{R}^d)$. This ensures that $V_{\mu,\lambda} \in H^1$. Indeed, (4.4.10) shows that the Fourier transform of $V_{\lambda,\nu}$ is given by $\widehat{V}_{\lambda,\mu}(k) = (|k|^2 + \lambda)^{-1} \widehat{\mu}(k)$. Hence the H^{-1} norm of $V_{\lambda,\nu}$

is given by

$$\int_{\mathbb{R}^3} (1+|k|^2)\left|\widehat{V}_{\mu,\lambda}(k)\right|^2 dk \lesssim \int_{\mathbb{R}^2} \frac{(1+|k|^2)}{\lambda^2+|k|^2}\frac{|\widehat{\mu}(k)|^2}{\lambda^2+|k|^2} dk \lesssim \int_{\mathbb{R}^3} \frac{|\widehat{\mu}(k)|^2}{\lambda^2+|k|^2} dk < \infty \, .$$

The last integral is finite for any $\lambda > 0$ since, by assumption, $\mu \in H^{-1}$. In particular, we also have $\varphi_\varepsilon V_{\mu,\lambda} \in H^1$ for any $\varepsilon, \lambda > 0$ as a product of an $W^{1,\infty}$ and an H^1 function. Note that if we split a probability measure $\rho \in H^{-1}(\mathbb{R}^3)$ as $\rho = \overline{\rho} + \nu$, with $\overline{\rho}$ the radial and ν the non–radial parts, the same holds for the potential $V_{\overline{\rho}}$ and V_ν. Thus, all potentials we need are in $H^1(\mathbb{R}^3)$. By monotone convergence

$$\begin{aligned} I_s(\rho) &= \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s+|y|^s}{2|x-y|} d\rho(x)d\rho(y) \\ &= \lim_{\lambda\to 0} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{(|x|^s+|y|^s)e^{-\lambda|x-y|}}{2|x-y|} d\rho(y)d\rho(x) \\ &= \lim_{\lambda\to 0}\lim_{\varepsilon\to 0} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{(\varphi_{\varepsilon,s}(x)+\varphi_{\varepsilon,s}(y))e^{-\lambda|x-y|}}{2|x-y|} d\rho(y)d\rho(x) \, . \end{aligned} \tag{4.4.11}$$

Define

$$I_s^{\lambda,\varepsilon}(\rho) = \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{(\varphi_{\varepsilon,s}(x)+\varphi_{\varepsilon,s}(y))e^{-\lambda|x-y|}}{|x-y|} d\rho(y)d\rho(x)$$

and its bilinear version

$$I_s^{\lambda,\varepsilon}(\rho_1,\rho_2) = \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{(\varphi_{\varepsilon,s}(x)+\varphi_{\varepsilon,s}(y))e^{-\lambda|x-y|}}{|x-y|} d\rho_1(y)d\rho_1(x) \, .$$

Split ρ into its radial part $\overline{\rho}$ and its non–radial part $\nu = \rho - \overline{\rho}$. Then as in (4.4.7) one sees

$$I_s^{\lambda,\varepsilon}(\rho) = I_s^{\lambda,\varepsilon}(\overline{\rho}) + 2I_s^{\lambda,\varepsilon}(\overline{\rho},\nu) + I_s^{\lambda,\varepsilon}(\nu) \, .$$

Again, we have that the potentials

$$\widetilde{V}_1 = (-\Delta_\lambda)^{-1}\overline{\rho} \quad \text{and } \widetilde{V}_2 = (-\Delta_\lambda)^{-1}\varphi_{\epsilon,s}\overline{\rho}$$

are rotationally symmetric. Thus as in (4.4.8) we have

$$8\pi I_s^{\lambda,\varepsilon}(\overline{\rho},\nu) = \int_{\mathbb{R}^3} \widetilde{V}_1(|y|)d\nu(y) + \int_{\mathbb{R}^3} \widetilde{V}_2(|y|)|y|^s d\nu(y) = 0$$

since ν is a bounded measure orthogonal to radial functions. Thus we have

$$I_s^{\lambda,\varepsilon}(\rho) = I_s^{\lambda,\varepsilon}(\overline{\rho}) + I_s^{\lambda,\varepsilon}(\nu) \tag{4.4.12}$$

and the claim follows once we show that $I_s^{\lambda,\varepsilon}(\nu) \geq 0$ for $\nu = \rho - \overline{\rho}$.

We claim that for any probability measure $\mu \in P(\mathbb{R}^3) \cap H^{-1}(\mathbb{R}^3)$

$$\frac{1}{4\pi} I_s^{\lambda,\varepsilon}(\mu,\mu) = \left\langle \nabla(\varphi_{\varepsilon,s} V_{\lambda,\mu}), \nabla(V_{\lambda,\mu}) \right\rangle + \lambda \left\langle \varphi_{\varepsilon,s}^{1/2} V_{\lambda,\mu}, \varphi_{\varepsilon,s}^{1/2} V_{\lambda,\mu} \right\rangle \tag{4.4.13}$$

where $V_{\lambda,\mu} = (-\Delta + \lambda)^{-1}\mu$ and $\varphi_{\varepsilon,s} V_{\lambda,\nu} \in H^1(\mathbb{R}^3)$. Assuming this representation allows us to finish the proof since now, we can apply the IMS localization formula. Since the right–hand side of (4.4.13) is real, we have

$$\begin{aligned} \frac{1}{4\pi} I_s^{\lambda,\varepsilon}(\mu,\mu) &= \mathrm{Re} \left\langle \nabla(\varphi_{\varepsilon,s} V_\mu), \nabla(V_\mu) \right\rangle + \lambda \left\langle \varphi_{\varepsilon,s}^{1/2} V_{\lambda,\mu}, \varphi_{\varepsilon,s}^{1/2} V_{\lambda,\mu} \right\rangle \\ &= \left\langle \nabla(\varphi_{\varepsilon,s}^{1/2} V_\mu), \nabla(\varphi_{\varepsilon,s}^{1/2} V_\mu) \right\rangle - \left\langle V_\mu, |\nabla \varphi_{\varepsilon,s}^{1/2}|^2 V_\mu \right\rangle + \lambda \left\langle \varphi_{\varepsilon,s}^{1/2} V_{\lambda,\mu}, \varphi_{\varepsilon,s}^{1/2} V_{\lambda,\mu} \right\rangle \end{aligned} \tag{4.4.14}$$

from the IMS localization formula. Computing the derivative shows

$$|\nabla \varphi_{\varepsilon,s}^{1/2}|^2 = \varphi_{\varepsilon,s} \left| \frac{\nabla \varphi_{\varepsilon,s}(x)}{2\varphi_{\varepsilon,s}(x)} \right|^2 = \varphi_{\varepsilon,s} \frac{s^2}{4|x|^2},$$

so, since $\lambda \geq 0$,

$$\frac{1}{4\pi} I_s^{\lambda,\varepsilon}(\mu,\mu) \geq \left\langle \nabla(\varphi_{\varepsilon,s}^{1/2} V_\mu), \nabla(\varphi_{\varepsilon,s}^{1/2} V_\mu) \right\rangle - \left\langle \varphi_{\varepsilon,s}^{1/2} V_\mu, \frac{s^2}{4|x|^2} \varphi_{\varepsilon,s}^{1/2} V_\mu \right\rangle .$$

We use this for $\mu = \nu = \rho - \overline{\rho} \in H^{-1}(\mathbb{R}^d)$. Note that ν being orthogonal to radial functions implies that its potential $V_\nu = (\Delta + \lambda)^{-1}\nu$ is orthogonal to radial functions in $L^2(\mathbb{R}^3)$. Also, since both ρ and $\overline{\rho} \in H^{-1}(\mathbb{R}^3)$ we also have that $\nu \in H^{-1}(\mathbb{R}^3)$, so we can use the representation (4.4.13) for $\mu = \nu$.
Hence, with the improved Hardy inequality $\widetilde{C}_d^H = d^2/4$ (see [29, Lemma 2.4]), valid for functions orthogonal to radial functions, we get

$$\frac{1}{4\pi} I_s^{\lambda,\varepsilon}(\nu,\nu) \geq \left(\widetilde{C}_3^H - s^2/4 \right) \left\langle \varphi_{\varepsilon,s}^{1/2} V_\nu, |x|^{-2} \varphi_{\varepsilon,s}^{1/2} V_\nu \right\rangle . \tag{4.4.15}$$

In our case $d = 3$, so (4.4.15) shows that $I_s(\nu,\nu) \geq 0$ as long as $s \leq 3$. Together with (4.4.12) we get

$$I_s(\rho) = \lim_{\varepsilon \to 0} \lim_{\lambda \to 0} I_s^{\lambda,\varepsilon}(\rho) \geq \lim_{\varepsilon \to 0} \lim_{\lambda \to 0} I_s^{\lambda,\varepsilon}(\overline{\rho}) = I_s(\overline{\rho}) \tag{4.4.16}$$

for any measure $\rho \in P(\mathbb{R}^3) \cap H^{-1}(\mathbb{R}^3)$ and all $0 \leq s \leq 3$.
It remains to prove the representation (4.4.13). First, note that by symmetry, we have

$$\frac{1}{4\pi} I_S^{\lambda\varepsilon}(\mu,\mu) = \iint \frac{\varphi_{\varepsilon,s}(x) e^{-\lambda|x-y|}}{4\pi|x-y|} d\mu(y)\, d\mu(x) = \int \varphi_{\varepsilon,s}(x) V_{\lambda,\mu}(x) d\mu(x) .$$

To show that this leads to (4.4.13) we use the the Lax-Milgram theorem [31, Chapter 6.2.1, Theorem 1]. For any $\lambda > 0$, define the bilinear, or better sesquilinear, form

$$B[\cdot,\cdot] : H^1 \times H^1 \to \mathbb{R}, \quad (u,v) \mapsto B[u,v] \coloneqq \langle \nabla u, \nabla v \rangle_{L^2} + \lambda^2 \langle u, v \rangle_{L^2}.$$

Then B is coercive and bounded (with respect to the H^1 norm) and thus fulfills the conditions of the Lax-Milgram Theorem. Let

$$f(\cdot) : H^1 \to \mathbb{C}, \quad g \mapsto f(g) \coloneqq \int_{\mathbb{R}^3} g(x) d\mu(x)$$

for $\mu \in H^{-1}$ a bounded measure. Then f is a bounded linear functional on H^1, and by the Lax-Milgram theorem, there exists a unique $v_0 \in H^1$ such that

$$\int_{\mathbb{R}^3} g d\mu = f(g) = B[g, v_0] = \langle \nabla g, \nabla v_0 \rangle_{L^2} + \lambda^2 \langle g, v_0 \rangle_{L^2}. \tag{4.4.17}$$

Recall that this solution v_0 is the weak solution of Equation (4.4.10), hence

$$\int_{\mathbb{R}^3} g d\mu = \langle \nabla g, \nabla V_{\mu,\lambda} \rangle_{L^2} + \lambda^2 \langle g, V_{\mu,\lambda} \rangle_{L^2}. \tag{4.4.18}$$

for all $g \in H^1(\mathbb{R}^3)$. Using $g = \varphi_{\varepsilon,s} V_{\lambda,\mu}$ proves

$$\frac{1}{4\pi} I_s^{\lambda,\varepsilon}(\mu,\mu) = \int \varphi_{\varepsilon,s} V_{\lambda,\mu} d\mu = \left\langle \nabla(\varphi_{\varepsilon,s} V_{\lambda,\mu}), \nabla V_{\lambda,\mu} \right\rangle + \lambda \left\langle \varphi_{\varepsilon,s} V_{\lambda,\mu}, V_{\lambda,\mu} \right\rangle$$

which is (4.4.13). ∎

4.5 Mean–Field Type Bound

In this section, we analyze $\alpha_{N,s}$ defined in (4.3.9) and derive lower bounds for $\alpha_{N,s}$ in terms of its mean–field version β_s. Clearly, the quotient in the definition of $\alpha_{N,s}$ is infinite if two points coincide. So let

$$A \coloneqq \{(x_1, x_2, \dots x_N) \in \mathbb{R}^{3N} : x_i \neq x_j \text{ whenever } i \neq j\}$$

then

$$\alpha_{N,s} = \inf \left\{ \frac{\sum_{\substack{1 \le i,k \le N \\ i \neq k}} \frac{|x_k|^s + |x_i|^s}{|x_i - x_k|}}{2(N-1) \sum_{k=1}^N |x_k|^{s-1}} : (x_1, x_2, \dots x_N) \in A \right\}. \tag{4.5.1}$$

Note that the mapping

$$(x_1, x_2, \dots x_N) \mapsto \frac{\sum_{\substack{1\le i,k\le N\\ i\neq k}} \frac{|x_k|^s+|x_i|^s}{|x_i-x_k|}}{2(N-1)\sum_{k=1}^N |x_k|^{s-1}}$$

is continuous on A. The set

$$A_0 := \{(x_1, x_2, \dots x_N) \in A : x_k \neq 0 \text{ for } 1 \le k \le N\} \tag{4.5.2}$$

is dense in A, thus

$$\alpha_{N,s} = \inf \left\{ \frac{\sum_{\substack{1\le j,k\le N\\ i\neq k}} \frac{|x_j|^s+|x_k|^s}{|x_i-x_k|}}{2(N-1)\sum_{k=1}^N |x_k|^{s-1}} : (x_1, x_2, \dots x_N) \in A_0 \right\} . \tag{4.5.3}$$

For completeness, we prove this in the Appendix in Lemma A.1.1. In order to prove that $\alpha_{N,s} \to \beta_s$ for $N \to \infty$, with β_s given by (4.4.1) we need some preparations.

Lemma 4.5.1. *Let $r > 0$, $x \in \mathbb{R}^3 \setminus \{0\}$ and μ be the measure defined by*

$$\int_{\mathbb{R}^3} f d\mu := \int_{S^2} f(x + r|x|\omega)\frac{d\omega}{4\pi} \tag{4.5.4}$$

for any measurable function f. Then $\mu \in H^{-1}(\mathbb{R}^3)$.

Remark 4.5.2. *This lemma shows that convex combinations of probability measures of the form* (4.5.4) *are allowed in the computation of upper bounds for β_s since they clearly are in $P(\mathbb{R}^3) \cap M_{s-1}(\mathbb{R}^3)$ and the lemma shows that they are also in $H^{-1}(\mathbb{R}^3)$.*

Proof. Let $r > 0$, $\Omega := \{x \in \mathbb{R}^3 : |x| < r\}$ and $T : H^1(\Omega) \to L^2(\partial\Omega)$ the trace operator as for example defined in [31, Chapter 5.5]. Furthermore, let $f \in H^1(\mathbb{R}^3)$ then

$$\left|\int_{\mathbb{R}^3} f d\mu\right| = \left|\int_{S^2} f(x + r|x|\omega)\frac{d\omega}{4\pi}\right| \le \frac{1}{4\pi}\int_{\partial\Omega} |(Tf)(\omega)|d\omega \le r^{1/2}\|Tf\|_{L^2(\partial\Omega)}.$$

The Trace Theorem [31, Chapter 5.5 Theorem 1] shows that there exists a $C > 0$ such that

$$\|Tf\|_{L^2(\partial\Omega)} \le C\|f\|_{H^1(\Omega)} < \infty .$$

Consequently, μ is in the dual space of $H^1(\mathbb{R}^3)$ by definition of the dual space. That is, $\mu \in H^{-1}(\mathbb{R}^3)$. ∎

We continue by comparing $\alpha_{N,s}$ to β_s. Let $r > 0$ and $(x_1, \ldots, x_N) \in \mathbb{R}^{3N}$ with $x_j \neq x_k$ for $j \neq k$. Following [81] we define

$$\mu := \frac{1}{N}\sum_{i=1}^{N} d\mu_i, \quad \int_{\mathbb{R}^3} f\, d\mu_i := \int_{S^2} f(x_j + r|x_j|\omega)\frac{d\omega}{4\pi} \tag{4.5.5}$$

for any measurable function f. By Lemma 4.5.1 $x_i \neq 0$ implies that $\mu_i \in H^{-1}$. In our analysis, we will use a refinement of the following Lemma 4.5.3. We provide this bound since it allows us to compare $\alpha_{N,s}$ and β_s for all $s > 0$ and large N, while the refinements only work for $s \geq 2$.

Lemma 4.5.3 (Comparison of $\alpha_{N,s}$ with β_s, all $s \geq 0$)**.** *Let $\alpha_{N,s}$ and β_s be defined as in* (4.4.1) *and* (4.5.1) *then for every $N \geq 2$, $r > 0$, and $s \geq 0$*

$$\frac{(r+1)^{s+1} - (1-r)^{s+1}}{2r(s+1)} N\beta_s \leq (1+r)^s \left(\alpha_{N,s}(N-1) + \frac{1}{r}\right). \tag{4.5.6}$$

Remark 4.5.4. *Note that the prefactors in front of $N\beta_s$ and $\alpha_{N,s}(N-1)$ in* (4.5.6) *converges to one as $r \to 0$. Thus* (4.5.6) *shows that for all $r > 0$*

$$\liminf_{N\to\infty} \alpha_{N,s} \geq \frac{(1+r)^{s+1} - (1-r)^{s+1}}{2r(s+1)(1+r)^s}\beta_s\,.$$

Taking the limit $r \to 0$ yields $\liminf_{N\to\infty} \alpha_{N,s} \geq \beta_s$ and with Lemma 4.3.3 this proves

$$\lim_{N\to\infty} \alpha_{N,s} = \beta_s$$

for all $s > 0$.

Proof of Lemma 4.5.3. Let $\mu = \sum_{j=1}^{N} \mu_j$ for points $x_1, \ldots, x_N \in A_0$, where A_0 is defined in (4.5.2), be the measure given by (4.5.5). By Lemma 4.5.1 we know that $\mu \in H^{-1}(\mathbb{R}^3)$. Recall the definition of I_s in Lemma 4.4.3. Then

$$\begin{aligned} N^2 I_s(\mu) &= \sum_{j,k=1}^{N} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s + |y|^s}{2|x-y|} d\mu_j(x)d\mu_k(y) \\ &= \sum_{j\neq k}^{N} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s + |y|^s}{2|x-y|} d\mu_j(x)d\mu_k(y) \\ &+ \sum_{j=1}^{N} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s + |y|^s}{2|x-y|} d\mu_j(x)d\mu_j(y)\,. \end{aligned} \tag{4.5.7}$$

Note that by construction of the measure μ_i

$$|x - x_i| = r|x_i|$$

and hence

$$|x| \leq |x - x_i| + |x_i| \leq (1+r)|x_i|. \tag{4.5.8}$$

for any $x \in \text{supp}(\mu_i)$ We first bound the diagonal terms with $j = k$. Note that

$$\begin{aligned}
\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s + |y|^s}{2|x-y|} d\mu_j(x) d\mu_j(y) &= \int_{\mathbb{R}^3} |x|^s \int_{\mathbb{R}^3} \frac{1}{|x-y|} d\mu_j(y) d\mu_j(x) \\
&\leq (1+r)^s |x_i|^s \int_{\mathbb{R}^3} \int_{S^2} \frac{1}{\left|x - x_j - r|x_i|\omega\right|} \frac{d\omega}{4\pi} d\mu_i(x) \\
&= (1+r)^s \left|x_j\right|^s \int_{S^2} \int_{S^2} \frac{1}{\left|r\left|x_j\right|\eta - r\left|x_j\right|\omega\right|} \frac{d\omega}{4\pi} \frac{d\eta}{4\pi} \\
&= \frac{\left|x_j\right|^{s-1}}{r} (1+r)^s.
\end{aligned} \tag{4.5.9}$$

Hence

$$\sum_{j=1}^{N} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s + |y|^s}{2|x-y|} d\mu_j(x) d\mu_j(y) \leq \frac{(1+r)^s}{r} \sum_{j=1}^{N} \left|x_j\right|^{s-1}. \tag{4.5.10}$$

Similarly, we can bound the off–diagonal terms $j \neq k$. We have

$$\begin{aligned}
&\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s + |y|^s}{2|x-y|} d\mu_j(x) d\mu_k(y) \\
&= \int_{\mathbb{R}^3} |x|^s \int_{\mathbb{R}^3} \frac{1}{|x-y|} d\mu_k(y) d\mu_j(x) \\
&\leq (1+r)^s \left|x_j\right|^s \int_{\mathbb{R}^3} \int_{S^2} \frac{1}{|x - x_k - r|x_k|\omega|} \frac{d\omega}{4\pi} d\mu_j(x) \\
&= (1+r)^s \left|x_j\right|^s \int_{\mathbb{R}^3} \frac{1}{\max\{\left|x - x_j\right|, r\left|x_j\right|\}} d\mu_j(x) \\
&\leq (1+r)^s |x_i|^s \int_{\mathbb{R}^3} \frac{1}{\left|x - x_j\right|} d\mu_j(x) \leq (1+r)^s \frac{|x_i|^s}{\left|x_i - x_j\right|}.
\end{aligned} \tag{4.5.11}$$

Thus

$$\sum_{j\neq k} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s + |y|^s}{2|x-y|} d\mu_j(x) d\mu_k(y) \leq (1+r)^s \sum_{j\neq k}^{N} \frac{\left|x_j\right|^s + |x_k|^s}{2\left|x_j - x_k\right|}. \tag{4.5.12}$$

Combining (4.5.7), (4.5.9) and (4.5.12) shows

$$N^2 I_s(\mu) \leq \frac{(1+r)^s}{r} \sum_{j=1}^{N} \left|x_j\right|^{s-1} + (1+r)^s \sum_{j\neq k}^{N} \frac{\left|x_j\right|^s + |x_k|^s}{2\left|x_j - x_k\right|}. \tag{4.5.13}$$

Let $t > -2$ then with Lemma A.2.2 we have

$$N\int_{\mathbb{R}^3}|x|^t d\mu = \sum_{j=1}^{N}\int_{S^2}\left|x_j + r\left|x_j\right|\omega\right|^t \frac{d\omega}{4\pi} = \frac{(1+r)^{t+2}-(1-r)^{t+2}}{2r(t+2)}\sum_{j=1}^{N}\left|x_j\right|^t . \tag{4.5.14}$$

Applying (4.5.14) for $t = s-1$ yields

$$N\int_{\mathbb{R}^3}|x|^{s-1}d\mu(x) = \frac{(1+r)^{s+1}-(1-r)^{s+1}}{2r(s+1)}\sum_{j=1}^{N}\left|x_j\right|^{s-1}. \tag{4.5.15}$$

Recall the definitions of β_s and $I_s(\mu)$ in (4.4.1) and (4.4.4) then $\beta_s \leq I_s(\mu)/\int |x|^{s-1}d\mu$ or

$$N\int_{\mathbb{R}^3}|x|^{s-1}d\mu(x)\,\beta_s N \leq N^2 I_s(\mu)\,, \tag{4.5.16}$$

which together with (4.5.13) and (4.5.15) implies the inequality

$$\frac{(1+r)^{s+1}-(1-r)^{s+1}}{2r(s+1)(1+r)^s}\beta_s N \leq \frac{1}{r} + \frac{\sum_{j\neq k}\frac{\left|x_j\right|^s+|x_k|^s}{2\left|x_j-x_k\right|}}{\sum_{j=1}^{N}\left|x_j\right|^{s-1}} .$$

Taking the infimum in the positions $(x_1, x_2, \ldots, x_N) \in A_0$ together with the definition of $\alpha_{N,s}$ and applying Lemma A.1.1 we conclude

$$\frac{(1+r)^{s+1}-(1-r)^{s+1}}{2r(s+1)(1+r)^s}\beta_s N \leq \frac{1}{r} + \alpha_{N,s}(N-1)\,.$$

This proves (4.5.6). ∎

Lemma 4.5.5 (Refined comparison I of $\alpha_{N,s}$ with β_s, $s \geq 2$)**.** *For $s \geq 2$ and all $N \in \mathbb{N}$ and $r > 0$ we have*

$$\left(\frac{s+2}{s+1}\right)\frac{(1+r)^{s+1}-|1-r|^{s+1}}{(1+r)^{s+2}-|1-r|^{s+2}}N\beta_s - \frac{1}{r} \leq \frac{2r(s+2)}{(1+r)^{s+2}-|1-r|^{s+2}}g(r)\alpha_{N,s}(N-1) \tag{4.5.17}$$

where

$$g(r) = (1+r^2)^{s/2}\left(\frac{(1+q)^{s/2}+(1-q)^{s/2}}{2} - \frac{s\,(s-2)}{15}q^2(1+q)^{\frac{s-4}{2}}\right), \quad q = \frac{2r}{1+r^2}\,. \tag{4.5.18}$$

Remark 4.5.6. *For $s = 2$, the bound* (4.5.17) *is similar to the refined bound (27) in [81]. The main challenge in establishing a relationship between $\alpha_{N,s}$ and β_s arises from the weighted Coulomb interaction term in* (4.5.11)*. In the proof of Lemma 4.5.5, we improve the estimate of these terms using a convexity argument.*
Since obtaining optimal estimates between $\alpha_{N,s}$ and β_s is technically challenging, we present the proof of Lemma 4.5.5 here, relying only on standard arguments. A further refinement

is provided in Lemma 4.5.9. This improvement, which is more difficult to prove as it involves a multipole expansion and estimates for all multipole moments using certain nontrivial properties of Legendre polynomials, yields a better constant in front of $\beta_s N$.

Before we give the proof of Lemma 4.5.5, we state and prove a result, which is extremely helpful in dropping certain terms when deriving a bound on $\alpha_{N,s}$ in terms of β_s when $s \geq 2$.

Lemma 4.5.7. *Let $\gamma : (0,\infty) \times (0,\infty) \to [0,\infty)$ a function such that $\gamma(u,v)$ is increasing in v for any fixed $u > 0$. Then for any N distinct points $x_1, \ldots, x_N$ in $\mathbb{R}^3 \setminus \{0\}$ we have*

$$\sum_{j \neq k} \frac{\gamma(|x_j - x_k|, r|x_j|)}{|x_j|} x_j \cdot (x_j - x_k) \geq 0 \tag{4.5.19}$$

for all $r > 0$

Proof. Since the sum is over pais $j \neq k$ it is enough to consider the case $N = 2$ and $i = 1$, $j = 2$. Set $a = x_1 - x_2$. We have $x_1 \cdot (x_1 - x_2) = |x_1|^2 - x_1 \cdot x_2 \geq |x_1|^2 - |x_1||x_2|$ and, similarly, $x_2 \cdot (x_2 - x_1) \geq |x_2|^2 - |x_2||x_1|$. Since $\gamma \geq 0$ $\gamma(|a|, v_1) \geq \gamma(|a|, v_2)$ if $v_1 \geq v_2$, by assumption, this implies

$$\begin{aligned}
&\frac{\gamma(|x_1 - x_2|, r|x_1|)}{|x_1|} x_1 \cdot (x_1 - x_2) + \frac{\gamma(|x_2 - x_1|, r|x_2|)}{|x_2|} x_2 \cdot (x_2 - x_1) \\
&\geq \gamma(|a|, r|x_1|) \left(|x_1| - |x_2|\right) + \gamma(|a|, r|x_2|) \left(|x_2| - |x_1|\right) \\
&= \left(\gamma(|a|, r|x_1|) - \gamma(|a|, r|x_2|)\right)\left(|x_1| - |x_2|\right) \geq 0\,.
\end{aligned}$$

∎

Remark 4.5.8. *We note that unlike the proof in [81], we do not need the explicit form of $\gamma(u,v)$ in* (4.5.35) *for* (4.5.19). *Our argument shows that it is enough that $\gamma(u,v) \geq 0$ is increasing in $v > 0$ for fixed $u > 0$.*

Proof of Lemma 4.5.5. The diagonal terms are easy to calculate. Without loss of generality, let $j = 1$. Then by symmetry, the definition of the measures μ_j, and Newton's theorem, we have

$$\begin{aligned}
\iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|x|^s + |y|^s}{2|x-y|} d\mu_1(x) d\mu_1(y) &= \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|x|^s}{|x-y|} d\mu_1(x) d\mu_1(y) \\
&= \frac{1}{(4\pi)^2} \int_{S^2} \int_{S^2} \frac{|x_1 + r|x_1|\omega_1|^s}{r|x_1||\omega_1 - \omega_2|} d\omega_1 d\omega_2 \\
&= \frac{1}{4\pi r|x_1|} |x_1|^{s-1} \int_{S^2} |\widehat{x}_1 + r\omega|^s d\omega \\
&= \frac{|x_1|^{s-1}}{r} \frac{(1+r)^{s+2} - |1-r|^{s+2}}{2r(s+2)}\,.
\end{aligned} \tag{4.5.20}$$

See Lemma A.2.2 for the explicit calculation of the last integral in (4.5.20). Thus, the diagonal sum is given by

$$\sum_{j=1}^{N} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s+|y|^s}{2|x-y|} d\mu_j(x) d\mu_k(y) = \frac{(1+r)^{s+2}-|1-r|^{s+2}}{2r^2(s+2)} \sum_{j=1}^{N} \left|x_j\right|^{s-1} . \tag{4.5.21}$$

For the off–diagonal sum, we use symmetry and Newton's theorem – the measure μ_j is radially symmetric around the point x_j – to see that

$$\begin{aligned} \sum_{j\neq k} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s+|y|^s}{2|x-y|} d\mu_j(x) d\mu_k(y) &= \sum_{j\neq k} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|x|^s}{|x-y|} d\mu_k(y) d\mu_j(x) \\ \leq \sum_{j\neq k} \int_{\mathbb{R}^3} \frac{|x|^s}{\left|x-x_j\right|} d\mu_j(x) &= \sum_{j\neq k} \frac{1}{4\pi} \int_{S^2} \frac{\left|x_j+r\left|x_j\right|\omega\right|^s}{\left|x_j-x_k+r\left|x_j\right|\omega\right|} d\omega . \end{aligned} \tag{4.5.22}$$

To bound the integral in the last sum for $s \neq 2$, the estimates presented in [81, Section 4] can not easily be applied. We will proceed differently. With $\widehat{x} = x/|x|$ for $x \in \mathbb{R}^3 \setminus \{0\}$ and $q = 2r/(1+r^2)$ we have for the numerator in the last term of (4.5.22)

$$\begin{aligned} \left|x_j+r\left|x_j\right|\omega\right|^s = \left|x_j\right|^s (\hat{x}_j+r\omega)^s &= \left|x_j\right|^s (1+r^2+2r\hat{x}_j\cdot\omega)^{s/2} \\ &= \left|x_j\right|^s (1+r^2)^{s/2} (1+q\hat{x}_j\cdot\omega)^{s/2} . \end{aligned} \tag{4.5.23}$$

Set for $t \in [-1,1]$ and $d \in \mathbb{R}$

$$F(t) \coloneqq (1+qt)^{s/2}, \quad H_d(t) \coloneqq F(t) - d(t^2-1) \tag{4.5.24}$$

We determine $d \in \mathbb{R}$ depending on $q, s \in \mathbb{R}$ such that H is convex. Note that $H_d'' = F'' - 2d$. Consequently, to ensure the convexity of H_d, we need

$$d \leq \frac{1}{2}F''(t) = \frac{s}{4}\left(\frac{s}{2}-1\right) q^2 (1+qt)^{\frac{s-4}{2}} \leq \frac{s}{4}\left(\frac{s}{2}-1\right) q^2 (1+q)^{\frac{s-4}{2}} .$$

We fix

$$d_0 \coloneqq \frac{s}{4}\left(\frac{s}{2}-1\right) q^2 (1+q)^{\frac{s-4}{2}} \tag{4.5.25}$$

such that H_{d_0} is convex. Due to the convexity of H_{d_0} we have

$$H_{d_0}(t) \leq \frac{H_{d_0}(1)-H_{d_0}(-1)}{2} t + \frac{H_{d_0}(1)+H_{d_0}(-1)}{2} .$$

Since $H_{d_0} = F(t) - d_0(t^2-1)$ this yields

$$F(t) \leq \frac{F(1)-F(-1)}{2} t + \frac{F(1)+F(-1)}{2} + d_0(t^2-1) \tag{4.5.26}$$

Inserting $F(t) = (1 + qt)^{s/2}$ and d_0 from (4.5.25) into (4.5.26) we arrive at

$$\begin{aligned}(1+qt)^{s/2} \leq & \frac{(1+q)^{s/2} - (1-q)^{s/2}}{2} t + \frac{(1+q)^{s/2} + (1-q)^{s/2}}{2} \\ & + \frac{s}{4}\left(\frac{s}{2} - 1\right) q^2 (1+q)^{\frac{s-4}{2}} (t^2 - 1) \,.\end{aligned} \tag{4.5.27}$$

Combining (4.5.22), (4.5.23) and (4.5.27) yields

$$\begin{aligned}&\sum_{j \neq k} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|x|^s + |y|^s}{2|x-y|} d\mu_j(x) d\mu_k(y) \\ &\leq (1+r^2)^{s/2} \frac{(1+q)^{s/2} - (1-q)^{s/2}}{2} \sum_{j \neq k} \left|x_j\right|^s \int_{S^2} \frac{\hat{x}_j \cdot \omega}{\left|x_j - x_k + r\left|x_j\right|\omega\right|} \frac{d\omega}{4\pi} \\ &\quad + (1+r^2)^{s/2} \frac{(1+q)^{s/2} + (1-q)^{s/2}}{2} \sum_{j \neq k} \left|x_j\right|^s \int_{S^2} \frac{1}{\left|x_j - x_k + r\left|x_j\right|\omega\right|} \frac{d\omega}{4\pi} \\ &\quad + (1+r^2)^{s/2} \frac{s}{4}\left(\frac{s}{2} - 1\right) q^2 (1+q)^{\frac{s-4}{2}} \sum_{j \neq k} \left|x_j\right|^s \int_{S^2} \frac{(\hat{x}_j \cdot \omega)^2 - 1}{\left|x_j - x_k + r\left|x_j\right|\omega\right|} \frac{d\omega}{4\pi} \,.\end{aligned} \tag{4.5.28}$$

We proceed by estimating each of the summands in the right–hand side of (4.5.28) independently. We begin by showing that the first summand is negative. Let $a_{jk} := (x_k - x_j)/\left|x_j\right|$ then

$$\left|x_j\right|^s \int_{S^2} \frac{\hat{x}_j \cdot \omega}{\left|x_j - x_k + r\left|x_j\right|\omega\right|} \frac{d\omega}{4\pi} = \left|x_j\right|^{s-1} \int_{S^2} \frac{\hat{x}_j \cdot \omega}{\left|a_{jk} - r\omega\right|} \frac{d\omega}{4\pi} \tag{4.5.29}$$

which either can be solved in polar coordinates directly or using multipol expansion, that is, expanding the Coulomb–kernel in terms of the Legendre Polynomials $P_l(t)$, $l \in \mathbb{N}_0$. Using the generating function

$$(1 + \delta^2 - 2\delta t)^{-1/2} = \sum_{n=0}^{\infty} \delta^n P_n(t)$$

which is valid for $|t| \leq 1$ and $|\delta| < 1$. We can always assume that $r \neq \left|a_{jk}\right|$ since otherwise we replace r with $r_\varepsilon = r + \varepsilon$ and take the limit $\varepsilon \to 0$ after solving the integral. Expanding $\left|a_{jk} - r\omega\right|^{-1}$ yields

$$\left|a_{jk} - r\omega\right|^{-1} = \sum_{n=0}^{\infty} \frac{\min\{\left|a_{jk}\right|, r\}^n}{\max\{\left|a_{jk}\right|, r\}^{n+1}} P_n(\omega \cdot \hat{a}_{jk}) \,. \tag{4.5.30}$$

Using $P_1(\hat{x}_j \cdot \omega) = \hat{x}_j \cdot \omega$ and inserting (4.5.30) into (4.5.29) we arrive at

$$
\begin{aligned}
&|x_j|^s \int_{S^2} \frac{\hat{x}_j \cdot \omega}{|x_j - x_k + r|x_j|\omega|} \frac{d\omega}{4\pi} \\
&\quad = |x_j|^{s-1} \int_{S^2} \sum_{n=0}^{\infty} \frac{\min\{|a_{jk}|, r\}^n}{\max\{|a_{jk}|, r\}^{n+1}} P_n(\omega \cdot \hat{a}_{jk}) P_1(\hat{x}_j \cdot \omega) \frac{d\omega}{4\pi} \\
&\quad = |x_j|^{s-1} \sum_{n=0}^{\infty} \frac{\min\{|a_{jk}|, r\}^n}{\max\{|a_{jk}|, r\}^{n+1}} \int_{S^2} P_n(\omega \cdot \hat{a}_{jk}) P_1(\hat{x}_j \cdot \omega) \frac{d\omega}{4\pi} \,.
\end{aligned}
\tag{4.5.31}
$$

Legendre Polynomials are orthogonal in the following sense

$$
\int_{-1}^{1} P_n(t) P_m(t)\, dt = \frac{2\delta_{mn}}{2n+1}, \tag{4.5.32}
$$

and consequently, by the Funk-Hecke formula in Lemma A.2.1, we arrive at

$$
\int_{S^2} P_n(\hat{x}_j \cdot \omega) P_m(\omega \cdot \hat{a}_{jk}) \frac{d\omega}{4\pi} = \frac{\delta_{mn}}{2n+1} \,. \tag{4.5.33}
$$

Inserting (4.5.33) into (4.5.31) we arrive at

$$
\begin{aligned}
&|x_j|^s \int_{S^2} \frac{\hat{x}_j \cdot \omega}{|x_j - x_k + r|x_j|\omega|} \frac{d\omega}{4\pi} \\
&\quad = |x_j|^{s-1} \frac{\min\{|a_{jk}|, r\}}{\max\{|a_{jk}|, r\}^2} \frac{\hat{a}_{jk} \cdot \hat{x}_j}{3} \\
&\quad = -|x_j|^{s-1} \frac{\min\{|a_{jk}|, r\}}{\max\{|a_{jk}|, r\}^2} \frac{(x_j - x_k) \cdot \hat{x}_j}{3|x_k - x_j|} \\
&\quad = -|x_j|^{s} \frac{\min\{|x_j - x_k|, r|x_j|\}}{\max\{|x_j - x_k|, r|x_j|\}^2} \frac{1}{3|x_k - x_j|} (x_j - x_k) \cdot \hat{x}_j \\
&\quad = -r^{-s} \gamma\left(|x_j - x_k|, r|x_j|\right) (x_j - x_k) \cdot \hat{x}_j
\end{aligned}
\tag{4.5.34}
$$

with

$$
\gamma(u, v) = \frac{v^s \min(u, v)}{3u \max(u, v)^2} \,. \tag{4.5.35}
$$

for $u, v > 0$. Summing (4.5.31) over $j \neq k$ yields

$$
\sum_{j \neq k} |x_j|^s \int_{S^2} \frac{\hat{x}_j \cdot \omega}{|x_j - x_k + r|x_j|\omega|} \frac{d\omega}{4\pi} = -r^{-s} \sum_{j \neq k} \gamma\left(|x_j - x_k|, r|x_j|\right) (x_j - x_k) \cdot \hat{x}_j \,. \tag{4.5.36}
$$

Applying Lemma 4.5.7 and noting Remark 4.5.8 we find

$$\sum_{j\neq k}\gamma(|x_j-x_k|,r|x_j|)\,\widehat{x}_j\cdot(x_j-x_k)\geq 0\,.$$

Thus, the first summand in the right–hand side of (4.5.28) is not positive and consequently

$$\begin{aligned}&\sum_{j\neq k}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|x|^s+|y|^s}{2|x-y|}d\mu_j(x)d\mu_k(y)\\ \leq\;&(1+r^2)^{s/2}\frac{(1+q)^{s/2}+(1-q)^{s/2}}{2}\sum_{j\neq k}|x_j|^s\int_{S^2}\frac{1}{|x_j-x_k+r|x_j|\omega|}\frac{d\omega}{4\pi}\\ &+(1+r^2)^{s/2}\frac{s}{4}\left(\frac{s}{2}-1\right)q^2(1+q)^{\frac{s-4}{2}}\sum_{j\neq k}|x_j|^s\int_{S^2}\frac{(\hat{x}_j\cdot\omega)^2-1}{|x_j-x_k+r|x_j|\omega|}\frac{d\omega}{4\pi}\,.\end{aligned}\tag{4.5.37}$$

The first integral in the right–hand side of (4.5.37) can be solved since due to Newton's theorem

$$\int_{S^2}\frac{1}{|x_j-x_k+r|x_j|\omega|}\frac{d\omega}{4\pi}=\frac{1}{\max\{|x_j-x_k|,r|x_j|\}}\,.\tag{4.5.38}$$

Inserting (4.5.38) into (4.5.37) yields

$$\begin{aligned}&\sum_{j\neq k}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|x|^s+|y|^s}{2|x-y|}d\mu_j(x)d\mu_k(y)\\ \leq\;&(1+r^2)^{s/2}\frac{(1+q)^{s/2}+(1-q)^{s/2}}{2}\sum_{j\neq k}\frac{|x_j|^s}{\max\{|x_j-x_k|,r|x_j|\}}\\ &+(1+r^2)^{s/2}\frac{s}{4}\left(\frac{s}{2}-1\right)q^2(1+q)^{\frac{s-4}{2}}\sum_{j\neq k}|x_j|^s\int_{S^2}\frac{(\hat{x}_j\cdot\omega)^2-1}{|x_j-x_k+r|x_j|\omega|}\frac{d\omega}{4\pi}\,.\end{aligned}\tag{4.5.39}$$

Next, we estimate the remaining integral on the right–hand side of (4.5.39). In particular we aim to solve

$$|x_j|^s\int_{S^2}\frac{(\hat{x}_j\cdot\omega)^2-1}{|x_j-x_k+r|x_j|\omega|}\frac{d\omega}{4\pi}=|x_j|^{s-1}\int_{S^2}\frac{(\hat{x}_j\cdot\omega)^2-1}{|a_{jk}-r\omega|}\frac{d\omega}{4\pi}\,.\tag{4.5.40}$$

We use

$$\frac{2}{3}P_2(t)-\frac{2}{3}=t^2-1,\quad\forall t\in[-1,1],\tag{4.5.41}$$

where P_2 is the second–order Legendre polynomial. Inserting (4.5.41) into (4.5.40) we find

$$\begin{aligned}|x_j|^s \int_{S^2} \frac{(\hat{x}_j\cdot\omega)^2-1}{|x_j-x_k+r|x_j|\omega|}\frac{d\omega}{4\pi} &= \frac{2}{3}|x_j|^{s-1}\int_{S^2}\frac{P_2(\hat{x}_j\cdot\omega)-1}{|a_{jk}-r\omega|}\frac{d\omega}{4\pi}\\ &= \frac{2}{3}|x_j|^{s-1}\left(\int_{S^2}\frac{P_2(\hat{x}_j\cdot\omega)}{|a_{jk}-r\omega|}\frac{d\omega}{4\pi}-\frac{1}{\max\{|a_{jk}|,r\}}\right).\end{aligned} \tag{4.5.42}$$

Where we have used Newton's theorem. To solve the integral involving the Legendre polynomial P_2 we use the multipole expansion in (4.5.30) and (4.5.33) to find

$$\begin{aligned}\int_{S^2}\frac{P_2(\hat{x}_j\cdot\omega)}{|a_{jk}-r\omega|}\frac{d\omega}{4\pi} &= \sum_{n=0}^{\infty}\frac{\min\{|a_{jk}|,r\}^n}{\max\{|a_{jk}|,r\}^{n+1}}\int_{S^2}P_n(\omega\cdot\hat{a}_{jk})P_2(\hat{x}_j\cdot\omega)\frac{d\omega}{4\pi}\\ &= \frac{\min\{|a_{jk}|,r\}^2}{\max\{|a_{jk}|,r\}^3}\frac{P_2(\hat{a}_{jk}\cdot\omega)}{5}\le\frac{1}{5\max\{|a_{jk}|,r\}}.\end{aligned} \tag{4.5.43}$$

Using $|a_{jk}|=|x_j-x_k|/|x_j|$ and inserting (4.5.43) into (4.5.42) shows

$$|x_j|^s\int_{S^2}\frac{(\hat{x}_j\cdot\omega)^2-1}{|x_j-x_k+r|x_j|\omega|}\frac{d\omega}{4\pi}\le\frac{-8}{15}\frac{|x_j|^s}{\max\{|x_j-x_k|,r|x_j|\}}. \tag{4.5.44}$$

Combining (4.5.39) and (4.5.44) we arrive at

$$\begin{aligned}&\sum_{j\neq k}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|x|^s+|y|^s}{2|x-y|}d\mu_j(x)d\mu_k(y)\\ &\le\ (1+r^2)^{s/2}\frac{(1+q)^{s/2}+(1-q)^{s/2}}{2}\sum_{j\neq k}\frac{|x_j|^s}{\max\{|x_j-x_k|,r|x_j|\}}\\ &\quad-\frac{8}{15}(1+r^2)^{s/2}\frac{s}{4}\left(\frac{s}{2}-1\right)q^2(1+q)^{\frac{s-4}{2}}\sum_{j\neq k}\frac{|x_j|^s}{\max\{|x_j-x_k|,r|x_j|\}}\\ &=\underbrace{(1+r^2)^{s/2}\left(\frac{(1+q)^{s/2}+(1-q)^{s/2}}{2}-\frac{s\,(s-2)}{15}q^2(1+q)^{\frac{s-4}{2}}\right)}_{=:g(r)}\sum_{j\neq k}\frac{|x_j|^s}{\max\{|x_j-x_k|,r|x_j|\}}.\end{aligned}$$

Using $q=2r/(1+r^2)$ one checks by direct computations that $g(r)\ge 0$. Consequently, we find

$$\sum_{j\neq k}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|x|^s+|y|^s}{2|x-y|}d\mu_j(x)d\mu_k(y)\le g(r)\sum_{j\neq k}\frac{|x_j|^s+|x_k|^s}{2|x_j-x_k|}. \tag{4.5.45}$$

Combining the estimates of the diagonal terms (4.5.20) and the off–diagonal terms (4.5.45) together with (4.5.7) yields

$$N^2 I_s(\mu) \leq \frac{(1+r)^{s+2} - |1-r|^{s+2}}{2r^2(s+2)} \sum_{j=1}^{N} \left|x_j\right|^{s-1} + g(r) \sum_{j\neq k} \frac{\left|x_j\right|^s + |x_k|^s}{2\left|x_j - x_k\right|} . \tag{4.5.46}$$

Applying Lemma A.2.2 we also get

$$N \int |x|^{s-1} d\mu(x) = \sum_{j=1}^{N} |x|^{s-1} d\mu_j(x) = \frac{(1+r)^{s+1} - |1-r|^{s+1}}{2r(s+1)} \sum_{j=1}^{N} \left|x_j\right|^{s-1} . \tag{4.5.47}$$

Combining (4.5.46) and (4.5.47) shows

$$\begin{aligned} N\beta_s &\leq \frac{N^2 I_s(\mu)}{N \int |x|^{s-1} d\mu(x)} \\ &\leq \frac{1}{r} \left(\frac{s+1}{s+2}\right) \frac{(1+r)^{s+2} - |1-r|^{s+2}}{(1+r)^{s+1} - |1-r|^{s+1}} \\ &\quad + \frac{2r(s+1)g(r)}{(1+r)^{s+1} - |1-r|^{s+1}} \frac{\sum_{1\leq j<k\leq N} \frac{\left|x_j\right|^s + |x_k|^s}{2\left|x_j - x_k\right|}}{\sum_{j=1}^N \left|x_j\right|^{s-1}} . \end{aligned} \tag{4.5.48}$$

Taking the infimum over the positions $x_1, x_2, \ldots x_N \in A_0$ together with the definition of $\alpha_{N,s}$ in (4.5.3) we conclude from (4.5.48)

$$N\beta_s \leq \frac{1}{r} \left(\frac{s+1}{s+2}\right) \frac{(1+r)^{s+2} - |1-r|^{s+2}}{(1+r)^{s+1} - |1-r|^{s+1}} + \frac{2r(s+1)g(r)}{(1+r)^{s+1} - |1-r|^{s+1}} \alpha_{N,s}(N-1) \tag{4.5.49}$$

and equivalently

$$\left(\frac{s+2}{s+1}\right) \frac{(1+r)^{s+1} - |1-r|^{s+1}}{(1+r)^{s+2} - |1-r|^{s+2}} N\beta_s - \frac{1}{r} \leq \frac{2r(s+2)g(r)}{(1+r)^{s+2} - |1-r|^{s+2}} \alpha_{N,s}(N-1) .$$

This completes the proof of Lemma 4.5.5. ∎

For small r, one can find a better bound than the one in Lemma 4.5.5 by estimating more carefully and not using convexity. But the argument is much more involved. However, since we are interested in bounds for small $r > 0$, in order to make the prefactor in (4.5.17) close to one, we will give this improved bound now.

Lemma 4.5.9 (Refined comparison II of $\alpha_{N,s}$ with β_s, $4 \geq s \geq 2$)**.** *Let $\alpha_{N,s}$ and β_s be defined as in* (4.5.1) *and* (4.4.1) *then for every $N \geq 2$, $r > 0$, and $4 \geq s \geq 2$*

$$\frac{(1+r)^{s+1} - (1-r)^{s+1}}{2r(s+1)} N\beta_s \leq \frac{(1+r)^{s+2} - (1-r)^{s+2}}{2r(s+2)} \left(\alpha_{N,s}(N-1) + \frac{1}{r}\right) + r^2 f(r,s)\alpha_{N,s}(N-1) \tag{4.5.50}$$

with

$$f(r,s) := \frac{s}{2}\left(\frac{s}{2} - 1\right)\left(\frac{4}{15} + \left(2 - \frac{s}{2}\right)\frac{8}{105}r + \left(2 - \frac{s}{2}\right)\frac{448}{625}r^2\right). \tag{4.5.51}$$

In particular, for $s = 3$ this gives

$$(1+r^2)N\beta_3 - \frac{1 + 2r^2 + r^4/5}{r} \leq \alpha_{N,3}(N-1)\left(1 + \frac{r^2}{5} + \frac{r^3}{35} + \frac{168}{625}r^4\right). \tag{4.5.52}$$

Remark 4.5.10. *Note that $f(r,2)$ vanishes for all $r > 0$, and for $s \in (2,3]$, it adds a positive correction to the leading order term in the prefactor of $\alpha_{N,s}$. For later usage, we note that one has the rough estimate $f(r,s) \leq f(r,3) < \frac{1}{2}$ for $r \in [0,1]$ any $s \in (2,3]$.*

Proof. We again use the bounds (4.5.7) together with (4.5.21) and (4.5.22). In order to improve on Lemma 4.5.5, we have to bound the integral in the last sum of (4.5.22) more carefully. Recalling $a_{jk} = (x_k - x_j)/|x_j|$ and $\widehat{x}_j = x_j/|x_j|$ we can rewrite

$$\int_{S^2} \frac{|x_j + r|x_j|\omega|^s}{|x_j - x_k + r|x_j|\omega|} \frac{d\omega}{4\pi} = |x_j|^{s-1} \int_{S^2} \frac{(1 + r^2 + 2r\hat{x}_j \cdot \omega)^{s/2}}{|a_{jk} - r\omega|} \frac{d\omega}{4\pi}. \tag{4.5.53}$$

Such integrals can be solved by multipole expansion, that is, expanding the Coulomb–kernel in terms of the Legendre Polynomials $P_l(t)$, $l \in \mathbb{N}_0$. Using the generating function

$$(1 + \delta^2 - 2\delta t)^{-1/2} = \sum_{n=0}^{\infty} \delta^n P_n(t) \tag{4.5.54}$$

which is valid for $|t| \leq 1$ and $|\delta| < 1$, and expanding $|a_{jk} - r\omega|^{-1}$ in (4.5.53) with the help of (4.5.54) and using Lemma A.2.1 yields

$$\begin{aligned} &|x_j|^{s-1} \int_{S^2} \frac{(1 + r^2 + 2r\hat{x}_j \cdot \omega)^{s/2}}{|a_{jk} - r\omega|} \frac{d\omega}{4\pi} \\ &= |x_j|^{s-1} \sum_{l=0}^{\infty} \frac{\min(|a_{jk}|, r)^l}{\max(|a_{jk}|, r)^{l+1}} \int_{S^2} (1 + r^2 + 2r\hat{x}_j \cdot \omega)^{s/2} P_l(\langle \hat{a}_{jk}, \omega \rangle) \frac{d\omega}{4\pi} \\ &= |x_j|^{s-1} \sum_{l=0}^{\infty} \frac{\min(|a_{jk}|, r)^l}{\max(|a_{jk}|, r)^{l+1}} \lambda_{l,s}(r) P_l(\hat{a}_{jk} \cdot \hat{x}_j) \end{aligned} \tag{4.5.55}$$

with

$$\lambda_{l,s}(r) = \frac{1}{2}\int_{-1}^{1}(1+r^2+2rt)^{s/2}P_l(t)dt\,.$$

We will see shortly that the sum $\sum_{l=0}^{\infty}\left|\lambda_{l,s}(r)\right|$ converges – see (4.5.68) – so the series in the last line of (4.5.55) converges for all $r > 0$ since $-1 \leq P_l(t) \leq 1$ for $-1 \leq t \leq 1$.
Using $P_0(t) \equiv 1$ the first multipole moment $l = 0$ is easy to compute,

$$\lambda_{0,s}(r) = \frac{(1+r)^{s+2}-(1-r)^{s+2}}{2(s+2)r}\,. \tag{4.5.56}$$

Note that with $P_1(t) = t$ and consequently the second multipole moment is positive non–negative since

$$\lambda_{1,s}(r) = \frac{1}{2}\int_{-1}^{1}(1+r^2+2rt)^{s/2}t\,dt > 0\,. \tag{4.5.57}$$

The calculation for higher moments is a bit involved. Before we embark on this, let us note that if $\sum_{l\geq 0}\lambda_{l,s}(r)$ converges absolutely, we can further bound (4.5.55) as follows.

$$\begin{aligned}
&\left|x_j\right|^{s-1}\sum_{l=0}^{\infty}\frac{\min(\left|a_{jk}\right|,r)^l}{\max(\left|a_{jk}\right|,r)^{l+1}}\lambda_{l,s}(r)P_l\left(\hat{a}_{jk}\cdot\hat{x}_j\right)\\
&\quad\leq \lambda_{0,s}(r)\frac{\left|x_j\right|^{s-1}}{\max(\left|a_{jk}\right|,r)} + \lambda_{1,s}(r)\frac{\left|x_j\right|^{s-1}\min(\left|a_{jk}\right|,r)}{\max(\left|a_{jk}\right|,r)^2}\left(\hat{a}_{jk}\cdot\hat{x}_j\right)\\
&\qquad + \frac{\left|x_j\right|^{s-1}}{\max(\left|a_{jk}\right|,r)}\sum_{l=2}^{\infty}\left|\lambda_{l,s}(r)\right|.
\end{aligned}$$

Using $a_{jk} = (x_k - x_j)/\left|x_j\right|$ we arrive at

$$\begin{aligned}
&\left|x_j\right|^{s-1}\sum_{l=0}^{\infty}\frac{\min(\left|a_{jk}\right|,r)^l}{\max(\left|a_{jk}\right|,r)^{l+1}}\lambda_{l,s}(r)P_l\left(\hat{a}_{jk}\cdot\hat{x}_j\right)\\
&\quad\leq\left(\lambda_{0,s}(r)+\sum_{l=2}^{\infty}\left|\lambda_{l,s}(r)\right|\right)\frac{\left|x_j\right|^s}{\left|x_j-x_k\right|}-\\
&\qquad\lambda_{1,s}(r)\frac{\left|x_j\right|^s\min(\left|x_j-x_k\right|,r\left|x_j\right|)}{\left|x_j-x_k\right|\max(\left|x_j-x_k\right|,r\left|x_j\right|)^2}\hat{x}_j\cdot(x_j-x_k)\,.
\end{aligned}$$

Let $C_s(r) = \sum_{l=2}^{\infty}\left|\lambda_{l,s}(r)\right|$ and

$$\widetilde{\gamma}(u,v) = \frac{v^s\min(u,v)}{u\max(u,v)^2},$$

then

$$\left|x_j\right|^{s-1}\sum_{l=0}^{\infty}\frac{\min(\left|a_{jk}\right|,r)^l}{\max(\left|a_{jk}\right|,r)^{l+1}}\lambda_{l,s}(r)P_l\big(\hat{a}_{jk}\cdot\hat{x}_j\big)$$
$$\leq \big(\lambda_{0,s}(r)+C_s(r)\big)\,\frac{\left|x_j\right|^s}{\left|x_j-x_k\right|}-\lambda_{1,s}(r)r^{-s}\widetilde{\gamma}(\left|x_j-x_k\right|,r\left|x_j\right|)\,\hat{x}_j\cdot(x_j-x_k)\,.$$

Note that $\widetilde{\gamma}(u,v)$ is increasing in v for fixed $u>0$. Applying Lemma 4.5.7 and noting Remark 4.5.8 we find

$$\sum_{j\neq k}\widetilde{\gamma}(\left|x_j-x_k\right|,r\left|x_j\right|)\,\widehat{x}_j\cdot\big(x_j-x_k\big)\geq 0\,. \tag{4.5.58}$$

As in (4.5.22) one sees

$$\sum_{j\neq k}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|x|^s+|x|^s}{2|x-y|}d\mu_j(x)d\mu_k(y)$$
$$\leq \big(\lambda_{0,s}(r)+C_s(r)\big)\sum_{j\neq k}\frac{\left|x_j\right|^s}{\left|x_j-x_k\right|}-\lambda_{1,s}(r)r^{-s}\sum_{j\neq k}\widetilde{\gamma}(\left|x_j-x_k\right|,r\left|x_j\right|)\,\hat{x}_j\cdot(x_j-x_k)$$
$$\leq \big(\lambda_{0,s}(r)+C_s(r)\big)\sum_{j\neq k}\frac{\left|x_j\right|^s+\left|x_j\right|^s}{2\left|x_j-x_k\right|}$$

where we used (4.5.58) to drop the second sum. In the last line, we symmetrized the remaining expression. Thus we get a similar bound as (4.5.45), with $g(r)$ replaced by $\lambda_{0,s}(r)+C_s(r)$. Thus, as in the proof of Lemma 4.5.5, a bound similar to (4.5.46), but with $g(r)$ in (4.5.46) replaced by $\lambda_{0,s}(r)+C_s(r)$, follows from this. In particular, it follows

$$\left(\frac{s+2}{s+1}\right)\frac{(1+r)^{s+1}-|1-r|^{s+1}}{(1+r)^{s+2}-|1-r|^{s+2}}N\beta_s-\frac{1}{r}\leq\left(1+\frac{2r(s+2)C_s(r)}{(1+r)^{s+2}-|1-r|^{s+2}}\right)\alpha_{N,s}(N-1)\,. \tag{4.5.59}$$

Hence the claimed bound (4.5.50) follows as soon as we can show that

$$C_s(r)\leq r^2 f(r,s) \tag{4.5.60}$$

with f given in (4.5.51). We will do this in the rest of this proof.

To get a grip on the higher order moments $\lambda_{l,s}(r)$ for $l\geq 2$ we expand $\left|\hat{x}_j+r\omega\right|^s$ in a binomial series. With $t=\widehat{x}_j\cdot\omega$ and

$$q=2r/(1+r^2)\leq 1 \tag{4.5.61}$$

we have

$$\big(1+r^2+2rt\big)^{s/2}=\big(1+r^2\big)^{s/2}\big(1+qt\big)^{s/2}=\big(1+r^2\big)^{s/2}\sum_{n=0}^{\infty}\binom{s/2}{n}q^nt^n\,. \tag{4.5.62}$$

According to [35, Satz 22.8] the binomial series converges absolutely and uniformly for $-1 \le t \le 1$ and all $0 \le q \le 1$. Hence, we can interchange the summation and integration in (4.5.55) to see that

$$\lambda_{l,s}(r) = (1+r^2)^{s/2} \sum_{n=0}^{\infty} \binom{s/2}{n} q^n \frac{1}{2} \int_{-1}^{1} t^n P_l(t)dt \quad l \ge 2\,. \tag{4.5.63}$$

Write

$$t^n = \sum_{m=0}^{n} c_{n,m} P_m(t) \quad \text{for } t \in [-1,1]\,. \tag{4.5.64}$$

Using that the Legendre polynomials are orthogonal in $L^2([-1,1])$ and normalized by $\frac{1}{2}\int_{-1}^{1} P_l(t)^2 dt = \frac{1}{2l+1}$, and P_l has degree l, one sees that $\int_{-1}^{1} t^n P_l(t)dt = 0$ if $n < l$ and for $n \ge l$ we have $\frac{1}{2}\int_{-1}^{1} t^n P_l(t)dt = \frac{c_{n,l}}{1l+1}$. Thus

$$\lambda_{l,s}(r) = (1+r^2)^{s/2} \sum_{n=l}^{\infty} \binom{s/2}{n} \frac{q^n c_{n,l}}{2l+1}, \quad l \ge 2\,. \tag{4.5.65}$$

We will use that the coefficients $c_{n,l}$ for $n, l \in \mathbb{N}_0$ are non–negative, see (A.2.6) in Appendix A. Moreover,

$$\sum_{m=0}^{n} c_{n,m} = 1\,,$$

which follows from setting $t = 1$ in (4.5.64) and using $P_l(1) = 1$ for $l \in \mathbb{N}_0$. Together with $c_{n,m} \ge 0$, this also shows $c_{n,m} \le 1$. From [35, Hilfssatz 22.8a] we have the bound

$$\left| \binom{s/2}{n} \right| \le \frac{c}{n^{1+s/2}}\,. \tag{4.5.66}$$

This implies that the series on the right–hand–side of (4.5.65) converges absolutely for all $0 \le q \le 1$, since $0 \le c_{n,l} \le 1$ and hence

$$\sum_{n=l}^{\infty} \left| \binom{s/2}{n} \right| \frac{q^n c_{n,l}}{2l+1} \lesssim \sum_{n=l}^{\infty} \frac{1}{2l+1} \frac{1}{n^{1+s/2}} < \infty \tag{4.5.67}$$

for any $s > 0$. Moreover, we also have

$$\begin{aligned} \sum_{l\ge 2} \left|\lambda_{l,s}(r)\right| &\le (1+r^2)^{s/2} \sum_{l=2}^{\infty}\sum_{n=l}^{\infty} \left| \binom{s/2}{n} \right| \frac{q^n c_{n,l}}{2l+1} \lesssim \sum_{l=2}^{\infty}\sum_{n=l}^{\infty} \frac{1}{n^{1+s/2}} \frac{1}{2l+1} \\ &= \sum_{n=2}^{\infty}\sum_{l=2}^{n} \frac{1}{n^{1+s/2}} \frac{1}{2l+1} \lesssim \sum_{n=2}^{\infty} \frac{\ln(2+n)}{n^{1+s/2}} < \infty\,. \end{aligned} \tag{4.5.68}$$

For $n \in \mathbb{N}$ define

$$A_n := \left|\binom{s/2}{n}\right| \sum_{l=2}^{n} \frac{c_{n,l}}{2l+1}.$$

We have

$$\sum_{l=2}^{\infty} \left|\lambda_{l,s}(r)\right| \leq (1+r^2)^{s/2} \sum_{l=2}^{\infty} \sum_{n=l}^{\infty} \left|\binom{s/2}{n}\right| \frac{c_{n,l}}{2l+1} q^n = (1+r^2)^{s/2} \sum_{n=2}^{\infty} A_n q^n. \tag{4.5.69}$$

Since $q = 2r/(1+r^2)$ (see (4.5.61)) we get

$$\sum_{n=2}^{\infty} A_n q^n \leq \frac{4r^2}{\left(1+r^2\right)^2} A_2 + \frac{8r^3}{\left(1+r^2\right)^3} A_3 + \frac{16r^4}{\left(1+r^2\right)^4} \sum_{n=4}^{\infty} A_n. \tag{4.5.70}$$

In Lemma A.2.4 in Appendix A we show that

$$A_2 = \left|\binom{s/2}{2}\right| \frac{2}{15}, \quad A_3 = \left|\binom{s/2}{3}\right| \frac{2}{35}, \quad \sum_{k=4}^{\infty} A_k \leq \frac{s}{2}\left(\frac{s}{2}-1\right)\left(2-\frac{s}{2}\right)\frac{28}{625}.$$

It follows that

$$\sum_{k=2}^{\infty} A_k q^k \leq \frac{r^2}{\left(1+r^2\right)^2} f(r,s). \tag{4.5.71}$$

with f defined in (4.5.51). Combining (4.5.71) with (4.5.69) proves for $s \leq 4$

$$C_s(r) = \sum_{l=2}^{\infty} \left|\lambda_{l,s}(r)\right| \leq (1+r^2)^{(s-4)/2} r^2 f(r,s) \leq r^2 f(r,s). \tag{4.5.72}$$

This proves (4.5.60), which finishes the proof of Lemma 4.5.9. ∎

Remark 4.5.11. *We truncate the series in* (4.5.70) *at the fourth power because we will later choose $r \lesssim Z^{-1/3}$. As a result, even terms like Zr^4 become negligible as Z increases. For further refinements at small Z respectively large r, it is more appropriate to evaluate the inequality using computational methods.*

4.6 Upper Bounds on the Weighted Kinetic Energy

In this section, we derive an upper bound on

$$Z - \frac{1}{2} \frac{\left\langle |x_1|^s \psi_{N,Z}, P_1^2 \psi_{N,Z} \right\rangle}{\left\langle |x_1|^{s-1} \psi_{N,Z}, \psi_{N,Z} \right\rangle} \tag{4.6.1}$$

which is the right–hand side of (4.3.10). Note that

$$\left\langle |x_1|^s \psi_{N,Z}, P_1^2 \psi_{N,Z} \right\rangle = \int_{\mathbb{R}^{3(N-1)}} \langle |x_1|^s \psi_{N,Z}, P_1^2 \psi_{N,Z} \rangle_{L^2(dx_1)} dx_2 \ldots dx_N \,.$$

In the case $s = 1$ Lieb used in [71] the fact that

$$\langle \varphi, (\Phi^{-1}\Delta + \Delta\Phi^{-1})\varphi \rangle_{L^2(\mathbb{R}^3)} \leq 0 \tag{4.6.2}$$

for any $\varphi \in L^2(\mathbb{R}^3)$ if Φ is a non negativ superharmonic function (see [76, Lemma 12.2]). In particular this covers $\Phi(x) = |x|^{-1}$ and proves

$$Z - \frac{1}{2} \frac{\left\langle |x_1| \psi_{N,Z}, P_1^2 \psi_{N,Z} \right\rangle}{\left\langle \psi_{N,Z}, \psi_{N,Z} \right\rangle} \leq Z \,. \tag{4.6.3}$$

Remark 4.6.1. *Combining* (4.3.10) *and* (4.6.3) *together with* $\alpha_{N,1} \geq 1/2$ *recovers the bound* $N_c < 2Z + 1$.

In [24] Chen and Siedentop showed that in dimension $d = 3$ for any $b \in [0, 1]$

$$\langle \varphi, (|x|^b \Delta + \Delta |x|^b)\varphi \rangle \leq 0 \tag{4.6.4}$$

for any $\varphi \in L^2(\mathbb{R}^3)$. For $b > 1$ (4.6.4) does not hold in general. Before we proceed, let us clarify in what sense we understand the inner product in (4.6.1). Recall that $\psi_{N,Z} \in \mathcal{H}_N^f$ is the normalized many particle ground state of $H_{N,Z}$ in (4.2.1) and does depend on the positions of particles $(x_1, x_2, \ldots, x_n)$ and the spin degrees of freedom $(\sigma_1, \sigma_2, \ldots, \sigma_N)$ with $\sigma_i \in \{1/2, -1/2\}$. Following [76, Chapter 3] we define the one-particle density by

$$\rho_{\psi_{N,Z}}(x) := \sum_{i=1}^{N} \rho^i_{\psi_{N,Z}}(x)$$

where

$$\rho^i_{\psi_{N,Z}}(x) := \int_{\mathbb{R}^{3(N-1)}} |\psi(x_1, \ldots x_{i-1}, x, x_{i+1}, \ldots x_N)|^2 dx_1 \ldots \hat{dx_i} \ldots dx_N \,.$$

where $\hat{dx_i}$ means that the integration of x_i is omitted. Remember that we ignore any degrees of freedom related to spin. Due to (4.2.3) we have $\rho^i = \rho^1$ for any $i \in \{1, 2, \ldots, N\}$ and thus

$$\rho_{\psi_{N,Z}}(x_1) := N \rho^1_{\psi_{N,Z}}(x_1) \tag{4.6.5}$$

with

$$\int_{\mathbb{R}^3} \rho_{\psi_{N,Z}}(x_1)\, dx_1 = N \,.$$

Consequently for any $p \in \mathbb{R}$

$$\left\langle |x_1|^p \psi_{N,Z}, \psi_{N,Z} \right\rangle = \frac{1}{N} \int_{R^3} |x_1|^p \rho_{\psi_{N,Z}}(x_1)\, dx_1 \tag{4.6.6}$$

As a substitute for the negativity in (4.6.2), we prove

Lemma 4.6.2. *For any $s \geq 2$*

$$\frac{-1}{2} \frac{\left\langle |x_1|^s \psi_{N,Z}, P_1^2 \psi_{N,Z} \right\rangle}{\left\langle |x_1|^{s-1} \psi_{N,Z}, \psi_{N,Z} \right\rangle} \leq \frac{s^2-1}{8} \left\langle |x_1|^{s-1} \psi_{N,Z}, \psi_{N,Z} \right\rangle^{\frac{-1}{s-1}} . \tag{4.6.7}$$

Proof. We drop the indices N, Z for readability so that $\psi = \psi_{N,Z}$. Applying the IMS-localization formula, see for example [27, Theorem 3.2], yields

$$\begin{aligned}
\mathrm{Re}\langle |x_1|^s \psi, P_1^2 \psi \rangle_{L^2(dx_1)} &= \left\langle |x_1|^{s/2} \psi, \left[P_1^2 - \left| \frac{\nabla_1 |x_1|^s}{2|x_1|} \right|^2 \right] |x_1|^{s/2} \psi \right\rangle_{L^2(dx_1)} \\
&= \left\langle |x_1|^{s/2} \psi, \left[P_1^2 - \frac{s^2}{4} |x_1|^{-2} \right] |x_1|^{s/2} \psi \right\rangle_{L^2(dx_1)} \\
&\geq \frac{1-s^2}{4} \left\langle |x_1|^{s-2} \psi, \psi \right\rangle_{L^2(dx_1)} .
\end{aligned} \tag{4.6.8}$$

Due to (4.6.6) we have

$$\left\langle |x_1|^{s-2} \psi, \psi \right\rangle = \frac{1}{N} \int_{R^3} |x_1|^{s-2} \rho_\psi(x_1)\, dx_1 .$$

Applying Hölder's inequality for

$$p = \frac{s-1}{s-2},\ q = s-1$$

yields

$$\left\langle |x_1|^{s-2} \psi, \psi \right\rangle_{L^2(dx_1)} \leq \left(\frac{1}{N} \int_{\mathbb{R}^3} |x_1|^{s-1} \rho_\psi(x_1)\, dx_1 \right)^{\frac{s-2}{s-1}} = \left(\left\langle |x_1|^{s-1} \psi, \psi \right\rangle_{L^2(dx_1)} \right)^{\frac{s-2}{s-1}} .$$

Note that we used $s > 2$ in this step. To cover the cases $s \in (1, 2)$, one needs to estimate the expression above differently. Consequently

$$\frac{\left\langle |x_1|^{s-2} \psi, \psi \right\rangle_{L^2(dx_1)}}{\left\langle |x_1|^{s-1} \psi, \psi \right\rangle_{L^2(dx_1)}} \leq \left(\left\langle |x_1|^{s-1} \psi, \psi \right\rangle_{L^2(dx_1)} \right)^{\frac{-1}{s-1}} . \tag{4.6.9}$$

Combining (4.6.8) and (4.6.9) proves Lemma (4.6.2). The case $s = 2$ follows in the limit $s \to 2$. ∎

Remark 4.6.3. *There exists a straightforward simplification of the inequality in Lemma 4.6.2 since by Jensen's Inequality*

$$\left\langle |x_1|^{s-1}\psi_{N,Z}, \psi_{N,Z} \right\rangle^{\frac{-1}{s-1}} \leq \left\langle |x_1|^{-1}\psi_{N,Z}, \psi_{N,Z} \right\rangle \tag{4.6.10}$$

The right–hand side of (4.6.7) *is growing quadratic in s, which is unfortunate since the bound on $b(s)$ in Theorem 4.2.2 is decreasing. Note that the right–hand side of* (4.6.10) *can be interpreted as the inverse expectation of the radius of the atom, which in Thomas–Fermi Theory grows as $Z^{-1/3}$ (see [72, p. 560]) but should be bounded in Z for real atoms. In [81], Nam did control the right-hand side of* (4.6.10)*. We follow a similar approach to his proof.*

We continue by estimating the right–hand side of (4.6.7). We want to apply the following inequality introduced by Lieb in [72, p. 563]

$$\left(\int_{\mathbb{R}^3} f(x)^{\frac{5}{3}} dx\right)^{\frac{p}{2}} \int_{\mathbb{R}^3} |x|^p f(x) dx \geq C_p \left(\int_{\mathbb{R}^3} f(x) dx\right)^{1+\frac{5p}{6}} \tag{4.6.11}$$

which holds for any non negative measurable function f and $p \geq 0$ where the sharp constant C_p is attained for

$$f_p(x) := \begin{cases} (1 - |x|^p)^{\frac{3}{2}} & |x| \leq 1 \\ 0 & \text{elsewise} \end{cases} . \tag{4.6.12}$$

We give the explicit constant C_p in the Appendix in equation (A.3.1). We prove

Lemma 4.6.4. *Let $p \geq 0$ then*

$$\left(\frac{1}{N}\int_{\mathbb{R}^3} |x_1|^p \rho_{\psi_{N,Z}}(x_1)\, dx_1\right)^{-1/p} \leq \kappa C_p^{-1/p} Z N^{-2/3}$$

where $\kappa = \sqrt{5}\left(\frac{2}{9\pi^2}1.456\right)^{1/3}$ and C_p the constant in (4.6.11).

Proof. Applying (4.6.11) for $f = \rho_{\psi_{N,Z}}$ yields

$$\left(\frac{1}{N}\int_{\mathbb{R}^3} |x_1|^p \rho_{\psi_{N,Z}}(x_1) dx_1\right)^{-1/p} \leq C_p^{-1/p} N^{-5/6} \left(\int_{\mathbb{R}^3} \rho_{\psi_{N,Z}}(x_1)^{\frac{5}{3}} dx_1\right)^{\frac{1}{2}} .$$

By the fermionic kinetic energy inequality in [39, Theorem 1]

$$\frac{u^{\frac{-2}{3}}}{2} K_3 \int_{\mathbb{R}^3} \rho_{\psi_{N,Z}}(x)^{\frac{5}{3}} dx \leq \sum_{i=1}^{N} \frac{1}{2}\langle \psi_{N,Z}, [-\Delta_i]\psi_{N,Z}\rangle \tag{4.6.13}$$

with $K_3 = \frac{3}{5}\left(\frac{1.456}{6\pi^2}\right)^{-2/3} \approx 7.096$. Here, u denotes the degrees of freedom in the spin components. We consider spin $1/2$ particles (for example, electrons) and thus $u = 2$. By the quantum mechanic virial theorem (see [122], [7])

$$-E_{N,Z} = \sum_{i=1}^{N} \frac{1}{2} \langle \psi_{N,Z}, [-\Delta_i] \psi_{N,Z} \rangle \, . \tag{4.6.14}$$

Combining (4.6.13) and (4.6.14) for $u = 2$ we arrive at

$$\int_{\mathbb{R}^3} \rho_{\psi_{N,Z}}(x)^{\frac{5}{3}} dx_1 \le -\frac{2^{5/3}}{K_3} E_{N,Z} \, .$$

Together with

$$-E_{N,Z} \le A Z^2 N^{1/3}$$

for $A = (3/2)^{1/3}$ (see Lemma A.4.1) this yields

$$\begin{aligned} \left(\frac{1}{N} \int_{\mathbb{R}^3} |x_1|^p \rho_{\psi_{N,Z}}(x_1) dx_1 \right)^{-1/p} &\le C_p^{-1/p} \left(\frac{2^{5/3}}{K_3} A \right)^{1/2} Z N^{-2/3} \\ &= C_p^{-1/p} \sqrt{5} \left(\frac{2}{9\pi^2} 1.456 \right)^{1/3} Z N^{-2/3} \, . \end{aligned}$$

∎

Combining Lemma 4.6.7 and Lemma 4.6.4 we can prove

Lemma 4.6.5. *Let $s \ge 2$ then*

$$Z + \frac{1}{2} \frac{\left\langle |x_1|^s \psi_{N,Z}, \Delta_1 \psi_{N,Z} \right\rangle}{\left\langle |x_1|^{s-1} \psi_{N,Z}, \psi_{N,Z} \right\rangle} \le Z + \frac{s^2 - 1}{8} C_{s-1}^{-1/(s-1)} \kappa Z N^{-2/3} \tag{4.6.15}$$

with $\kappa = \sqrt{5} \left(\frac{2}{9\pi^2} 1.456 \right)^{1/3}$ and C_{s-1} the constant in (4.6.11).

Proof. The inequality (4.6.15) follows directly by combining Lemma 4.6.2 and Lemma 4.6.4. The fact that we can either apply Lemma 4.6.4 for $p = 1$ or $p = s - 1$ is due to Jensen's inequality as explained in Remark 4.6.3. An explicit calculation shows

$$\begin{aligned} C_1^{-1} &= \left(3^{\frac{5}{3}} 5^{\frac{5}{6}} \frac{\left(\frac{7}{\pi} \right)^{\frac{1}{3}}}{22\sqrt{11}} \right)^{-1} \approx 2.341 \ldots \\ C_2^{-1/2} &= 4 \frac{\pi^{2/3}}{\sqrt{15}} \approx 2.215 \ldots \end{aligned}$$

and $t \mapsto C_t^{-1/t}$ is decreasing. We give in Appendix Lemma A.3.1 the explicit constant C_p for any $p \in [1, 2]$. ∎

4.7 Bounds on Maximal Excess Charge

From Lemma 4.5.9 and Lemma 4.6.5, it is straightforward to prove the inequality in Theorem 4.2.2. We begin with the general inequality for $s \in [2, 3]$ before we discuss some refinements in the cases $s = 2$ and $s = 3$.

4.7.1 Main Theorem

Proof of Theorem 4.2.2. We aim to solve (4.5.50) namely

$$\begin{aligned} \frac{(1+r)^{s+1} - (1-r)^{s+1}}{2r(s+1)} N\beta_s \leq & \frac{(1+r)^{s+2} - (1-r)^{s+2}}{2r(s+2)} \left(\alpha_{N,s}(N-1) + \frac{1}{r} \right) \\ & + r^2 f(r,s) \alpha_{N,s}(N-1) \end{aligned} \tag{4.7.1}$$

for N. Note that the fraction on the left–hand side of (4.7.1) is positive for all $r > 0$ and $s > 0$ and consequently we can use the lower bound $b(s)^{-1}$ from Proposition 4.4.5 to bound the left–hand side β_s.
Direct computations show for $r \in [0, 1]$ and $p \geq 2$

$$2rp \leq (1+r)^p - (1-r)^p \,.$$

Consequently

$$\frac{2r(s+2)}{(r+1)^{s+2} - (1-r)^{s+2}} \leq 1$$

together with $f(r, s) < 1/2$

$$\frac{2r(s+2)}{(r+1)^{s+2} - (1-r)^{s+2}} r^2 f(r,s) \leq r^2 f(r,s) \leq \frac{r^2}{2} \,.$$

Consequently from 4.5.9 we conclude

$$\left(\frac{s+2}{s+1} \frac{(r+1)^{s+1} - (1-r)^{s+1}}{(r+1)^{s+2} - (1-r)^{s+2}} \frac{N}{b(s)} - \frac{1}{r} \right) \leq \alpha_{N,s}(N-1) \left(1 + \frac{r^2}{2} \right) . \tag{4.7.2}$$

We prove in the appendix as Lemma A.5.1 that for any $r \in (0, 1)$ and $s \geq 0$

$$\frac{s+2}{s+1} \frac{(r+1)^{s+1} - (1-r)^{s+1}}{(r+1)^{s+2} - (1-r)^{s+2}} \geq 1 - \frac{s}{3} r^2 \,. \tag{4.7.3}$$

Combining the (4.7.2) and (4.7.3) we conclude

$$\left(1 - \frac{s}{3} r^2 \right) \frac{N}{b(s)} - \frac{1}{r} < \alpha_{N,s}(N-1) \left(1 + \frac{r^2}{2} \right) . \tag{4.7.4}$$

We minimize the left-hand side of (4.7.4), and therefore we choose

$$r = \left(\frac{3}{2s}\right)^{1/3} \left(\frac{N}{b(s)}\right)^{-1/3} =: \lambda N^{-1/3} . \tag{4.7.5}$$

Combining (4.7.4) and (4.7.5) to find

$$\frac{N}{b(s)} \le \alpha_{N,s}(N-1)\left(1+\frac{\lambda^2}{2}N^{-2/3}\right) + \left(\lambda^{-1} + \frac{s}{3}\frac{\lambda^2}{b(s)}\right) N^{1/3} .$$

Applying Lemma 4.6.15 shows

$$\begin{aligned} \frac{N}{b(s)} \le\ & Z\left(1+AN^{-2/3}\right)(1+(\lambda^2/2)N^{-2/3}) + \left(\lambda^{-1}+\frac{s}{3}\frac{\lambda^2}{b(s)}\right)N^{1/3} \\ &= Z + \left(A+(\lambda^2/2)\right) ZN^{-2/3} + \left(\lambda^{-1}+\frac{s}{3}\frac{\lambda^2}{b(s)}\right)N^{1/3} + \frac{\lambda^2 A}{2} ZN^{-4/3} \end{aligned}$$

where

$$A := \frac{s^2-1}{8} C_{s-1}^{-1/(s-1)} \kappa$$

is the parameter in Lemma 4.6.15. Note that $Z \le N \le 3Z$ and thus there exists some $c(s) > 0$ such that

$$N_c < b(s)\, Z + c(s) Z^{1/3} .$$

Since the calculations hold for any lower bound $b(s)^{-1} < \beta_s$, the statement of Theorem 4.2.2 follows. ∎

4.7.2 The Case of a Quadratic Weight

Proof of Proposition 4.2.4. Applying Lemma 4.5.9 yields

$$\frac{r^2/3+1}{r^2+1} N\beta_2 - \frac{1}{r} \le \alpha_{N,2}(N-1) < Z + \frac{3}{8} C_1^{-1}\kappa Z N^{-2/3} . \tag{4.7.6}$$

Note that by a straightforward calculation

$$N\beta_2\left(1-\frac{2r^2}{3}\right) \le \frac{r^2/3+1}{r^2+1} N\beta_2 \tag{4.7.7}$$

and consequently by inserting (4.7.7) into (4.7.6) we arrive at

$$N\beta_2\left(1-\frac{2r^2}{3}\right) - \frac{1}{r} \le Z + \frac{3}{8} C_1^{-1}\kappa Z N^{-2/3} . \tag{4.7.8}$$

Optimizing the left–hand side of (4.7.8) in $r > 0$ gives

$$r = \left(\frac{3}{4}\right)^{1/3} (N\beta_2)^{-1/3} . \tag{4.7.9}$$

Note that $r < 1$ for $N > 1$. Inserting (4.7.9) into (4.7.8) yields

$$N\beta_2 - \left(\frac{9}{2}\right)^{1/3} (N\beta_2)^{1/3} \leq Z + \frac{3}{8} C_1^{-1} \kappa Z N^{-2/3} .$$

Applying Lemma 4.6.5 we arrive at

$$N\beta_2 \leq Z + \frac{3}{8} C_1^{-1} \kappa Z N^{-2/3} + \left(\frac{9}{2}\beta_2\right)^{1/3} N^{1/3} .$$

We define

$$\lambda := \frac{3}{8} C_1^{-1} \kappa \approx 0.6284 .$$

Then

$$N\beta_2 \leq Z + \lambda Z N^{-2/3} + \left(\frac{9}{2}\beta_2\right)^{1/3} N^{1/3} . \tag{4.7.10}$$

Let $a > 0$ and assume that

$$N\beta_2 \geq Z + \beta_2 a Z^{1/3} . \tag{4.7.11}$$

Combining (4.7.10) and (4.7.11) yields

$$Z + \beta_2 a Z^{1/3} \leq Z + \lambda Z N^{-2/3} + \left(\frac{9}{2}\beta_2\right)^{1/3} N^{1/3} . \tag{4.7.12}$$

Dividing by $Z^{1/3}$ gives

$$a \leq \beta_2^{-1} \lambda \left(\frac{N}{Z}\right)^{-2/3} + \beta_2^{-1} \left(\frac{9}{2}\beta_2\right)^{1/3} \left(\frac{N}{Z}\right)^{1/3} .$$

From Lieb's bound, we conclude $N/Z < 5/2$ for any $Z \geq 2$. Maximizing the right hand side of (4.7.12) for $N/Z \in [1, 5/2]$ yields

$$a \leq \beta_2^{-1} \lambda \left(\frac{N}{Z}\right)^{-2/3} + \beta_2^{-1} \left(\frac{9}{2}\beta_2\right)^{1/3} \left(\frac{N}{Z}\right)^{1/3} \leq 2.953 .$$

Thus for $a := 2.96$ assumption (4.7.11) cannot hold and thus

$$N \leq \frac{1}{\beta_2} Z + 2.96 Z^{1/3} < b(2) Z + 2.96 Z^{1/3}$$

for any $Z \geq 2$. The assertion in Proposition 4.2.4 follows. ∎

4.7.3 The Case of a Cubic Weight

Proof of Proposition 4.2.5. By application of Lemma 4.5.9 we find

$$\frac{(1+r)^{s+1}-(1-r)^{s+1}}{2r(s+1)} N\beta_s \leq \frac{(1+r)^{s+2}-(1-r)^{s+2}}{2r(s+2)} \left(\alpha_{N,s}(N-1)+\frac{1}{r}\right) + r^2 f(r,s)\alpha_{N,s}(N-1) \tag{4.7.13}$$

or equivalently

$$\left(\frac{s+2}{s+1}\right) \frac{(1+r)^{s+1}-|1-r|^{s+1}}{(1+r)^{s+2}-|1-r|^{s+2}} N\beta_s - \frac{1}{r} \leq \left(1+\frac{2r(s+2)r^2 f(r,s)}{(1+r)^{s+2}-|1-r|^{s+2}}\right)\alpha_{N,s}(N-1)\,. \tag{4.7.14}$$

In Appendix A as Lemma A.5.1 we show that for any $r \in (0,1)$ and $s \geq 0$

$$1-\frac{s}{3}r^2 \leq \frac{s+2}{s+1}\frac{(r+1)^{s+1}-(1-r)^{s+1}}{(r+1)^{s+2}-(1-r)^{s+2}}\,. \tag{4.7.15}$$

Combining (4.7.15) and (4.7.14) with $s = 3$ proves

$$(1-r^2)N\beta_3 - \frac{1}{r} \leq \left(1+\frac{5}{r^2(r^2+10)+5} r^2 f(r,3)\right)\alpha_{N,3}(N-1)\,.$$

where

$$f(r,3) = \frac{1}{5}+\frac{1}{35}r+\frac{168}{625}r^2\,. \tag{4.7.16}$$

By direct computations, one shows for any $r \geq 0$

$$\frac{5}{r^2(r^2+10)+5} \leq 1-2r^2+\frac{19}{5}r^4\,. \tag{4.7.17}$$

Assume $r < 0.5$ then by combining (4.7.16) and (4.7.17) we find

$$\begin{aligned}\left(1+\frac{5}{r^2(r^2+10)+5} r^2 f(r,3)\right) &\leq 1+\frac{r^2}{5}+\frac{r^3}{35}\underbrace{-\frac{82r^4}{625}-\frac{2r^5}{35}+\frac{139r^6}{625}+\frac{19r^7}{175}+\frac{3192r^8}{3125}}_{\leq 0,\text{ for } r<0.53} \\ &\leq 1+\frac{r^2}{5}+\frac{r^3}{35}\,.\end{aligned} \tag{4.7.18}$$

Inserting (4.7.18) into (4.7.14) we arrive at

$$(1-r^2)N\beta_3 - \frac{1}{r} \leq \left(1+\frac{r^2}{5}+\frac{r^3}{35}\right)\alpha_{N,3}(N-1)\,. \tag{4.7.19}$$

for any $r \leq 0.5$. Applying Lemma 4.6.5 for $s = 3$ yields

$$(1 - r^2)N\beta_3 - \frac{1}{r} \leq \left(1 + \frac{r^2}{5} + \frac{r^3}{35}\right)\left(Z + cZN^{-2/3}\right), \quad c = C_2^{-1/2}\kappa\,.$$

We continue by choosing $r \in (0, 0.5]$. As in the previous cases, let

$$r = \lambda(N\beta_3)^{-1/3}, \quad \lambda > 0\,. \tag{4.7.20}$$

Inserting (4.7.20) into (4.6.5) yields

$$\begin{aligned} N\beta_3 \leq \quad & Z + \lambda^{-1}(N\beta_3)^{1/3} + \lambda^2(N\beta_3)^{1/3} + \frac{\lambda^2}{5}(N\beta_3)^{-2/3}Z + cZN^{-2/3} \\ & + \frac{\lambda^3}{35}(N\beta_3)^{-1}Z + c\frac{\lambda^2}{5}(N\beta_3)^{-2/3}ZN^{-2/3} \\ & + c\frac{\lambda^3}{35}(N\beta_3)^{-1}ZN^{-2/3}\,. \end{aligned} \tag{4.7.21}$$

We can always assume $Z < N\beta_3$ (since otherwise $N \leq \beta_3^{-1}Z$ already proves an inequality than the statement), and consequently we find

$$\begin{aligned} N\beta_3 \leq \quad & Z + \left(\lambda^{-1} + \frac{6\lambda^2}{5}\right)(N\beta_3)^{1/3} + cZN^{-2/3} \\ & + \frac{\lambda^3}{35} + c\frac{\lambda^2}{5}(\beta_3)^{1/3}N^{-1/3} + c\frac{\lambda^3}{35}N^{-2/3}\,. \end{aligned} \tag{4.7.22}$$

To optimize the leading correction term that grows as $N^{1/3}$, we minimize

$$\lambda \mapsto \lambda^{-1} + \frac{6}{5}\lambda^2,$$

and consequently, we choose

$$\lambda = \left(\frac{5}{12}\right)^{1/3}, \quad \text{such that} \quad \lambda^{-1} + \frac{6}{5}\lambda^2 = 3\left(\frac{3}{10}\right)^{1/3}. \tag{4.7.23}$$

To ensure $r < 0.5$ as assumed after (4.7.23) we need to have

$$N > \frac{10}{3\beta_3} > \frac{10}{3}\,. \tag{4.7.24}$$

We always assume $N \geq Z$, and consequently, the result will hold for $Z \geq 4$. Inserting (4.7.23) into (4.7.22) yields

$$\begin{aligned} N\beta_3 \leq \quad & Z + 3\left(\frac{3}{10}\right)^{1/3} (N\beta_3)^{1/3} + cZN^{-2/3} \\ & + \frac{1}{84} + \frac{c}{5}\left(\frac{5}{12}\right)^{2/3} (\beta_3)^{1/3} N^{-1/3} + c\frac{1}{84} N^{-2/3} . \end{aligned} \tag{4.7.25}$$

We can always assume $N \geq \beta_3^{-1} Z$ because otherwise $N \leq \beta_3^{-1} Z$ and we are done. Inserting $N \geq \beta_3^{-1} Z$ into the last two summands in the right–hand side of (4.7.25) yields

$$\begin{aligned} N\beta_3 \leq \quad & Z + 3\left(\frac{3}{10}\right)^{1/3} (N\beta_3)^{1/3} + cZN^{-2/3} \\ & + \frac{1}{84} + \frac{c}{5}\left(\frac{5}{12}\right)^{2/3} (\beta_3)^{2/3} Z^{-1/3} + c\frac{\beta_3^{2/3}}{84} Z^{-2/3} . \end{aligned}$$

To prove the desired inequality

$$N \leq \beta_3^{-1} Z + a_1 Z^{1/3} + a_2 + a_3 Z^{-1/3} + a_4 Z^{-2/3}$$

for optimal $a_1, a_2, a_3, a_4 \geq 0$ and all $N \geq 3$ we assume that for any arbitrary but fixed N, Z with $N \geq 3$ holds

$$N\beta_3 \geq Z + \beta_3 a_1 Z^{1/3} + \beta_3 a_2 + \beta_3 a_3 Z^{-1/3} + \beta_3 a_4 Z^{-2/3} \tag{4.7.26}$$

and bring this to a contradiction by choosing $a_1, a_2, a_3, a_4 \geq 0$ and comparing (4.7.26) with (4.7.25). We do this now to finish the proof. Combining (4.7.26) with (4.7.25) yields

$$\begin{aligned} & \beta_3 a_1 Z^{1/3} + \beta_3 a_2 + \beta_3 a_3 Z^{-1/3} + \beta_3 a_4 Z^{-2/3} \\ & \qquad \leq \quad 3\left(\frac{3}{10}\right)^{1/3} (N\beta_3)^{1/3} + cZN^{-2/3} \\ & \qquad \quad + \frac{1}{84} + \frac{c}{5}\left(\frac{5}{12}\right)^{2/3} (\beta_3)^{2/3} Z^{-1/3} + c\frac{\beta_3^{2/3}}{84} Z^{-2/3} . \end{aligned} \tag{4.7.27}$$

After comparing both sides of (4.7.27) we choose

$$a_2 = \beta_3^{-1}/84, \quad a_3 = \frac{c}{5}\left(\frac{5}{12}\right)^{2/3} \beta_3^{-1/3}, \quad a_4 = c\frac{\beta_3^{-1/3}}{84} . \tag{4.7.28}$$

Using $\beta_3^{-1} < 1.1185$ and $c < 1.5855$ this gives

$$a_2 \leq 0.0134, \quad a_3 \leq 0.184, \quad a_4 \leq 0.0196 . \tag{4.7.29}$$

For this choice of a_2, a_3, a_4 we arrive at

$$\beta_3 a_1 Z^{1/3} \leq \; 3\left(\frac{3}{10}\right)^{1/3} (N\beta_3)^{1/3} + cZN^{-2/3}\,. \tag{4.7.30}$$

Dividing (4.7.30) by $\beta_3 Z^{1/3}$ we find

$$a_1 \leq \; 3\left(\frac{3}{10}\right)^{1/3} \beta_3^{-2/3}\left(\frac{N}{Z}\right)^{1/3} + c\beta_3^{-1}\left(\frac{N}{Z}\right)^{-2/3}\,. \tag{4.7.31}$$

We can always assume $N \geq \beta_3^{-1}Z$ as explained earlier and $N < 2Z+1$ due to Lieb's result and consequently we can assume $N/Z \in [\beta_3^{-1}, 5/2]$ for $Z \geq 2$. Thus

$$a_1 \leq \sup\left\{3\left(\frac{3}{10}\right)^{1/3} \beta_3^{-2/3} x^{1/3} + c\beta_3^{-1} x^{-2/3} : x \in [\beta_3^{-1}, 5/2]\right\}\,. \tag{4.7.32}$$

Following Lemma 4.6.5 we have

$$c = \sqrt{5}\left(\frac{2}{9\pi^2}1.456\right)^{1/3} 4\frac{\pi^{2/3}}{\sqrt{15}}, \tag{4.7.33}$$

and since $\beta_3^{-1} \in [1.0, 1.1185]$ one can show that the supremum in the right–hand side of (4.7.32) is attained at $x = \beta_3^{-1}$ and consequently

$$a_1 \leq 3\left(\frac{3}{10}\right)^{1/3} \beta_3^{-1} + c\beta_3^{-1/3} < 3.893\,. \tag{4.7.34}$$

For the choice $a_1 = 3.90$ and a_2, a_3, a_4 as in (4.7.27) the inequality (4.7.26) fails and therefore we find

$$N \leq \beta_3^{-1}Z + 3.90Z^{1/3} + 0.0134 + 0.184Z^{-1/3} + 0.0196Z^{-2/3}, \quad Z \geq 4\,.$$

this proves the statement of Proposition 4.2.5. ∎

4.8 Bosonic Atoms

So far, our discussion has focused exclusively on fermionic systems. We now turn our attention to bosonic atoms by considering the Hamiltonian $H_{N,Z}$ in (4.2.1) on the bosonic Hilbert space $\mathcal{H}_N^b$. Contrary to the fermionic case the result on the excess charge will not depend on the spin of the particles. Therefore, we restrict our analysis to spinless bosons. In this context, let $\psi_{N,Z}$ denote the ground state of $H_{N,Z}$ on $\mathcal{H}_N^b$, and let $N_c(Z)$ represent the critical number of bosonic particles that can be bound.

By comparison to the Hartree model, it was shown by Benguria and Lieb in [17] that

$$\lim_{Z\to\infty} \frac{N_c(Z)}{Z} = t_c \tag{4.8.1}$$

for some $t_c > 1$ where the numerical value was computed by Baumgartner in [15] to be $t_c \approx 1.21$. In the appendix as Lemma A.7.1, we prove the analytic bound $t_c \leq 1.47$.
Up to our knowledge, for finite $Z > 0$, Lieb's bound of $N_c < 2Z + 1$ remains the best bound so far. The mean-field arguments presented in Section 4.5 remain valid in the bosonic case without modification. The only part of the previous proofs that relied on the fermionic symmetry of the ground state was Lemma 4.6.4, which is used to find in the fermionic case the bound

$$\left\langle |x_1|^{-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle \lesssim ZN^{-2/3} \lesssim Z^{1/3}\,. \tag{4.8.2}$$

Here, the left-hand side of (4.8.2) represents the expectation value of one electron's inverse position. For a fermionic atom, the average distance between the electrons and the nucleus with charge Z scales as $Z^{-1/3}$. However, in the case of bosonic atoms, this distance is proportional to Z^{-1}. This can be derived by comparing $H_{N,Z}$ with $H_{N,kZ}$ for some $k > 0$, together with estimates of the ground state energy $E_{N,Z}$, see [98, Proof of Theorem 1].
In Section 4.8.1, we present an initial estimate that can be derived by applying our previous findings while optimizing the parameter $s \geq 1$ in the Benguria–Lieb–Nam argument. Specifically, we prove the following bound:

$$N_c(Z) < 1.54141\,Z + 3.50\,Z^{1/2} + 2.43 + 0.494\,Z^{-1/2}, \quad \forall Z \geq 2$$

as stated in Theorem 4.8.1.
In Section 4.8.2, we build on an approach developed by Benguria et al. in [19] to establish new bounds on the ground state energy $E_{N,Z}$ for bosonic systems. These refined estimates enable us to improve the result on the maximal excess charge of bosonic atoms. Our main objective is to prove Theorem 4.2.7.

4.8.1 A first Inequality

The techniques derived earlier can be applied to the case of bosonic atoms. We show

Theorem 4.8.1. *Let $s \in (1, 2]$ and $Z \geq 2$, then*

$$\begin{aligned} N_c(Z) < b(s)d(s)Z &+ 2b(s)\,(d(s)s)^{1/2}\,Z^{1/2} \\ &+ b(s)(s + 1 - s^{-1}) \\ &+ b(s)(s-1)\,(d(s)s)^{-1/2}\,Z^{-1/2} \end{aligned} \tag{4.8.3}$$

where

$$b(s) := \frac{s-1}{st_0}, \quad d(s) = 1 + \frac{s^2-1}{8}$$

with t_0 the unique solution of $t^s + st + 1 - s = 0$ in $(0, 1)$.

Remark 4.8.2. *In Figure 4.3, we have plotted the behavior of* $s \mapsto b(s)d(s)$. *The minimum is attained at* $s \approx 1.480$. *Let* $s_0 = 1.48$ *then for* $t_1 = 0.241715$ *it follows* $t_1^{s_0} + s_0 t_1 + 1 - s_0 < 0$ *and consequently*

$$b(s_0) < \frac{s_0 - 1}{s_0 t_1} = 1.34176, \text{ and } d(s_0) = 1.1488\,.$$

By direct computations,

$$\begin{aligned} &b(s_0)d(s_0) < 1.54141, \\ &2b(s_0)\,(d(s_0)s_0)^{1/2} < 3.50, \\ &b(s_0)(s_0 + 1 - s_0^{-1}) < 2.43, \\ &b(s_0)(s_0 - 1)\,(d(s_0)s_0)^{-1/2} < 0.494\,. \end{aligned}$$

Inserting these numbers into (4.8.3) *proves*

$$N_c(Z) < 1.54141\,Z + 3.50\,Z^{1/2} + 2.43 + 0.494\,Z^{-1/2}\,.$$

which improves Lieb's result of $N_c(Z) < 2Z + 1$ *for* $Z > 64.6$.

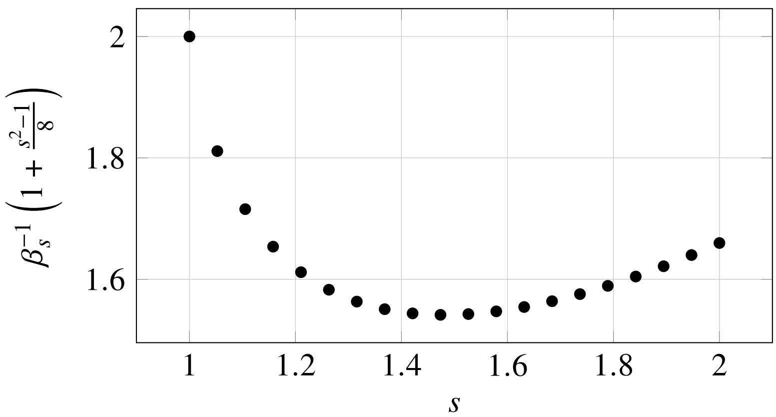

FIGURE 4.3: Sample values of the prefactor in the term linear in Z in (4.8.11) .

Proof. Without any changes (4.2.2) and (4.6.9) still hold, so that for any $s \geq 2$ and Jensen's inequality

$$\begin{aligned} \alpha_{N,s}(N-1) &< Z + \frac{s^2-1}{8}\left(\left\langle |x_1|^{s-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle\right)^{\frac{-1}{s-1}} \\ &< Z + \frac{s^2-1}{8}\left\langle |x_1|^{-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle\,. \end{aligned} \tag{4.8.4}$$

Indeed (4.8.4) does also hold for $s \geq 1$, and we prove this as Lemma 4.8.8 below. Following [76] the energy of a single electron atom with nuclear charge λ is bounded from below by

$$\left\langle f, \frac{-\Delta}{2} f \right\rangle - \left\langle f, \frac{\lambda}{|x|} f \right\rangle \geq -\frac{\lambda^2}{2} \langle f, f \rangle$$

for every $f \in H^1$ and $\lambda \in \mathbb{R}$. Recall the definition of $\rho_{\psi_{N,Z}}$ in (4.6.5). Then $\rho_{\psi_{N,Z}} \geq 0$ by construction. Choose

$$\lambda = \frac{\int |x|^{-1} \rho_{\psi_{N,Z}(x)} dx}{N}, \; f = \sqrt{\rho_{\psi_{N,Z}}(x)} .$$

Consequently, we arrive at Coulomb's uncertainty principle

$$\int |x|^{-1} \rho_{\psi_{N,Z}(x)} dx \leq N^{1/2} \left\| \nabla \sqrt{\rho_{\psi_{N,Z}}} \right\|_2 . \tag{4.8.5}$$

By the Hoffmann-Ostenhof inequality (see, [46, Lemma 2]) and the virial theorem

$$\left\| \nabla \sqrt{\rho_{\psi_{N,Z}}} \right\|_2^2 \leq \sum_{i=1}^{N} \langle \psi_{N,Z}, -\Delta_i \psi_{N,Z} \rangle = -2E_{N,Z} . \tag{4.8.6}$$

For the bosonic ground state we have $-E_{N,Z} \leq NZ^2/2$ by ignoring the electron–electron repulsion which together with (4.8.5) yields

$$\langle |x_1|^{-1} \psi_{N,Z}, \psi_{N,Z} \rangle \leq N^{-1/2} \sqrt{-2E_{N,Z}} \leq Z . \tag{4.8.7}$$

Combining (4.8.4) and (4.8.7) we arrive at

$$\alpha_{N,s}(N-1) < \left(1 + \frac{s^2-1}{8}\right) Z .$$

Applying Lemma 4.5.3 for every $N \geq 2$, $r > 0$ and $s \geq 1$ we find

$$\frac{(r+1)^{s+1} - (1-r)^{s+1}}{2r(s+1)(1+r)^s} N\beta_s \leq \left(1 + \frac{s^2-1}{8}\right) Z + \frac{1}{r} . \tag{4.8.8}$$

Let $p \geq 2$ and $r > 0$ then by standard arguments, the following inequality is valid

$$(1+r)^p - (1-r)^p \geq 2rp . \tag{4.8.9}$$

Let $p = s + 1$ for $s \geq 1$ and insert (4.8.9) into (4.8.8) to find

$$N\beta_s \leq \left(1 + \frac{s^2-1}{8}\right) Z(1+r)^s + \frac{(1+r)^s}{r} . \tag{4.8.10}$$

Choose $r = \lambda Z^{-1/2}$ for some $\lambda > 0$, then by standard estimates one can find $c(\lambda, s) > 0$ with

$$N \le \beta_s^{-1}\left(1 + \frac{s^2-1}{8}\right) Z + c(\lambda, s) Z^{1/2} . \tag{4.8.11}$$

Optimizing in $\lambda > 0$ can improve the result. For $s \in [1,2]$ we give a rough estimate on $c(\lambda, s)$. For $q \in [0,1]$, the following Bernoulli's inequality is true

$$(1+x)^q \le 1 + qx, \quad \forall x \ge -1 . \tag{4.8.12}$$

Let $|r| < 1$ then together with Bernoulli's inequality we find

$$(1+r)^s = (1+r)(1+r)^{s-1} \le (1+r)(1+(s-1)r) = 1 + sr + (s-1)r^2 . \tag{4.8.13}$$

Let

$$d := d(s) := 1 + \frac{s^2-1}{8} = \frac{s^2+7}{8} \tag{4.8.14}$$

then by inserting (4.8.14) and (4.8.13) into the right–hand side of (4.8.10) we arrive at

$$\begin{aligned}\left(1 + \frac{s^2-1}{8}\right) Z(1+r)^s + \frac{(1+r)^s}{r} &= \left(dZ + \frac{1}{r}\right)(1+r)^s \\ &\le (dZ + r^{-1})(1 + sr + (s-1)r^2) \\ &= dZ + dsZr + r^{-1} + d(s-1)Zr^2 + s + (s-1)r .\end{aligned}$$

Choose now $r = \lambda Z^{-1/2}$ for some $\lambda > 0$ then

$$\begin{aligned}\left(1 + \frac{s^2-1}{8}\right) Z(1+r)^s + \frac{(1+r)^s}{r} \le\ & dZ + [ds\lambda + \lambda^{-1}]Z^{1/2} \\ &+ [d(s-1)\lambda^2 + s] \\ &+ \lambda(s-1)Z^{-1/2} .\end{aligned}$$

It remains to choose the free parameter $\lambda > 0$ optimally. We decide to optimize the expression that grows as $Z^{1/2}$ in the free parameter $\lambda > 0$ to find

$$\lambda = (ds)^{-1/2}$$

and consequently

$$\begin{aligned}\left(1 + \frac{s^2-1}{8}\right) Z(1+r)^s + \frac{(1+r)^s}{r} \le\ & dZ + 2\,(ds)^{1/2}\, Z^{1/2} \\ &+ \left[s + 1 - s^{-1}\right] \\ &+ (s-1)\,(ds)^{-1/2}\, Z^{-1/2} .\end{aligned}$$

Inserting this into (4.8.10) proves the statement of Theorem 4.8.1. ∎

4.8.2 Comparison with the Hartree Model

We begin by analyzing a recent technique by Benguria et al. in [19] to derive new bounds to the ground state energy $E_{N,Z}$ in the bosonic case. It has come to our attention that there appears to be an inconsistency in [19]. Upon careful examination, we have identified a potential error. We deeply appreciate the approach introduced by Benguria et al. and hope that our contribution will be seen as a constructive enhancement to their valuable work.

We study the Hartree Model, which is given by

$$\mathcal{E}_Z^{\mathrm{H}}(f) := \frac{1}{2}\int (\nabla f)^2 \,\mathrm{d}x - Z\int \frac{|f|^2}{|x|}\,\mathrm{d}x + \frac{1}{2}\iint \frac{|f(x)|^2|f(y)|^2}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y\,, \quad f \in H^1\,. \tag{4.8.15}$$

The energy in the Hartree model is defined as

$$E_{N,Z}^{\mathrm{H}} := \inf\left(\mathcal{E}_Z^{H}(f) : f \in H^1(\mathbb{R}^3), \|f\|_2^2 = N\right)\,. \tag{4.8.16}$$

By rescaling

$$E_{N,Z}^{\mathrm{H}} = Z^3 e(N/Z) \tag{4.8.17}$$

where $e(\cdot)$ is defined as

$$e(t) := \inf\left\{\mathcal{E}_1^{\mathrm{H}}(g) : g \in H^1(\mathbb{R}^3), \|g\|_2^2 = t\right\}, \text{ for } t > 0 \text{ and } e(0) := 0\,. \tag{4.8.18}$$

We give this rescaling argument in Appendix A as Lemma A.6.1.

Remark 4.8.3. *The mapping $t \mapsto e(t)$ is strictly decreasing and strictly convex for $t \in [0, t_c]$ (see [17]) and constant for $t \geq t_c$ (see [110, p. 166]). In particular*

$$\min e(t) = e(t_c)\,. \tag{4.8.19}$$

Note that this behavior of $e(\cdot)$ directly clarifies the maximal excess charge in the Hartree model since, for any $\delta > 0$, we have due to (4.8.17)

$$E_{N-\delta,Z}^{H} > E_{N,Z}^{H} \Leftrightarrow e\left(\frac{N-\delta}{Z}\right) > e\left(\frac{N}{Z}\right) \Leftrightarrow \frac{N-\delta}{Z} < t_c$$

and in the limit $\delta \to 0$ this proves $N \leq t_c Z$. Due to Baumgartner [15] we know numerically $t_c \approx 1.21$. In Lemma A.7.1, we prove analytically $t_c \leq 1.47$ and consequently $N < 1.47Z$ in the Hartree model.

In Section 4.8.3 we show

Lemma 4.8.4. *Let $e(\cdot)$ be defined as in* (4.8.18) *and let t_c the asymptotic constant in* (4.8.1) *then*

$$e(t_c) \geq -\frac{2t_c}{9}\,.$$

Remark 4.8.5. *Combining Lemma 4.8.4 and* (4.8.17) *together with* (4.8.19) *shows*

$$E^H_{N,Z} \geq -\frac{2t_c}{9}Z^3 \tag{4.8.20}$$

Equipped with Lemma 4.8.4, we show a lower bound to the ground state energy $E_{N,Z}$. In particular, we show

Corollary 4.8.6. *For the ground state energy $E_{N,Z}$ we find*

$$E_{N,Z} \geq -\frac{2t_c}{9}Z^3 - D\frac{2\sqrt{t_c}}{3}N^{5/6}Z^{3/2} - D^2\frac{3}{2\sqrt{t_c}}N^{13/6}Z^{-3/2}.$$

where $D = C_{LO}C_{GN}$ with $C_{GN} = 0.2793$ and $C_{LO} = 1.58$.

Remark 4.8.7. *To derive estimates on $N_c(Z)$, we can always assume $N \geq Z$. In the proof of Theorem 4.8.1, we used the bound*

$$-E_{N,Z} < \frac{NZ^2}{2}\,.$$

However, the estimate provided in Corollary 4.8.6 improves upon this, since it proves

$$-E_{N,Z} < \frac{2t_c}{9}Z^3 + O(Z^{2+1/3}),$$

where $t_c \leq 2$, as established by Lieb's result $N_c(Z) < 2Z + 1$ and numerically $t_c \approx 1.21$ due to Baumgartner [15]. Following the steps of the proof of Theorem 4.8.1 and applying this refined estimate for $E_{N,Z}$, we obtain an improved bound on $N_c(Z)$. The remainder of our analysis will focus on proving Corollary 4.8.6 and deriving a new estimate on $N_c(Z)$.

We prove Corollary 4.8.6 in section section 4.8.4. We continue by proving Lemma 4.8.4.

4.8.3 Proof of Lemma 4.8.4

Proof. Following [110, p. 166] there exists $f_H = \sqrt{u}$ with $\sqrt{u} \in H^1$ such that

$$e(t_c) = \mathcal{E}^{\mathrm{H}}_1(\sqrt{u}), \quad \|f\|_2^2 = \int_{\mathbb{R}^3} |u(x)|\,\mathrm{d}x = t_{\mathrm{c}} \tag{4.8.21}$$

where f_H is the unique positive solution to

$$\frac{-\Delta f_H}{2} = \Phi f_H$$

with

$$\Phi(x) = |x|^{-1} - (u * |\cdot|^{-1})(x)\,.$$

The Hartree energy functional is strictly convex. The fact that the function

$$u \mapsto \int \left|\nabla\sqrt{u}\right| dx$$

is convex, can be for instance found in [16, Lemma 4]. Due to the strict convexity of $\mathcal{E}_1^{\mathrm{H}}$ there is no minimizer of $\mathcal{E}_1^{\mathrm{H}}$ with $\|f\|_2^2 = t > t_c$ and $\mathcal{E}_1^{\mathrm{H}}(f) = e(t_c)$ (choose $\gamma = 0$ in [73, Theorem 2.4 and Theorem 2.5], where the more general Thomas-Fermi-von Weizsäcker theory is studied). Consequently $f_H = \sqrt{u}$ is the unique minimizer of $\mathcal{E}_1^H$ without restriction on $\|u\|_1$. Let $\lambda, s > 0$, and define

$$u_{\lambda,s}(x) \coloneqq s^{-1/2}\lambda^{-3/2}u\Big(\lambda^{-1}x\Big), \tag{4.8.22}$$

then by direct calculations

$$\begin{aligned}\mathcal{E}_1^H\big(\sqrt{u_{\lambda,s}}\big) =& \frac{1}{s\lambda^2 2}\int \big(\nabla\sqrt{u}\big)^2\,\mathrm{d}x - \frac{1}{s\lambda}\int \frac{|u(x)|}{|x|}\,\mathrm{d}x \\ &+ \frac{1}{s^2\lambda}\frac{1}{2}\iint \frac{|u(x)||u(y)|}{|x-y|}\,\mathrm{d}y\,\mathrm{d}x\,.\end{aligned} \tag{4.8.23}$$

As $f_H = \sqrt{u}$ is the unique minimizer it follows

$$\frac{\partial}{\partial s}\mathcal{E}_1^H\big(\sqrt{u_{\lambda,s}}\big)\bigg|_{s=\lambda=1} = \frac{\partial}{\partial\lambda}\mathcal{E}_1^H\big(\sqrt{u_{\lambda,s}}\big)\bigg|_{s=\lambda=1} = 0\,. \tag{4.8.24}$$

These conditions define several virial theorems. To reduce notation, we define,

$$K \coloneqq \frac{1}{2}\int_{\mathbb{R}^3}\big(\nabla\sqrt{u}\big)^2\,\mathrm{d}x\,, \tag{4.8.25}$$

$$A \coloneqq \int_{\mathbb{R}^3}\frac{|u(x)|}{|x|}\,\mathrm{d}x\,, \tag{4.8.26}$$

$$R \coloneqq \frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|u(x)||u(y)|}{|x-y|}\,\mathrm{d}y\,\mathrm{d}x\,. \tag{4.8.27}$$

Taking the derivatives in (4.8.23) according to (4.8.24) and inserting K, A and R we find

$$0 = \left(-\frac{2}{s\lambda^3}K + \frac{1}{s\lambda^2}A - \frac{1}{s^2\lambda^2}R\right)\bigg|_{s=\lambda=1} = -2K + A - R, \tag{4.8.28}$$

$$0 = \left(-\frac{1}{s^2\lambda^2}K + \frac{1}{s^2\lambda}A - \frac{2}{s^3\lambda}R\right)\bigg|_{s=\lambda=1} = -K + A - 2R\,. \tag{4.8.29}$$

By definition of K, A and R together with (4.8.21) and the definition of $e(t_c)$ in (4.8.17) we have

$$e(t_{\mathrm{c}}) = K - A + R\,.$$

Combining this with (4.8.28) we find

$$K = A/3, \quad e(t_c) = -K. \tag{4.8.30}$$

We apply the Coulomb Uncertainty Principle (see [76, Equation 2.2.18]) which yields

$$\int_{\mathbb{R}^3} \frac{|u(x)|}{|x|}\,\mathrm{d}x \le \left(\int_{\mathbb{R}^3} (\nabla\sqrt{u})^2\,\mathrm{d}x\right)^{1/2}\left(\int_{\mathbb{R}^3} |u(x)|\,\mathrm{d}x\right)^{1/2}. \tag{4.8.31}$$

Since $3K = A$,

$$A^2 = \left(\int_{\mathbb{R}^3} \frac{|u(x)|}{|x|}\,\mathrm{d}x\right)^2 \le \left(\left(\int_{\mathbb{R}^3} (\nabla\sqrt{u})^2\,\mathrm{d}x\right)^{1/2} t_c^{1/2}\right)^2 \Rightarrow A^2 \le Kt_c \Rightarrow A \le \frac{1}{3}t_c \tag{4.8.32}$$

Combining (4.8.30) and (4.8.32) we arrive at

$$K \le \frac{1}{9}t_c\,. \tag{4.8.33}$$

Together with $e(t_c) = -K$ we find

$$e(t_c) \ge -\frac{2t_c}{9} \tag{4.8.34}$$

which completes the proof. ∎

We continue by proving Corollary 4.8.6.

4.8.4 Proof of Corollary 4.8.6

Proof. Let $\psi_{N,Z}$ denote the ground state of $H_{N,Z}$, and recall the definition of the one-particle density $\rho_{\psi_{N,Z}}$ given in (4.6.5). For brevity, we write $\rho = \rho_{\psi_{N,Z}}$. Following [17], the Hartree energy $\mathcal{E}_Z^H$ and the ground state energy $E_{N,Z}$ of the Schrödinger operator $H_{N,Z}$ can be related via the Lieb-Oxford inequality (see [75]). In particular, we have

$$E_{N,Z} \ge \mathcal{E}_Z^H(\sqrt{\rho}) - C_{\mathrm{LO}} \int_{\mathbb{R}^3} \rho(x)^{4/3}\,\mathrm{d}x. \tag{4.8.35}$$

We use the improved Lieb-Oxford constant $C_{LO} = 1.5765$, which was recently derived in [68, Equation 79]. Applying the Gagliardo–Nirenberg inequality to the Lieb-Oxford term, we find

$$\int_{\mathbb{R}^3} (\rho(x))^{4/3} dx \le C_{GN}\|\nabla\sqrt{\rho}\|_2 \left(\int_{\mathbb{R}^3} \rho(x) dx\right)^{5/6} = C_{GN}\|\nabla\sqrt{\rho}\|_2 N^{5/6} \tag{4.8.36}$$

where C_{GN} can be computed numerically to get $C_{GN} < 0.2793$ (see [19]). By the Hoffmann-Ostenhof Inequality (see, [46, Lemma 2])) and the virial theorem

$$\left\|\nabla\sqrt{\rho}\right\|_2^2 \le \sum_{i=1}^{N} \langle \psi_{N,Z}, -\Delta_i \psi_{N,Z}\rangle = -2E_{N,Z}\,.$$

Using the definition of the Hartree energy in (4.8.16) and combining (4.8.35), (4.8.36) and (4.8.6) shows

$$E_{N,Z} \ge E^{\mathrm{H}}_{N,Z} - C_{LO}C_{GN}(-2E_{N,Z})^{1/2}N^{5/6}$$

Define $D := C_{LO}C_{GN}$ then by application of (4.8.20) we arrive at

$$E_{N,Z} \ge -\frac{2t_{\mathrm{c}}}{9}Z^3 - D(-2E_{N,Z})^{1/2}N^{5/6}\,. \tag{4.8.37}$$

Inserting equation (4.8.37) into itself yields

$$E_{N,Z} \ge -\frac{2t_{\mathrm{c}}}{9}Z^3 - D\left(\frac{4t_{\mathrm{c}}}{9}Z^3 + 2D(-2E_{N,Z})^{1/2}N^{5/6}\right)^{1/2} N^{5/6}\,. \tag{4.8.38}$$

Ignoring the electron–electron repulsion, there is always the inequality

$$-E_{N,Z} \le \frac{1}{2}NZ^2\,. \tag{4.8.39}$$

Combining (4.8.39) and (4.8.38) we arrive at

$$\begin{aligned}
E_{N,Z} &\ge -\frac{2t_{\mathrm{c}}}{9}Z^3 - D\left(\frac{4t_{\mathrm{c}}}{9}Z^3 + 2DN^{4/3}Z\right)^{1/2} N^{5/6}\\
&= -\frac{2t_{\mathrm{c}}}{9}Z^3 - D\frac{2\sqrt{t_{\mathrm{c}}}}{3}N^{5/6}Z^{3/2}\left(1 + \frac{9D}{2t_{\mathrm{c}}}N^{4/3}Z^{-2}\right)^{1/2}\\
&\ge -\frac{2t_{\mathrm{c}}}{9}Z^3 - D\frac{2\sqrt{t_{\mathrm{c}}}}{3}N^{5/6}Z^{3/2}\left(1 + \frac{9D}{4t_{\mathrm{c}}}N^{4/3}Z^{-2}\right)\\
&= -\frac{2t_{\mathrm{c}}}{9}Z^3 - D\frac{2\sqrt{t_{\mathrm{c}}}}{3}N^{5/6}Z^{3/2} - D^2\frac{3}{2\sqrt{t_{\mathrm{c}}}}N^{13/6}Z^{-3/2}\,.
\end{aligned}$$

In the third line, we applied Bernoulli's Inequality (4.8.12). This proves the assertion of Corollary 4.8.6. ∎

Equipped with Corollary 4.8.6, we can continue to prove bounds to the Excess Charge in the bosonic case.

4.8.5 Maximal Excess Charge In The Bosonic Case

We want to apply Lemma 4.6.2, but for $s < 2$, this is not directly possible. We show

Lemma 4.8.8. *For any $s \in (1, 2]$*

$$\frac{1}{2}\frac{\left\langle |x_1|^s \psi_{N,Z}, \Delta_1 \psi_{N,Z}\right\rangle}{\left\langle |x_1|^{s-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle} \le \frac{s^2-1}{8}\left\langle |x_1|^{-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle . \tag{4.8.40}$$

Proof. With the same arguments as in Lemma 4.6.2

$$\frac{1}{2}\frac{\left\langle |x_1|^s \psi_{N,Z}, \Delta_1 \psi_{N,Z}\right\rangle}{\left\langle |x_1|^{s-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle} \le \frac{s^2-1}{8}\frac{\left\langle |x_1|^{s-2}\psi_{N,Z}, \psi_{N,Z}\right\rangle}{\left\langle |x_1|^{s-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle} .$$

Note that

$$\left\langle |x_1|^{s-2}\psi_{N,Z}, \psi_{N,Z}\right\rangle = \frac{1}{N}\int_{R^3} |x_1|^{s-1}|x_1|^{-1}\rho_{\psi_{N,Z}}(x_1)\, dx_1 .$$

Instead of applying Hölder's inequality directly, we define the probability measure

$$d\varphi(x) := \frac{1}{N}\frac{|x|^{-1}\rho_{\psi_{N,Z}}(x)\, dx}{\left\langle |x_1|^{-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle}$$

then by Hölder's inequality

$$\begin{aligned}\left\langle |x_1|^{s-2}\psi_{N,Z}, \psi_{N,Z}\right\rangle &= \int_{\mathbb{R}^3} |x|^{s-1} d\varphi(x) \left\langle |x_1|^{-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle \\ &\le \left(\int_{\mathbb{R}^3} |x|^s d\varphi(x)\right)^{(s-1)/s} \left\langle |x_1|^{-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle .\end{aligned} \tag{4.8.41}$$

Inserting the definition of $d\varphi$ in the second line of (4.8.41) we arrive at

$$\left\langle |x_1|^{s-2}\psi_{N,Z}, \psi_{N,Z}\right\rangle \le \left(\left\langle |x_1|^{s-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle\right)^{\frac{s-1}{s}} \left(\left\langle |x_1|^{-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle\right)^{\frac{1}{s}}$$

and consequently

$$\frac{\left\langle |x_1|^{s-2}\psi_{N,Z}, \psi_{N,Z}\right\rangle}{\left\langle |x_1|^{s-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle} \le \left(\left\langle |x_1|^{s-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle\right)^{\frac{-1}{s}} \left(\left\langle |x_1|^{-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle\right)^{\frac{1}{s}} . \tag{4.8.42}$$

To simplify the expression on the right–hand side of (4.8.42) we use Jensen's inequality. Let $s \in (1, 2]$ and $\mu \in P(\mathbb{R}^3)$. We show

$$\left(\int_{\mathbb{R}^3} |x|^{s-1} d\mu(x)\right)^{-\frac{1}{s}} \le \left(\int_{\mathbb{R}^3} |x|^{-1} d\mu(x)\right)^{1-\frac{1}{s}} . \tag{4.8.43}$$

This is equivalent to

$$\int_{\mathbb{R}^3} |x|^{s-1} d\mu(x) \ge \left(\int_{\mathbb{R}^3} |x|^{-1} d\mu(x)\right)^{1-s} . \tag{4.8.44}$$

The mapping $(0,\infty) \ni t \mapsto t^{1-s}$ is convex for any $s \in (1,2]$ since $(t^{1-s})'' = s(s-1)t^{-(s+1)}$. Equation (4.8.44) and consequently (4.8.43) then follows directly from Jensen's inequality. Note that

$$d\mu = N^{-1} d\rho_{\psi_{N,Z}}$$

is a probability measure, and thus, applying (4.8.43), we conclude

$$\left(\left\langle |x_1|^{s-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle\right)^{\frac{-1}{s}} \leq \left(\left\langle |x_1|^{-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle\right)^{1-\frac{1}{s}}$$

which combining with (4.8.42) yields

$$\frac{\left\langle |x_1|^{s-2}\psi_{N,Z}, \psi_{N,Z}\right\rangle}{\left\langle |x_1|^{s-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle} \leq \left\langle |x_1|^{-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle .$$

This finishes the proof of Lemma 4.8.8. ∎

With Corollary 4.8.6 and Lemma 4.8.8, we now have the necessary tools to establish a more refined version of Theorem 4.8.1, namely Theorem 4.2.7. Before proceeding with the proof of Theorem 4.2.7, it is helpful to summarize our findings in the form of the following lemma.

Lemma 4.8.9. *Let $\psi_{N,Z}$ the ground state of $H_{N,Z}$ in* (4.2.1) *on $\mathcal{H}_N^b$ then*

$$\begin{aligned}&\left\langle |x_1|^{-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle \\ &\leq \frac{2\sqrt{t_c}}{3}\left(\frac{Z}{N}\right)^{1/2} Z\left(1 + D\frac{3}{2\sqrt{t_c}}\left(\frac{N}{Z}\right)^{5/6} Z^{-2/3} + D^2\left(\frac{3}{2\sqrt{t_c}}\right)^2\left(\frac{N}{Z}\right)^{13/6} Z^{-7/3}\right)\end{aligned} \tag{4.8.45}$$

Proof. We already have proven

$$\left\langle |x_1|^{-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle \leq N^{-1/2}\sqrt{-2E_{N,Z}} \tag{4.8.46}$$

in the proof of Theorem 4.8.1 (see (4.8.7)). Combining (4.8.46) together with the estimate on $E_{N,Z}$ found in Corollary 4.8.6 we arrive at

$$
\begin{aligned}
&\left\langle |x_1|^{-1}\psi_{N,Z}, \psi_{N,Z}\right\rangle \\
&= \frac{1}{N}\int_{R^3} |x_1|^{-1}\rho(x_1)\, dx_1 \\
&\leq N^{-1/2}\left(\frac{4t_c}{9}Z^3 + D\frac{4\sqrt{t_c}}{3}N^{5/6}Z^{3/2} + D^2\frac{6}{2\sqrt{t_c}}N^{13/6}Z^{-3/2}\right)^{1/2} \\
&= \frac{2\sqrt{t_c}}{3}\left(\frac{Z}{N}\right)^{1/2} Z\left(1 + \frac{3D}{\sqrt{t_c}}N^{5/6}Z^{-3/2} + 2D^2\left(\frac{3}{2\sqrt{t_c}}\right)^2 N^{13/6}Z^{-9/2}\right)^{1/2} \\
&\leq \frac{2\sqrt{t_c}}{3}\left(\frac{Z}{N}\right)^{1/2} Z\left(1 + D\frac{3}{2\sqrt{t_c}}N^{5/6}Z^{-3/2} + D^2\left(\frac{3}{2\sqrt{t_c}}\right)^2 N^{13/6}Z^{-9/2}\right) \\
&= \frac{2\sqrt{t_c}}{3}\left(\frac{Z}{N}\right)^{1/2} Z\left(1 + D\frac{3}{2\sqrt{t_c}}\left(\frac{N}{Z}\right)^{5/6} Z^{-2/3} + D^2\left(\frac{3}{2\sqrt{t_c}}\right)^2\left(\frac{N}{Z}\right)^{13/6} Z^{-7/3}\right).
\end{aligned}
$$

∎

4.8.6 Proof of Theorem 4.2.7

Remark 4.8.10. *As in previous cases, $s \geq 1$ will appear as a free parameter in our analysis. However, unlike the fermionic case, increasing s does not necessarily yield better results. In Lemma A.7.1, we prove the bound*

$$
t_c = \lim_{Z\to\infty}\frac{N_c(Z)}{Z} \leq \inf_{s\in[1,2]} b(s)\left(1 + \frac{s^2-1}{12}\right) \leq 1.47,
$$

where the infimum is attained at $s \approx 1.624$. This suggests that optimal results can be expected for $s \leq 2$.

In the fermionic case, we previously relied on Lemma 4.5.9, which is valid only for $s \geq 2$. Here, we instead use Lemma 4.5.3, which applies to $s \leq 2$. Consequently, we cannot establish

$$
\frac{N_c(Z)}{Z} \in O(Z^{1/3}),
$$

and instead, we obtain a $Z^{1/2}$ behavior for the correction terms.

While extending the analysis to $s \geq 2$ in conjunction with Lemma 4.5.3 might improve our results for finite Z, we restrict our consideration to $s \in (1,2)$.

Proof of Theorem 4.2.7. We combine (4.3.10) with Lemma 4.5.3 and the estimate on β_s in (4.4.5) to prove the Theorem. Combining Lemma 4.5.3, Lemma 4.8.8 and (4.3.10) yields

$$\begin{aligned}&\frac{(r+1)^{s+1}-(1-r)^{s+1}}{2r(s+1)(1+r)^s}N\beta_s-\frac{1}{r}\\&\le Z+\frac{s^2-1}{12}\sqrt{t_c}\left(\frac{Z}{N}\right)^{1/2}Z\left(1+\frac{3D}{2\sqrt{t_c}}\left(\frac{N}{Z}\right)^{5/6}Z^{-2/3}+\frac{9D^2}{4t_c}\left(\frac{N}{Z}\right)^{13/6}Z^{-7/3}\right).\end{aligned}$$

Direct computations show for $r \ge 0$ and $s \ge 1$ that

$$(1+r)^{s+1}-(1-r)^{s+1}\ge 2r(s+1)(1-r)^s\,.$$

Thus, we arrive at

$$\begin{aligned}\left(\frac{1-r}{1+r}\right)^s N\beta_s-\frac{1}{r}\le&\left(1+\frac{s^2-1}{12}\sqrt{t_c}\left(\frac{Z}{N}\right)^{1/2}\right)Z\\&+\frac{s^2-1}{8}D\left(\frac{N}{Z}\right)^{7/6}Z^{1/3}\\&+\frac{s^2-1}{8}\frac{3D^2}{2\sqrt{t_c}}\left(\frac{N}{Z}\right)^{5/3}Z^{-4/3}\,.\end{aligned}\tag{4.8.47}$$

Note that by Bernoulli's inequality

$$\left(\frac{1-r}{1+r}\right)^s\ge 1-s\frac{2r}{1+r}\ge 1-2sr\tag{4.8.48}$$

for any $r\in(0,1)$. Combining (4.8.47) and (4.8.48) yields

$$\begin{aligned}(1-2sr)N\beta_s-\frac{1}{r}\le&\left(1+\frac{s^2-1}{12}\sqrt{t_c}\left(\frac{Z}{N}\right)^{1/2}\right)Z\\&+\frac{s^2-1}{8}D\left(\frac{N}{Z}\right)^{7/6}Z^{1/3}\\&+\frac{s^2-1}{8}\frac{3D^2}{2\sqrt{t_c}}\left(\frac{N}{Z}\right)^{5/3}Z^{-4/3}\,.\end{aligned}\tag{4.8.49}$$

We use that $N < 2Z+1$ by Lieb's result and hence $N \le 5/2Z$ for $Z \ge 2$. We define

$$c_1 := \frac{s^2-1}{8}D\left(\frac{5}{2}\right)^{7/6},\quad c_2 := \frac{s^2-1}{8}\frac{3D^2}{2\sqrt{t_c}}\left(\frac{5}{2}\right)^{5/3}\,.$$

Consequently, we arrive at

$$N\beta_s \le \left(1 + \frac{s^2-1}{12}\sqrt{t_{\mathrm{c}}}\left(\frac{Z}{N}\right)^{1/2}\right) Z + c_1 Z^{1/3} + c_2 Z^{-4/3} + \frac{1}{r} + 2srN\beta_s\,.$$

Optimizing in r yields

$$r = \left(\frac{1}{2s\beta_s}\right)^{1/2} N^{-1/2}\,.$$

Note that $r < 1$ if $N \ge 1$. Thus, we arrive at

$$N \le \frac{1}{\beta_s}\left(1 + \frac{s^2-1}{12}\sqrt{t_{\mathrm{c}}}\left(\frac{Z}{N}\right)^{1/2}\right) Z + \frac{c_1}{\beta_s} Z^{1/3} + \frac{c_2}{\beta_s} Z^{-4/3} + 2\sqrt{\frac{2s}{\beta_s}} N^{1/2}\,.$$

Using again that $N < 2Z + 1$ by Liebs result and hence $N \le 5/2Z$ for $Z \ge 2$ shows

$$N \le \frac{1}{\beta_s}\left(1 + \frac{s^2-1}{12}\sqrt{t_{\mathrm{c}}}\left(\frac{Z}{N}\right)^{1/2}\right) Z + \frac{c_1}{\beta_s} Z^{1/3} + \frac{c_2}{\beta_s} Z^{-4/3} + 2\sqrt{\frac{5s}{\beta_s}} Z^{1/2}\,. \tag{4.8.50}$$

It remains to turn (4.8.50) into the desired relation between N and Z. To this end let $\theta_0, \theta_1, \theta_2, \theta_3 > 0$ and assume for arbitrary but fixed $N \ge Z \ge 2$

$$N \ge \theta_0 Z + \theta_1 Z^{1/2} + \theta_2 Z^{1/3} + \theta_3 Z^{-4/3}\,. \tag{4.8.51}$$

To prove the theorem, we will now determine values of $\theta_0, \theta_1, \theta_2$ and θ_3 such that (4.8.50) together with (4.8.51) yields a contradiction. Fix

$$\theta_1 = 2\sqrt{\frac{5s}{\beta_s}}, \quad \theta_2 = \frac{c_1}{\beta_s}, \quad \theta_3 = \frac{c_2}{\beta_s}\,. \tag{4.8.52}$$

Then combining (4.8.50), (4.8.51) and (4.8.52) we arrive at

$$\theta_0 \le \frac{1}{\beta_s}\left(1 + \frac{s^2-1}{12}\sqrt{t_{\mathrm{c}}}\left(\frac{Z}{\theta_0 Z + \theta_1 Z^{1/2} + \theta_2 Z^{1/3} + \theta_3 Z^{-4/3}}\right)^{1/2}\right).$$

Consequently,

$$\theta_0 \le \frac{1}{\beta_s}\left(1 + \frac{s^2-1}{12}\left(\frac{t_{\mathrm{c}}}{\theta_0}\right)^{1/2}\right). \tag{4.8.53}$$

Recall that our goal is to determine the smallest possible value of θ_0 for a given $s > 1$ at which (4.8.53) no longer holds. Choose $\theta_0 = x^{-2}t_c$ then we need to find $x > 0$ such that

$$\beta_s t_c \le \left(1 + \frac{s^2-1}{12}x\right)x^2 \tag{4.8.54}$$

fails. For fixed $s \ge 1$, the cubic equation (4.8.54) has a unique positive solution that can be computed explicitly. A numerical investigation with $t_c \approx 1.21$ shows that at $s = 1.66$, one can prove the best results. Thus, we fix $s = 1.66$. In this case $\beta_{1.66} < 0.782$ and consequently we may choose $x = x_0$ as the unique positive solution of

$$0.782\, t_c = (1 + 0.1463 x_0)\, x_0^2$$

and consequently $\theta_0 = x_0^{-2}t_c$. For $t_c \approx 1.21$ one finds $x_0 \approx 0.913597\ldots$ which gives $\theta_0 < 1.45$ Thus we have found

$$N_c \le \frac{t_c}{x_0^2}Z + \theta_1 Z^{1/2} + \theta_2 Z^{1/3} + \theta_3 Z^{-4/3} \tag{4.8.55}$$

with

$$\theta_1 = 2\sqrt{\frac{5s}{\beta_s}}, \quad \theta_2 = \frac{c_1}{\beta_s}, \quad \theta_3 = \frac{c_2}{\beta_s}\,.$$

With $s = 1.66$ and $t_c \ge 1$

$$\theta_1 \le 6.52, \quad \theta_2 \le 0.361, \quad \theta_3 \le 0.378\,.$$

This proves Theorem 4.2.7. ∎

Chapter 5

Why a System of Three Bosons On Separate Lines Can Not Exhibit The Confinement Induced Efimov Effect

5.1 Introduction

5.1.1 The physical system

We study a system consisting of three quantum particles (bosons) with *short–range* interactions confined to move on separate lines within $\mathbb{R}^3$, see Figure 5.2 in Section 5.2. Two of these lines, L_2 and L_3, are parallel to each other within a plane P, while the first line, L_1, is constrained to a plane perpendicular to P which does not intersect L_2 or L_3. That is the intersection of the plane on which L_1 lies with the plane P forms a line parallel to L_2 and L_3. The line L_1 intersects P at an angle $\zeta \in (0, \pi/2]$. Without loss of generality, we can fix the point of intersection of the line L_1 and the plane P as the origin.
Recently the physicists Nishida and Tan predicted that this system might exhibit the so–called confinement induced Efimov effect. This, in particular, means that it should have an infinite number of negative eigenvalues if two–particle subsystems do not have bound states but have resonances at the bottom of the essential spectrum. the possible existence of Efimov type effects in such *geometrically constrained quantum systems*, see [87],[86]).

Our main result, see Theorem 5.2.1, shows that this prediction is *not correct*. We prove that the geometrically constrained three–particle system discussed above can have at most finitely many bound states for a large class of short–range potentials.

5.1.2 The Efimov effect.

It is well known that an one-particle Schrödinger operator $-\Delta + V(x)$ on $L^2(\mathbb{R}^d)$ with relatively bounded potential decaying faster than $|x|^{-2-\delta}$, $\delta > 0$ may have only a finite number of eingenvalues. It was proven by Zhislin [129] and Yafaev [59] using two different methods that N-particle Schrödinger operators, under the same conditions on the potentials, possess only a finite number of eigenvalues if at least one of the subsystems has a bound state below zero.

It was very surprising when physicist Efimov found in 1970 [28] that a system of three particles in $\mathbb{R}^3$ with short–range pairwise interactions may have an *infinite number* of eigenvalues when the two–particle subsystems do not have bound states, but have resonances at the bottom of the spectrum.
Beyond the infinite accumulation of bound states, the Efimov effect exhibits several remarkable properties, one of the most significant being its universality. This means that the discrete spectrum's asymptotic behavior remains the same, regardless of the microscopic specifics of the underlying pair–potentials. In particular, the number of bound states $N(E)$ below $E < 0$ satisfies the *universal* asymptotic behavior

$$\lim_{E \to 0^-} \frac{N(E)}{|\ln(|E|)|} = C_0 \tag{5.1.1}$$

for some constant $C_0 > 0$, which depends solely on the particle masses and not on the interaction potentials.
Both in mathematics and physics, the study of the Efimov effect became a highly recognized challenge. After Efimov's initial description, the first rigorous mathematical proof was provided by Yafaev in 1970 [59], followed by a variational proof by Ovchinnikov and Sigal in 1979 [89] and Tamura in [113]. The asymptotic behavior of the number of bound states, which was already predicted by Efimov, was later confirmed mathematically by Sobolev in 1993 [108]. Until the end of the 1990s, several significant physical and mathematical findings had emerged on this topic (see, e.g., [116], [66], [91], [90], [120] and [118])
Despite its universality property, the Efimov effect is an exceptionally rare phenomenon, primarily due to the necessary presence of virtual levels in two–particle subsystems. In experiments, it is difficult to create conditions where two–particle subsystems have zero–energy resonances. Moreover, the Efimov bound states have a large size and are very weakly bound. This makes the Efimov effect exceedingly challenging to observe.
However, technological advancements in the 1990s, such as improved laser cooling techniques, enabled the study of resonant systems through the application of magnetic fields and so–called *Feshbach resonances* (see, e.g., [116], [55], and [25]). The first experimental observation of the Efimov effect was achieved in 2002 in an ultracold gas of cesium atoms, which was published in 2006 [67]. Later, in experiments with potassium atoms, two consecutive Efimov states have been observed [126], obtaining data consistent with the universal scaling property in (5.1.1). By the late 2000s, evidence of the Efimov effect was found for various other particles, including cases beyond systems of three identical bosons (see, e.g., [43], [92], [10] and [124]). For a more detailed review of the experimental results on the Efimov effect, see [33] and the references therein. The experimental verification of the Efimov effect generated renewed and significant academic interest. For a comprehensive review, see [84] (published in 2017), which includes over 400 references, most of them from after 2009.
Experimental and theoretical studies have recently explored the existence of effects similar to the Efimov effect. A natural question is: does the Efimov effect extend to N–particle systems for $N > 3$ when the $(N-1)$–particle subsystems possess a virtual level? It is known that in systems with $N \geq 4$ bosons in three dimensions, the effect is absent [4], [12], [42].

Another question is whether the effect can exist in spatial dimensions other than three, which occur, for example, in configurations involving graphene or by confinement of particles via optical lattices. In systems of N bosons, the absence of the Efimov effect in dimension one has been established in [12]. In the same work, it was proved that for N two–dimensional bosons, the Efimov effect is absent, except in the case $N = 4$. Physicists predict that for $N = 4$, the Efimov effect exists only if the system interacts solely via three-particle forces. Mathematically, this is still an open problem.
For $N = 3$ in dimensions greater than five, virtual levels correspond to bound states of two–particle subsystems, resulting in the non–existence of the Efimov effect. The situation in dimension four is more complex since virtual levels in this case are resonances but not bound states, however, the decay rate is so high, that the resonance barely misses to be L^2. The non–existence of the Efimov effect for three bosons in dimension four was demonstrated by the use of so–called *Faddeev equations* in [11]. This completes the picture for the existence or non–existence of the Efimov effect for (bosonic) three–particle systems in all dimensions.
Recent advancements in experiments with ultracold gases have enabled the confinement of particles to lower–dimensional subspaces using strong optical lattices (see, e.g., [40], [112]). This development enables the study of systems with *mixed dimensionality*, where different species of particles are confined to distinct subspaces of dimension less than three. The physicists Nishida and Tan discussed the possible existence of Efimov type effects in such geometrically constrained systems (see [87],[86]). In [85], they examined the possibility of this effect occurring in a mixture of ^{40}K and ^{6}Li isotopes, where the conventional Efimov effect is known to be absent. They argued that confining ^{40}K particles to a one–dimensional subspace is a promising system for the so–called *confinement induced Efimov effect*. However, a rigorous mathematical description of these scenarios remains an open question. In [84], the predictions on the Efimov effect among various configurations of three particles with mixed dimensionality have been summarized. We present the table [84, page 44, Table 1] and these predictions in Figure 5.1 below. In this work, we examine one of the cases. Namely, the case (1D-1D x 1D) on the bottom right.
We prove that, contrary to the predictions made, this system can support only a finite number of bound states, even if there are virtual levels in the two–particle subsystems.
This configuration is particularly intriguing because it is a truly mixed dimensional system, consisting of one one–dimensional and two two–dimensional subsystems.
Our approach is based on methods developed by Vugalter and Zhislin (see, e.g., [129], [120], [118] and [119]), which were recently applied in [13] to establish the absence of the Efimov effect in unconstrained N–particle systems in dimensions one and two. As usual, an important part of the work is the study of the decay properties of resonances, which may occur at the bottom of the spectrum of subsystems. To the best of our knowledge, the decay of resonances has only been studied in the case of rotational symmetric potentials. However, for this mixed dimensional system, the subsystems are not necessarily rotational invariant, which tremendously complicates the analysis of the decay properties of zero–energy solutions. Although this solutions are not functions in $L^2(\mathbb{R}^2)$ using a modification of techniques from [49], [47], [12], [13] and [9], which extend the method of [2], we show that the projection of these solutions onto the subspace orthogonal to radially symmetric functions are in $L^2(\mathbb{R}^2)$.

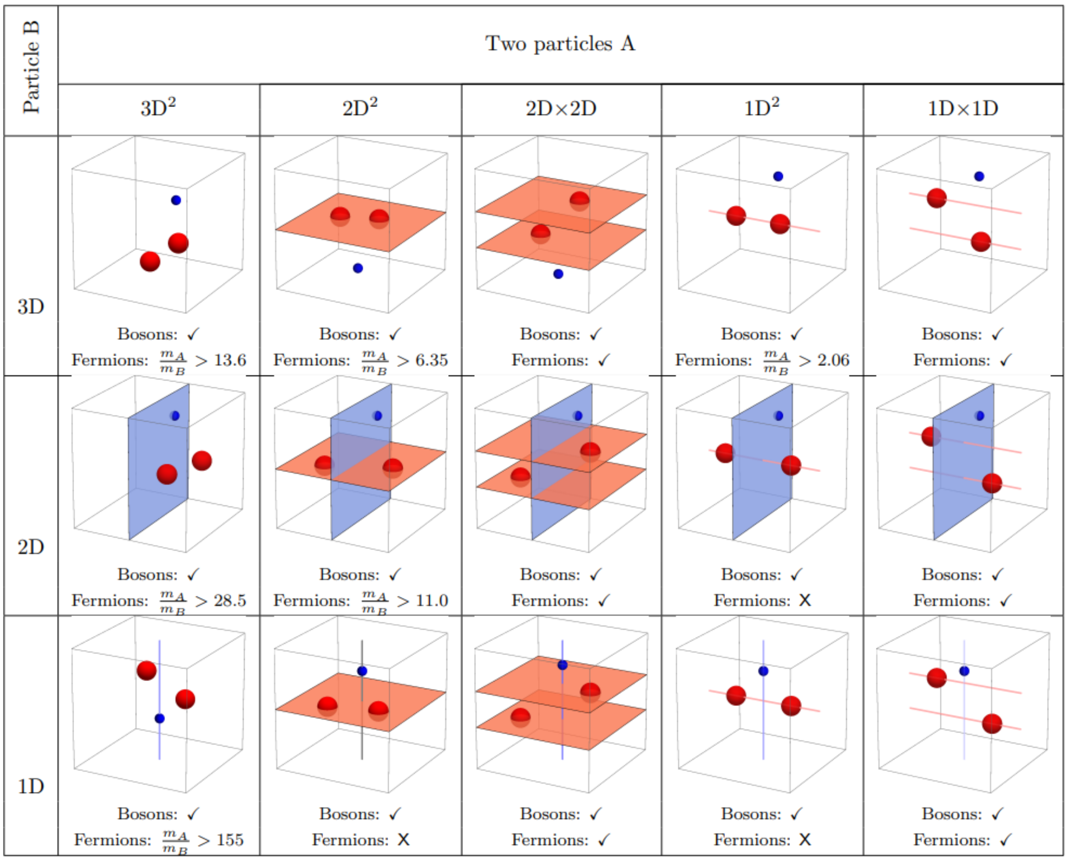

FIGURE 5.1: Predictions on the confinement induced Efimov effect. Table taken from [84, page 44, Table 1]. For each case, it is indicated whether the Efimov effect is predicted to occur (✓) or not (x).

The paper is structured as follows. In Section 5.2, we give main definitions, state our main result, and address the (lack of) symmetries within the two–particle subsystems. In Section 5.3.1, we state four lemmas and show how they lead to a proof of our main theorem regarding the finiteness of the discrete spectrum.

As preparation for proving these lemmas, Section 5.4 examines the decay properties of the zero–energy solutions within a given symmetry subspace. It turns out that the part of a resonance in angular momentum subspaces different from zero angular momentum has faster decay than the part in the zero angular momentum subspace (the s channel in physics language). We finish the proof of the main theorem by proving the remaining lemmas from Section 5.3.1 in Section 5.5.

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5.2 Definitions and Main Result

Let $y_i \in \mathbb{R}$ be the distance of the i-th particle from the origin along the line L_i, and let $\mathbf{r}_i \in \mathbb{R}^3$ be the three–dimensional position vector of this particle. Then

$$\mathbf{r}_1 = \begin{pmatrix} y_1 \cos(\zeta) \\ 0 \\ y_1 \sin(\zeta) \end{pmatrix}, \ \mathbf{r}_2 = \begin{pmatrix} y_2 \\ a_2 \\ 0 \end{pmatrix}, \ \mathbf{r}_3 = \begin{pmatrix} y_3 \\ a_3 \\ 0 \end{pmatrix},$$

where $a_j \in \mathbb{R}$ with $j \in \{2,3\}$ denotes the distances between the line L_j and the $\hat{e}_1$–axis as indicated in Figure 5.2.
Denote by $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ the distance between the particles i and j. The Schrödinger operator of the system, expressed in this coordinate system, is given by

$$H = -\sum_{i=1}^{3} \frac{1}{m_i} \frac{\partial^2}{\partial y_i^2} + \sum_{\alpha \in I} V_\alpha(|\mathbf{r}_\alpha|) \tag{5.2.1}$$

where $V_\alpha : \mathbb{R} \longrightarrow \mathbb{R}$ is the interaction potential between the particle pairs, indexed by $\alpha \in I$, with $I := \{(12), (13), (23)\}$ and $m_1, m_2, m_3 > 0$ are the masses of the particles. We study the

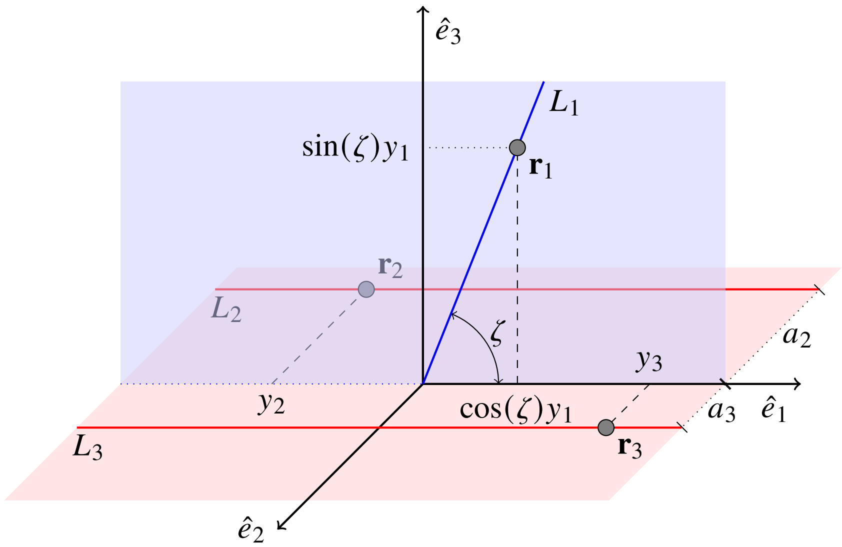

FIGURE 5.2: Geometrically constrained configuration space of particles.

system of three bosons given by the operator H in (5.2.1). Regarding the potentials we assume that $V_{1j} \in L^2_{\text{loc}}(\mathbb{R}^2)$ and $V_{23} \in L^2_{\text{loc}}(\mathbb{R})$ and there exist constants $C, \delta > 0$ and $A > 0$ such that for $|\mathbf{r}_\alpha| > A$.

$$|V_\alpha(|\mathbf{r}_\alpha|)| \le C(1 + |\mathbf{r}_\alpha|)^{-\nu_\alpha}, \tag{5.2.2}$$

where $\nu_{23} := 2 + \delta$ and $\nu_{12} := \nu_{13} := 3 + \delta$. Note that by short–range one typically refers to potentials which decay as $|\cdot|^{-2-\delta}$ at infinity. To ensure the applicability of specific decay

estimates on the so–called zero–energy resonances of two–particle subsystems, we assume a stronger decay condition on the interaction potentials V_{12} and V_{13}.
In addition, the particles always maintain a minimum distance, making the presence or absence of singularities in the potentials at very small distances irrelevant, except in the special cases where $a_2 = 0$ or $a_3 = 0$, when the particles 1 and 2, respectively, 1 and 3, can come arbitrarily close to each other. Denote by $\sigma_{\text{ess}}(H)$ the essential and by $\sigma_{\text{disc}}(H)$ the discrete spectrum of H. Our main result is

Theorem 5.2.1. *Let H be the operator defined in equation* (5.2.1) *with V_α fulfilling* (5.2.2) *for any $\alpha \in I = \{(12), (13), (23)\}$. Assume that $\sigma_{\text{ess}}(H) = [0, \infty)$. Then $\sigma_{\text{disc}}(H)$ is at most finite. Contrary to the prediction in [84], this system does not exhibit a confinement induced Efimov effect.*

Remarks 5.2.2. *The statement of Theorem 5.2.1 does not impose any conditions on the existence or absence of resonances in two–particle subsystems.*

For each $\alpha = (ij) \in I$ we denote by h_α the corresponding two–body Hamiltonian:

$$h_\alpha \coloneqq -\frac{1}{m_i}\frac{\partial^2}{\partial y_i^2} - \frac{1}{m_j}\frac{\partial^2}{\partial y_j^2} + V_\alpha(|\mathbf{r}_\alpha|)\,. \tag{5.2.3}$$

Let $\Sigma_{ij} \coloneqq \inf \sigma(h_{ij})$ be the bottom of the spectrum of h_{ij} and let $\Sigma \coloneqq \min\{\Sigma_\alpha : \alpha \in I\}$. Analogously to the HVZ theorem for systems without geometrical constraints [93, Theorem XIII.17], we have $\sigma_{\text{ess}}(H) = [\Sigma, \infty)$. Under the conditions of Theorem 5.2.1, $\Sigma = 0$ and consequently $h_\alpha \geq 0$.
By appropriate rescaling, we can remove the dependence on the masses from the kinetic part of the Hamiltonian H. Let $x = (x_1, x_2, x_3)$ with

$$x_i = \sqrt{m_i}\, y_i \text{ for } i \in \{1, 2, 3\}$$

and $|x| \coloneqq (x_1^2 + x_2^2 + x_3^2)^{1/2}$, then

$$H = -\sum_{i=1}^{3} \frac{\partial^2}{\partial x_i^2} + \sum_{\alpha\in I} V_\alpha(|\mathbf{r}_\alpha|) = -\Delta_x + \sum_{\alpha\in I} V_\alpha(|\mathbf{r}_\alpha|) \tag{5.2.4}$$

and

$$h_{ij} = -\frac{\partial^2}{\partial x_i^2} - \frac{\partial^2}{\partial x_j^2} + V_{ij}(|\mathbf{r}_{ij}|)\,.$$

In abuse of notation, we denote the transformed operator by the same letter. In this new set of coordinates the distances $|\mathbf{r}_\alpha|$ are

$$\begin{aligned} \left|\mathbf{r}_{1j}\right| &= \left(\frac{x_1^2}{m_1} + \frac{x_j^2}{m_j} - 2\frac{\cos(\zeta)}{\sqrt{m_1 m_j}} x_1 x_j + a_j^2\right)^{1/2}, \\ |\mathbf{r}_{23}| &= \left(\left(\frac{x_2}{\sqrt{m_2}} - \frac{x_3}{\sqrt{m_3}}\right)^2 + (a_2 - a_3)^2\right)^{1/2}. \end{aligned} \tag{5.2.5}$$

Note that $\left|\mathbf{r}_{1j}\right|$ remains unchanged under reflection $(x_1, x_j) \mapsto (-x_1, -x_j)$. This symmetry of the potentials will play an important role in our analysis.

5.3 Absence of the Efimov Effect

5.3.1 Proof of Theorem 5.2.1

By the min–max principle, it is sufficient to find a finite–dimensional subspace $\mathcal{M} \subset L^2(\mathbb{R}^3)$ such that for any $\psi \in L^2(\mathbb{R}^3)$ orthogonal to $\mathcal{M}$

$$\langle \psi, H\psi \rangle \geq 0 \,.$$

Such a space $\mathcal{M}$ exists, see for example the work by Zhislin [129], if there are constants $b, \tau > 0$ such that

$$L[\psi] := \int_{\mathbb{R}^3} \left(\sum_{i=1}^{3} \left|\partial_{x_i}\psi\right|^2 + \sum_{\alpha\in I} V_\alpha |\psi|^2 \right) dx - \int_{|x|\in[b,2b]} \frac{|\psi|^2}{|x|^{2+\tau}} dx \geq 0 \tag{5.3.1}$$

for any $\psi \in C_0^1(\mathbb{R}^3)$ with $\operatorname{supp}\psi \subset \{x \in \mathbb{R}^3 : |x| > b\}$. We emphasize that no smallness condition of the parameter $\tau > 0$ is needed. Everywhere below we assume that $b > 0$ is sufficiently large and $\tau > 0$ is a fixed number which is less than δ, where $\delta > 0$ is the parameter in the decay condition on the interaction potentials in (5.2.2). Let

$$\begin{aligned} K_{1j}(\gamma) &:= \{x \in \mathbb{R}^3 : \left(x_1^2 + x_j^2\right)^{1/2} \leq \gamma|x|\}, \quad j \in \{2,3\}\,, \\ K_{23}(\gamma) &:= \left\{x \in \mathbb{R}^3 : \left|\frac{x_2}{\sqrt{m_2}} - \frac{x_3}{\sqrt{m_3}}\right| \leq \gamma|x|\right\}, \\ \Omega(\gamma) &:= \mathbb{R}^3 \setminus \{K_{12}(\gamma) \cup K_{13}(\gamma) \cup K_{23}(\gamma)\}\,. \end{aligned} \tag{5.3.2}$$

In the following we denote by $\partial K_\alpha(\gamma)$ the boundary of $K_\alpha(\gamma)$. The sets $K_\alpha(\gamma)$ describe parts of the configuration space where the particles i and j in $\alpha = (ij)$ are close to each other compared to their distance from the third particle $k \neq \{i, j\}$. In Lemma B.2.1 in the Appendix B, we show that the sets $K_\alpha(\gamma)$ do not intersect, except for $x = 0$, for sufficiently small $\gamma > 0$.

Let $\mathbb{1}_A$ be the indicator function of the set $A \subset \mathbb{R}^3$ and define $\psi_\alpha := \psi \mathbb{1}_{K_\alpha(\gamma)}$ and $\psi_0 := \psi \mathbb{1}_{\Omega(\gamma)}$. We prove (5.3.1) by estimating for all $\alpha \in I$ the *local energies*

$$\begin{aligned} L_\alpha[\psi_\alpha] &:= \int_{K_\alpha(\gamma)} \left(|\nabla \psi_\alpha|^2 + \sum_{\beta \in I} V_\beta |\psi_\alpha|^2 \right) dx - \int_{K_\alpha(\gamma)} \frac{|\psi_\alpha|^2}{|x|^{2+\tau}} dx\,, \\ L_0[\psi_0] &:= \int_{\Omega(\gamma)} \left(|\nabla \psi_0|^2 + \sum_{\alpha \in I} V_\alpha |\psi_0|^2 \right) dx - \int_{\Omega(\gamma)} \frac{|\psi_0|^2}{|x|^{2+\tau}} dx\,, \end{aligned} \tag{5.3.3}$$

and noting

$$L[\psi] = L_0[\psi_0] + \sum_{\alpha \in I} L_\alpha[\psi_\alpha]\,. \tag{5.3.4}$$

Note that we use a hard cut–off in the definition of the local energies L_α and L_0. The analysis of these local energies will involve boundary terms on $\partial K_\alpha(\gamma)$ and $\partial\Omega(\gamma)$. The analysis will proceed in several steps. As a first step, we show that the functionals L_α for $\alpha \in I$ can be bounded in terms of boundary integrals over $\partial K_\alpha(\gamma)$. This is done in the following two lemmas.

Lemma 5.3.1. *Fix $\alpha \in \{(12), (13)\}$ and let $P_0[\alpha]$ be the projection in $L^2(\mathbb{R}^3)$ onto functions that are invariant under rotations of the coordinates (x_1, x_j) describing the position of the particle pair $\alpha = (ij)$. Under the conditions of Theorem 5.2.1 there exists a constant $c > 0$, independent of ψ, such that*

$$L_\alpha[\psi_\alpha] \geq -c \int_{\partial K_\alpha(\gamma)} \frac{|P_0[\alpha]\psi|^2}{|x|^{1+\tau}} d\sigma\,. \tag{5.3.5}$$

The statement of Lemma 5.3.1 is similar to [13, Lemma 6.7], whereas its proof is significantly more complex. It is based on a detailed analysis of properties of zero-energy resonances of two–dimensional systems, which will be done in Section 5.4.
For the functional $L_{23}[\psi_{23}]$, we prove the following bound, whose proof is similar to the proof of [13, Theorem 6.1].

Lemma 5.3.2. *Under the conditions of Theorem 5.2.1, there exists a constant $c > 0$ such that*

$$L_{23}[\psi_{23}] \geq -c \int_{\partial K_{23}(\gamma)} \frac{|\psi|^2}{|x|^{1+\tau}} d\sigma\,. \tag{5.3.6}$$

As the second step, applying the one–dimensional Trace Theorem (see, [31, Theorem 1, p. 272]) and Hardy Inequality, we show that the right–hand sides of (5.3.5) and (5.3.6) can be controlled by a small part of the kinetic energy term on the set $\Omega(\gamma)$. This is done in the following two lemmas.

Lemma 5.3.3. *For $\gamma_1 \in (\gamma, 1)$ and $\alpha \in \{(12), (13)\}$, we define $K_\alpha(\gamma, \gamma_1) := K_\alpha(\gamma_1) \setminus K_\alpha(\gamma)$. For any $\varepsilon > 0$, for sufficiently large $b > 0$ holds*

$$\int_{\partial K_\alpha(\gamma)} \frac{|P_0[\alpha]\psi|^2}{|x|^{1+\tau}} d\sigma \le \varepsilon \int_{K_\alpha(\gamma,\gamma_1)} |\nabla\psi|^2 dx\,. \tag{5.3.7}$$

Lemma 5.3.4. *Let $\gamma_1 \in (\gamma, 1)$ and define $K_{23}(\gamma,\gamma_1) := K_{23}(\gamma_1) \setminus K_{23}(\gamma)$. For any $\varepsilon > 0$ we have*

$$\int_{\partial K_{23}(\gamma)} \frac{|\psi|^2}{|x|^{1+\tau}} d\sigma \le \varepsilon \int_{K_{23}(\gamma,\gamma_1)} |\nabla\psi|^2 dx\,. \tag{5.3.8}$$

for all sufficiently large $b > 0$.

Assuming the Lemmas 5.3.1, 5.3.2, 5.3.3 and 5.3.4 for the moment, we give the

Proof of Theorem 5.2.1: Using the bounds of Lemma 5.3.3 and 5.3.4 in (5.3.4) and assuming that $\gamma_1 > \gamma$ is close enough to γ so that the regions $K_\alpha(\gamma,\gamma_1) = K_\alpha(\gamma_1) \setminus K_\alpha(\gamma)$ for $\alpha \in I$ do not overlap, we arrive at

$$\begin{aligned} L[\psi] &\ge L_0[\psi_0] - \varepsilon \sum_{\alpha\in\{(12),(13)\}} \int_{K_\alpha(\gamma,\gamma_1)} |\nabla\psi|^2 dx - \varepsilon \int_{K_{23}(\gamma,\gamma_1)} |\nabla\psi|^2 dx \\ &\ge L_0[\psi_0] - 3\varepsilon \int_{\Omega(\gamma)} |\nabla\psi|^2 dx\,. \end{aligned} \tag{5.3.9}$$

where $\varepsilon > 0$ is arbitrary small and $b > 0$ large. Choosing $b > 0$ large enough, Lemma B.2.2 shows that each of the potentials satisfies $|V_\alpha| \le C|x|^{-\nu_\alpha}$ for some constant $C > 0$ on $\Omega(\gamma) \cap \{x : |x| > b\}$. Thus, for fixed $\varepsilon > 0$ we have $|V_\alpha| \le \varepsilon|x|^{-2}$ for $x \in \Omega(\gamma)$ with $|x| > b$ and all sufficiently large $b > 0$. Hence,

$$L_0[\psi_0] - 3\varepsilon \int_{\Omega(\gamma)} |\nabla\psi|^2 dx \ge (1-3\varepsilon) \int_{\Omega(\gamma)} |\nabla\psi|^2 dx - \varepsilon \int_{\Omega(\gamma)} \frac{|\psi|^2}{|x|^2} dx\,. \tag{5.3.10}$$

The set $\Omega(\gamma) \subset \mathbb{R}^3$ is conical and applying the radial Hardy inequality for the last term on the right–hand side of (5.3.10) (see B.1.3) yields

$$L_0[\psi_0] - 3\varepsilon \int_{\Omega(\gamma)} |\nabla\psi|^2 dx \ge (1-7\varepsilon) \int_{\Omega(\gamma)} |\nabla\psi|^2 dx\,.$$

This completes the proof of Theorem 5.2.1. ∎

5.4 Zero–Energy Resonances

To prove Lemma 5.3.1, we will need some properties of zero–energy resonances of two–particle Schrödinger Operators in dimension two. The most important of them are the estimates on the decay of such resonances, which will be given in Lemma 5.4.3.
Let

$$h = -\Delta + V \text{ on } L^2(\mathbb{R}^2) \tag{5.4.1}$$

with V satisfying (5.2.2) with parameter $\nu_\alpha = 3 + \delta$ for some $\delta > 0$ and $V(x) = V(-x)$. Following [61], we say that h has a virtual level (zero–energy resonance) if $h \geq 0$ and for any $\varepsilon > 0$, $h + \varepsilon\Delta$ has an eigenvalue below zero.
Let $\dot{H}^1(\mathbb{R}^2)$ be the homogeneous Sobolev space defined as

$$\dot{H}^1(\mathbb{R}^2) \coloneqq \{u \in L^2_{\text{loc}}(\mathbb{R}^2) : \nabla u \in L^2(\mathbb{R}^2)\},$$

equipped with the norm

$$\|u\|_{\dot{H}^1(\mathbb{R}^2)} \coloneqq \left(\int_{\mathbb{R}^2} |\nabla u|^2 dx + \int_{|x|\leq 1} |u|^2 dx\right)^{1/2} .$$

We will use the following result of [13, Theorem 2.2]

Lemma 5.4.1. *Assume that h has a virtual level. Then*

1. *there exists a unique non–negative* $\varphi_0 \in \dot{H}^1(\mathbb{R}^2)$ *with* $\|\varphi_0\|_{\dot{H}^1(\mathbb{R}^2)} = 1$ *such that for any* $\psi \in \dot{H}^1(\mathbb{R}^2)$
$$\langle \nabla\psi, \nabla\varphi_0\rangle + \langle \psi, V\varphi_0\rangle = 0 . \tag{5.4.2}$$
2. *there exists* $\mu > 0$ *such that for any* $\psi \in H^1(\mathbb{R}^2)$ *with* $\langle \nabla\psi, \nabla\varphi_0\rangle = 0$
$$\langle \psi, h\psi\rangle \geq \mu\|\nabla\psi\|^2 . \tag{5.4.3}$$

Remark 5.4.2. *Note that, in general,* $\varphi_0 \notin L^2(\mathbb{R}^2)$*. Moreover, if the potential V is radially symmetric and compactly supported, it is easy to see that* φ_0 *is also a radially symmetric function that does not decay at infinity. If V is not radially symmetric, then* φ_0 *is not radially symmetric either. For this case, we prove that if V is symmetric under reflection, then the projection of* φ_0 *onto the subspace orthogonal to radially symmetric functions is in* $L^2(\mathbb{R}^2)$*. The proof is given in the next lemma.*

Let P_0 the projection onto radially symmetric functions in $L^2(\mathbb{R}^2)$ and $P_\perp \coloneqq 1 - P_0$ the projection onto its orthogonal complement. The next result shows that even though $\varphi_0 \notin L^2(\mathbb{R}^2)$ its projection $P_\perp\varphi_0$ is in a weighted L^2–space.

Lemma 5.4.3. *Let* φ_0 *be a virtual level of h, then there exists* $l(\delta) > 0$ *such that*

$$(1 + |\cdot|)^l P_\perp\varphi_0 \in L^2(\mathbb{R}^2) . \tag{5.4.4}$$

5.4.1 Proof of Lemma 5.4.3

Let $f \coloneqq P_0\varphi_0$ and $g \coloneqq P_\perp\varphi_0$. Since $V(x) = V(-x)$, a virtual level φ_0 can be either an even or odd function with respect to reflection. However, by Lemma 5.4.1, φ_0 is non–negative, which implies that it must be an even function. Consequently, for almost all $|x|$,

$$\int_0^{2\pi} e^{\pm i\theta} g(|x|, \theta) d\theta = 0 .$$

Note that for all functions $F(|x|,\theta) \in \dot{H}^1(\mathbb{R}^2)$ orthogonal to radially symmetric functions with

$$\int_0^{2\pi} e^{\pm i\theta} F(|x|,\theta) d\theta = 0 \tag{5.4.5}$$

the following inequality holds:

$$\int_{\mathbb{R}^2} |\nabla F|^2 \, dx \geq 4 \int_{\mathbb{R}^2} \frac{F(x)^2}{|x|^2} \, dx \,. \tag{5.4.6}$$

In particular (5.4.6) holds for $F = g$. To prove (5.4.4) it suffices now to show that

$$\nabla \left((1+|\cdot|)^{l+1} g \right) \in L^2(\mathbb{R}^2) \,. \tag{5.4.7}$$

Choose $\xi \in C^\infty([0,\infty))$ with $\xi(t) = 0$ for $t \leq 1$ and $\xi(t) = 1$ for $t \geq 2$, such that $\xi(t) \leq 1$ and $\xi'(t) \leq 2$ for any $t \in [0,\infty)$. For any $\omega, \kappa, \beta > 0$ we define

$$G(|x|) \coloneqq \frac{|x|^\kappa}{1+\omega|x|^\kappa} \xi(|x|/\beta) \,. \tag{5.4.8}$$

Inserting $\psi = G^2 g$ into (5.4.2) and writing $\varphi_0 = f + g$ yields

$$0 = \langle G^2 g, hf \rangle + \langle G^2 g, hg \rangle \,. \tag{5.4.9}$$

Since P_0 and $P_\perp$ commute with $-\Delta$, it holds

$$\langle G^2 g, hf \rangle = \langle Gg, VGf \rangle \,. \tag{5.4.10}$$

Observe that

$$\begin{aligned} \langle G^2 g, hg \rangle &= \langle Gg, hGg \rangle - \left\langle Gg, \frac{|\nabla G|^2}{G^2} Gg \right\rangle \\ &= \|\nabla(Gg)\|^2 + \langle Gg, VGg \rangle - \left\langle Gg, \frac{|\nabla G|^2}{G^2} Gg \right\rangle \,. \end{aligned} \tag{5.4.11}$$

Combining (5.4.9), (5.4.10) and (5.4.11) we arrive at

$$\|\nabla(Gg)\|^2 + \langle Gg, VGg \rangle - \left\langle Gg, \frac{|\nabla G|^2}{G^2} Gg \right\rangle + \langle Gg, VGf \rangle = 0 \,. \tag{5.4.12}$$

We claim, there exists some $\varepsilon > 0$ and a constant $c(\beta) > 0$ that both are independent of ω such that

$$\langle Gg, VGg \rangle - \left\langle Gg, \frac{|\nabla G|^2}{G^2} Gg \right\rangle + \langle Gg, VGf \rangle \geq -(1-\varepsilon)\|\nabla(Gg)\|^2 - c(\beta)\|\varphi_0\|_{\dot{H}^1}^2 \,. \tag{5.4.13}$$

Assuming this claim for the moment, we complete the proof of Lemma 5.4.3. Combining (5.4.12) with (5.4.13) yields

$$\varepsilon\|\nabla(Gg)\|^2 \le c(\beta)\|\varphi_0\|^2_{\dot{H}^1}$$

and consequently $\|\nabla(Gg)\|^2$ is bounded uniformly in ω, which proves (5.4.7) with $\kappa = l+1$. Then, taking the limit $\omega \to 0$ concludes the proof of Lemma 5.4.3. ∎

We prove the remaining statement in (5.4.13) by estimating each of the terms on the left–hand side of (5.4.13) separately.

5.4.2 First Term in (5.4.13)

The function G vanishes for $|x| < \beta$ and V fulfills (5.2.2) and therefore there exists $C > 0$ such that

$$|\langle Gg, VGg\rangle| \le \frac{C}{(1+\beta)^{1+\delta}} \int_{|x|>\beta} \frac{|Gg|^2}{|x|^2} dx \le \frac{4C}{(1+\beta)^{1+\delta}} \|\nabla(Gg)\|^2 . \tag{5.4.14}$$

5.4.3 Second Term in (5.4.13)

In Lemma B.3.1 in Appendix B we show for $|x| > 2\beta$ that

$$|\nabla G(x)| \le \kappa |x|^{-1} G(x) \quad \text{for} \quad |x| > 2\beta \tag{5.4.15}$$

and

$$|\nabla G(x)|^2 \le \beta^{\kappa-1}\left(2^{\kappa+1} + \kappa 2^{\kappa-1}\right) =: c_1(\beta) \quad \text{for} \quad |x| \in [\beta, 2\beta] . \tag{5.4.16}$$

Recall that the function Gg is orthogonal to radially symmetric functions and in addition satisfies (5.4.5), consequently (5.4.15) together with (5.4.6) yields

$$\int_{|x|\ge 2\beta} \frac{|\nabla G|^2}{G^2} |Gg|^2 dx \le \kappa^2 \int_{|x|\ge 2\beta} |x|^{-2}|Gg|^2 dx \le \frac{\kappa^2}{4}\|\nabla(Gg)\|^2 . \tag{5.4.17}$$

By combining (5.4.16) and (5.4.17), we obtain

$$\begin{aligned} \left\langle Gg, \frac{|\nabla G|^2}{G^2} Gg \right\rangle &\le \int_{\beta\le|x|\le 2\beta} |\nabla G|^2 |g|^2 dx + \int_{|x|\ge 2\beta} |\nabla G|^2 |g|^2 dx \\ &\le c_1(\beta) \int_{\beta\le|x|\le 2\beta} |g|^2 dx + \frac{\kappa^2}{4}\|\nabla(Gg)\|^2 . \end{aligned} \tag{5.4.18}$$

Applying (5.4.6) gives

$$\begin{aligned}\int_{\beta\le|x|\le 2\beta}|g|^2dx &\le (2\beta)^2\int_{\beta\le|x|\le 2\beta}|x|^{-2}|g|^2dx\\ &\le 4(2\beta)^2\int_{\mathbb{R}^2}|\nabla g|^2dx\\ &\le 4(2\beta)^2\|\varphi_0\|^2_{\dot H^1}\,.\end{aligned} \tag{5.4.19}$$

Inserting (5.4.19) into (5.4.18) yields

$$\left\langle Gg, \frac{|\nabla G|^2}{G^2}Gg\right\rangle \le \frac{\kappa^2}{4}\|\nabla(Gg)\|^2 + c_2(\beta)\|\varphi_0\|^2_{\dot H^1} \tag{5.4.20}$$

where $c_2(\beta) = 4(2\beta)^2 c_1(\beta)$.

5.4.4 Third Term in (5.4.13)

Let $\tilde\varepsilon > 0$. By (5.2.2) and Schwarz Inequality, we obtain

$$\begin{aligned}|\langle Gg, VGf\rangle| &\le C\int_{|x|>\beta}\frac{|Gg|}{|x|^{1+\delta/2}}\frac{|Gf|}{|x|^{2+\delta/2}}dx\\ &\le C\tilde\varepsilon\int_{|x|>\beta}\frac{|G|^2}{|x|^{2+\delta}}|g|^2dx + \frac{C}{\tilde\varepsilon}\int_{|x|>\beta}\frac{|G|^2}{|x|^{4+\delta}}|f|^2dx\,.\end{aligned} \tag{5.4.21}$$

Using (5.4.6) for Gg in the first term on the right–hand side of (5.4.21) we get

$$C\tilde\varepsilon\int_{|x|>\beta}\frac{|G|^2}{|x|^{2+\delta}}|g|^2dx \le \frac{C\tilde\varepsilon}{4}\|\nabla(Gg)\|^2\,. \tag{5.4.22}$$

To estimate the second term on the right–hand side of (5.4.21) we choose κ in the definition of G in (5.4.8) as $1 + \delta/4$, then for every $|x| > \beta$

$$\frac{|G(x)|^2}{|x|^{4+\delta}} \le |x|^{2\kappa-4-\delta}|\xi(|x|/\beta)|^2 \le |x|^{-2-\delta/2}|\xi(|x|/\beta)|^2\,. \tag{5.4.23}$$

Applying (5.4.23) yields

$$\int_{|x|>\beta}\frac{|G|^2}{|x|^{4+\delta}}|f|^2dx \le \int_{\mathbb{R}^2}|x|^{-2-\delta/2}|\xi(|x|/\beta)f(x)|^2dx\,. \tag{5.4.24}$$

Note that the function $\xi(|x|/\beta)f(x)$ vanishes for $|x| = \beta$ and consequently for $\beta > 0$ large enough we can apply the two–dimensional Hardy Inequality (see Lemma B.1.2) and get

$$\int_{\mathbb{R}^2}|x|^{-2-\delta/2}|\xi(|x|/\beta)f(x)|^2dx \le \int_{\mathbb{R}^2}|\nabla(\xi(|x|/\beta)f(x))|^2dx\,. \tag{5.4.25}$$

Since $\nabla\xi(|\cdot|/\beta)$ is supported in $\beta \leq |x| \leq 2\beta$ and $|\nabla\xi(|\cdot|/\beta)| \leq 2/\beta$ we get for the right–hand side of (5.4.25)

$$\int_{\mathbb{R}^2} |\nabla(\xi(|x|/\beta)f(x))|^2 dx \leq \frac{8}{\beta^2}\int_{\beta<|x|<2\beta} |f|^2 dx + 2\int_{|x|>\beta} |\nabla f|^2 dx \tag{5.4.26}$$

where we have used that $(a+b)^2 < a^2+b^2$. The function $\varphi_0 \in L^2_{\text{loc}}(\mathbb{R}^2)$ is normalized with respect to $\dot{H}^1(\mathbb{R}^2)$. Then, due to the orthogonality of f and g for fixed $|x|$, there exists a constant $c_3(2\beta) > 0$ such that

$$\|f\|^2_{|x|<2\beta} \leq \|\varphi_0\|^2_{|x|<2\beta} \leq c_3(2\beta)\|\varphi_0\|^2_{\dot{H}^1(\mathbb{R}^2)}\,. \tag{5.4.27}$$

Combining (5.4.26) and (5.4.27) shows there exits a constant $c_4(\beta) > 0$, such that

$$\int_{\mathbb{R}^2} |\nabla(\xi(|x|/\beta)f(x))|^2 dx \leq c_4(\beta)\|\varphi_0\|^2_{\dot{H}^1(\mathbb{R}^2)}\,.$$

Relations (5.4.24), (5.4.25) and (5.4.4) imply

$$\int_{|x|>\beta} \frac{|G|^2}{|x|^{4+\delta}}|f|^2 dx \leq c_4(\beta)\|\varphi_0\|^2_{\dot{H}^1}\,.$$

Substituting (5.4.22) and (5.4.4) into (5.4.21) gives

$$|\langle Gg, VGf\rangle| \leq \frac{C\tilde{\varepsilon}}{4}\|\nabla(Gg)\|^2 + c_5(\beta,\tilde{\varepsilon})\|\varphi_0\|^2_{\dot{H}^1},$$

where

$$c_5(\beta,\tilde{\varepsilon}) := \frac{C}{\tilde{\varepsilon}}\cdot c_4(\beta)$$

is a constant depending on β and $\tilde{\varepsilon}$. Note that $C > 0$ is a constant depending on the potential V only, and the parameter $\tilde{\varepsilon} > 0$ can be chosen small.

5.4.5 Completing the Proof of (5.4.13)

Combining the inequalities (5.4.14), (5.4.20) and (5.4.4) yields for a constant $c(\beta,\tilde{\varepsilon}) > 0$ that depends on β and $\tilde{\varepsilon}$ but is independent of ψ

$$\begin{aligned}\langle Gg, VGg\rangle - \left\langle Gg, \frac{|\nabla G|^2}{G^2}Gg\right\rangle + \langle Gg, VGf\rangle \\ \geq -\left(\frac{\kappa^2}{4} + \frac{4C}{(1+\beta)^{1+\delta}} + \frac{C\tilde{\varepsilon}}{4}\right)\|\nabla(Gg)\|^2 - c(\beta,\tilde{\varepsilon})\|\varphi_0\|^2_{\dot{H}_1}\,.\end{aligned}$$

Since we can always assume $\delta < 1$ and since $\kappa = 1+\delta/4$ we have $\kappa^2/4 < 1$. Consequently for $\beta > 0$ sufficiently large and by assuming that $\tilde{\varepsilon} > 0$ in (5.4.21) is chosen to be small we can have

$$\left(\frac{\kappa^2}{4}+\frac{4C}{(1+\beta)^{1+\delta}}+\frac{C\tilde{\varepsilon}}{4}\right)<1-\varepsilon\,.$$

The constant $c(\beta,\tilde{\varepsilon})$ for fixed β and $\tilde{\varepsilon}$ may be large but is finite and independent on ω. As explained earlier, taking the limit $\omega \to 0$ completes the proof of Lemma 5.4.3.

5.5 Proofs of the Lemmas for the Main Theorem

In this section, we prove the lemmas stated in Section 5.3.1.

5.5.1 Proof of Lemma 5.3.1

We show the statement for $L_\alpha[\psi_\alpha]$ with $\alpha = (12)$. The proof for $\alpha = (13)$ is similar. We drop the index α whenever possible.

Remark 5.5.1. *The proof of Lemma 5.3.1 is organized as follows. First, we introduce several new functions and state three lemmas corresponding to the proof's main steps, showing how they conclude Lemma 5.3.1. The proofs of these three lemmas are then provided in Section 5.5.2.*

Due to [120, Lemma 5.1] for given $\varepsilon > 0$ and fixed $\gamma > 0$ there exists a $\tilde{\gamma} \in (0,\gamma)$ and a piecewise continuously differentiable function $u : \mathbb{R}^3 \to [0,1]$ with

$$u(x) = \begin{cases} 1 & x \in K_{12}(\tilde{\gamma}) \\ 0 & x \notin K_{12}(\gamma) \end{cases} \tag{5.5.1}$$

such that for $v := \left(1-u^2\right)^{1/2}$

$$|\nabla u|^2 + |\nabla v|^2 \le \varepsilon\left(\frac{v^2}{|x|^2}+\frac{u^2}{|(x_1,x_2)|^2}\right) \tag{5.5.2}$$

for every $x = (x_1,x_2,x_3) \in \mathbb{R}^3$.
Let

$$\begin{aligned} \psi_1 &:= (P_\perp \psi_{12})v, \\ \psi_2 &:= (P_\perp \psi_{12})u + P_0\psi_{12}\,. \end{aligned} \tag{5.5.3}$$

Note that we use smooth localization for the function $P_\perp\psi_{12}$, which allows us to apply the IMS–Localization formula. For reasons that will be explained later, we can not do such a smooth localization for the function $P_0\psi_{12}$.
As the first step, we show that $L_{12}[\psi_{12}]$ can be estimated in terms of integrals involving ψ_2 only. Namely, we prove the following:

Lemma 5.5.2. *Let $K_{12}(\gamma,\tilde{\gamma}) \coloneqq K_{12}(\gamma) \setminus K_{12}(\tilde{\gamma})$ and $b > 0$ large enough. Then*

$$L_{12}[\psi_{12}] \geq \tilde{L}_{12}[\psi_2],$$

where

$$L_{12}[\psi_{12}] = \int_{K_{12}(\gamma)} \left(|\nabla\psi_{12}|^2 + \sum_{\alpha\in I} V_\alpha |\psi_{12}|^2 \right) dx - \int_{K_{12}(\gamma)\setminus S(0,b)} \frac{|\psi_{12}|^2}{|x|^{2+\tau}} dx$$

and

$$\begin{aligned} \tilde{L}_{12}[\psi_2] \coloneqq & \int_{K_{12}(\gamma)} \left(|\nabla\psi_2|^2 + \sum_{\alpha\in I} V_\alpha |\psi_2|^2 \mathbb{1}_{K_\alpha(\tilde{\gamma})} - 2\frac{|\psi_2|^2}{|x|^{2+\tau}} \right) dx \\ & - \varepsilon \int_{K_{12}(\gamma,\tilde{\gamma})} \frac{|P_\perp \psi_2|^2}{|(x_1,x_2)|^2} dx\,. \end{aligned} \tag{5.5.4}$$

As the next step we extend ψ_2 for fixed x_3 outside of $K_{12}(\gamma)$. Note that $\psi_2 = P_0\psi_{12}$ on $\partial K_{12}(\gamma)$ and thus is constant for fixed $x_3 \in \mathbb{R}$ on $\partial K_{12}(\gamma)$. This allows us to continuously extend ψ_2 to $\mathbb{R}^3$ by a function which does not depend on (x_1,x_2) outside of $K_{12}(\gamma)$. Let $\tilde{\psi}_2$ be this new function, then since $\psi \in C_0^1(\mathbb{R}^3)$ it follows that

$$\tilde{\psi}_2(\cdot,x_3) \in \dot{H}^1(\mathbb{R}^2), \quad \tilde{\psi}_2(x_1,x_2,\cdot) \in H^1(\mathbb{R}) \quad \text{and} \quad \tilde{\psi}_2 \in \dot{H}^1(\mathbb{R}^3)\,. \tag{5.5.5}$$

Denote by $\nabla_{12} = (\partial_{x_1}, \partial_{x_2})$ the gradient in the (x_1,x_2)–plane. If h_{12} has a virtual level let $\varphi_0 \in \dot{H}^1(\mathbb{R}^2)$ be the corresponding solution of $h_{12}\varphi_0 = 0$. We normalize φ_0 with respect to the seminorm corresponding to the sesquilinearform

$$\langle \nabla_{12} f, \nabla_{12}\, g\rangle_* = \int_{\mathbb{R}^2} (\nabla_{12} f \cdot \nabla_{12} g)\; d(x_1,x_2), \quad f,g \in H^1(\mathbb{R}^2)$$

such that

$$\|\varphi_0\|_*^2 = \int_{\mathbb{R}^2} |\nabla\varphi_0|^2 d(x_1,x_2) = 1\,.$$

For every $x_3 \in \mathbb{R}$ let

$$\Phi(x_3) \coloneqq \langle \nabla_{12}\varphi_0, \nabla_{12}\tilde{\psi}_2\rangle_{L^2(\mathbb{R}^2)}\,. \tag{5.5.6}$$

We show that the function Φ is in $L^2(\mathbb{R})$. Since $\nabla_{12}\tilde{\psi}_2$ vanishes outside of $\operatorname{supp}\psi_{12}$ and consequently outside of $\operatorname{supp}\psi$, applying Schwarz Inequality yields for some constant $C > 0$

$$\begin{aligned}
\|\Phi\|^2_{L^2(\mathbb{R})} &= \int \left| \iint \left(\nabla_{12}\varphi_0 \mathbb{1}_{\operatorname{supp}(\psi)} \cdot \nabla_{12}\tilde{\psi}_2\right) d(x_1,x_2)\right|^2 dx_3 \\
&\le \int_{\mathbb{R}} \left\|\nabla_{12}\varphi_0 \mathbb{1}_{\operatorname{supp}(\psi)}\right\|_{L^2(\mathbb{R}^2)} \cdot \left\|\nabla_{12}\tilde{\psi}_2(\cdot,x_3)\right\|_{L^2(\mathbb{R}^2)} dx_3 \\
&\le \frac{1}{2}\int_{\mathbb{R}} \left(\left\|\nabla_{12}\varphi_0 \mathbb{1}_{\operatorname{supp}(\psi)}\right\|^2_{L^2(\mathbb{R}^2)} + \left\|\nabla_{12}\tilde{\psi}_2(\cdot,x_3)\right\|^2_{L^2(\mathbb{R}^2)}\right) dx_3 \\
&\le C\|\nabla_{12}\varphi_0\|_* + \frac{1}{2}\left\|\tilde{\psi}_2\right\|_{\dot{H}^1(\mathbb{R}^3)} .
\end{aligned} \tag{5.5.7}$$

In the last line of 5.5.7, we have used that ψ is compactly supported.
Let $F(x_1,x_2,x_3)$ be defined by

$$\tilde{\psi}_2(x_1,x_2,x_3) = \varphi_0(x_1,x_2)\Phi(x_3) + F(x_1,x_2,x_3)\,. \tag{5.5.8}$$

For almost all $x_3 \in \mathbb{R}$ the function F satisfies

$$\langle \nabla_{12}\varphi_0, \nabla_{12}F\rangle_{L^2(\mathbb{R}^2)} = 0\,. \tag{5.5.9}$$

If the virtual level φ_0 does not exist we assume $\Phi(x_3) \equiv 0$ and consequently $F = \tilde{\psi}_2$.

Remark 5.5.3. *For fixed $x_3 \in \mathbb{R}$, the expression* (5.5.8) *is a projection of $\tilde{\psi}_2$ onto the virtual level φ_0 within $\dot{H}^1(\mathbb{R}^2)$. Note that, unlike $\tilde{\psi}_2(\cdot,x_3)$, the function $\psi_2(\cdot,x_3)$ is not in $\dot{H}^1(\mathbb{R}^2)$ and therefore such a projection would not be possible. That is the reason why we needed to extend ψ_2 introducing $\tilde{\psi}_2$.*

With these definitions in (5.5.6) and (5.5.8), we can state the following:

Lemma 5.5.4. *For the functional $\tilde{L}_{12}$ we have the estimate*

$$\begin{aligned}
\tilde{L}_{12}[\psi_2] \ge{} & \mu\|\nabla_{12}F\|^2 + \frac{1}{2}\int_{K_{12}(\gamma)} \left|\partial_{x_3}(P_\perp\psi_2)\right|^2 dx - \varepsilon \int_{K_{12}(\gamma,\tilde{\gamma})} \frac{|P_\perp\psi_2|^2}{|(x_1,x_2)|^2} dx \\
& - C\int_{\partial K_{12}(\gamma)} \frac{|P_0\psi|^2}{|x|^{1+\tau}} d\sigma
\end{aligned}$$

where $\mu > 0$ is the parameter in assertion (2) of Lemma 5.4.1 and $C > 0$ a constant independent of ψ.

Remark 5.5.5. *By comparing the statement of Lemma 5.3.1 with Lemma 5.5.4 we see that the assertion of Lemma 5.3.1 follows immediately if we can show that the sum of the first three terms on the right–hand side of* (5.5.4) *are positive. We give this in the following lemma, which is the last step in the proof of Lemma 5.3.1.*

Lemma 5.5.6. *For $\varepsilon \in (0, \mu/8)$ and $b > 0$ large enough we have*

$$\mu\|\nabla_{12}F\|^2 + \frac{1}{2}\int_{K_{12}(\gamma)} \left|\partial_{x_3}(P_\perp\psi_2)\right|^2 dx - \varepsilon\int_{K_{12}(\gamma,\tilde{\gamma})} \frac{|P_\perp\psi_2|^2}{|(x_1,x_2)|^2} dx \geq 0\,. \tag{5.5.10}$$

Remark 5.5.7. *Recall that for any fixed $\gamma > 0$, we can make $\varepsilon > 0$ arbitrarily small by choosing $\tilde{\gamma} \in (0, \gamma)$ small. In particular, we can always assume $\varepsilon < \mu/8$.*

5.5.2 Proofs of Lemmas 5.5.2, 5.5.4 and 5.5.6

Proof of Lemma 5.5.2

We aim to decompose the expression

$$L_{12}[\psi_{12}] = \int_{K_{12}(\gamma)} \left(|\nabla\psi_{12}|^2 + \sum_{\alpha\in I} V_\alpha|\psi_{12}|^2\right) dx - \int_{K_{12}(\gamma)\setminus S(0,b)} \frac{|\psi_{12}|^2}{|x|^{2+\tau}} dx \tag{5.5.11}$$

into terms that involve either ψ_1 or ψ_2 defined in (5.5.3). In the region $K_{12}(\gamma,\tilde{\gamma})$, the potentials V_α satisfy $|V_\alpha| \leq \tilde{C}|x|^{-2-\delta}$ for some constant $\tilde{C} > 0$, assuming $\gamma > 0$ is sufficiently small and $b > 0$ is sufficiently large (see Lemma B.2.2). Since $\tau < \delta$ we have

$$\int_{K_{12}(\gamma,\tilde{\gamma})} \sum_{\alpha\in I} V_\alpha|\psi_{12}|^2 dx \geq -\int_{K_{12}(\gamma)\setminus S(0,b)} \frac{|\psi_{12}|^2}{|x|^{2+\tau}} dx$$

and consequently

$$L_{12}[\psi_{12}] \geq \int_{K_{12}(\gamma)} \left(|\nabla\psi_{12}|^2 + \sum_{\alpha\in I} V_\alpha|\psi_{12}|^2 \mathbb{1}_{K_{12}(\tilde{\gamma})}\right) dx - 2\int_{K_{12}(\gamma)\setminus S(0,b)} \frac{|\psi_{12}|^2}{|x|^{2+\tau}} dx\,. \tag{5.5.12}$$

Due to the orthogonality of $P_0\psi_{12}$ and $P_\perp\psi_{12}$

$$\int_{K_{12}(\gamma)} |\nabla\psi_{12}|^2 dx = \int_{K_{12}(\gamma)} |\nabla(P_\perp\psi_{12})|^2 dx + \int_{K_{12}(\gamma)} |\nabla(P_0\psi_{12})|^2 dx\,. \tag{5.5.13}$$

With the bounds on the localization estimates in (5.5.2), we have

$$\begin{aligned} &\int_{K_{12}(\gamma)} |\nabla(P_\perp\psi_{12})|^2 dx \\ &\quad\geq \int_{K_{12}(\gamma)} |\nabla(P_\perp\psi_{12}u)|^2 dx - \varepsilon\int_{K_{12}(\gamma,\tilde{\gamma})} |P_\perp\psi_{12}|^2 \frac{u^2}{|(x_1,x_2)|^2} dx \\ &\quad+ \int_{K_{12}(\gamma)} |\nabla(P_\perp\psi_{12}v)|^2 dx - \varepsilon\int_{K_{12}(\gamma,\tilde{\gamma})} |P_\perp\psi_{12}|^2 \frac{v^2}{|x|^2} dx, \end{aligned} \tag{5.5.14}$$

where u, v are functions defined by (5.5.1). Due to the definition of functions ψ_1 and ψ_2 in (5.5.3) we have

$$\int_{K_{12}(\gamma)} |\nabla(P_\perp\psi_{12}u)|^2 dx + \int_{K_{12}(\gamma)} |\nabla(P_0\psi_{12})|^2 dx = \int_{K_{12}(\gamma)} |\nabla\psi_2|^2 dx \tag{5.5.15}$$

and since ψ_1 vanishes on $K_{12}(\tilde{\gamma})$ it follows

$$\int_{K_{12}(\gamma)} |\nabla(P_\perp\psi_{12}v)|^2 dx = \int_{K_{12}(\gamma,\tilde{\gamma})} |\nabla\psi_1|^2 dx\,. \tag{5.5.16}$$

Inserting (5.5.14) into (5.5.13) and applying the relations in (5.5.15) and (5.5.16) we arrive at

$$\begin{aligned}\int_{K_{12}(\gamma)} |\nabla\psi_{12}|^2 dx \geq \int_{K_{12}(\gamma,\tilde{\gamma})} |\nabla\psi_1|^2 dx - \varepsilon \int_{K_{12}(\gamma,\tilde{\gamma})} \frac{|\psi_1|^2}{|x|^2} dx \\ + \int_{K_{12}(\gamma)} |\nabla\psi_2|^2 dx - \varepsilon \int_{K_{12}(\gamma,\tilde{\gamma})} \frac{|P_\perp\psi_2|^2}{|(x_1,x_2)|^2} dx\,.\end{aligned} \tag{5.5.17}$$

The functions ψ_1, ψ_2 satisfy

$$P_0\psi_1 = 0 \quad \text{and} \quad |P_\perp\psi_1|^2 + |P_\perp\psi_2|^2 = |P_\perp\psi_{12}|^2\,. \tag{5.5.18}$$

Dividing by $|x|^{2+\tau}$ does not change the symmetry of the functions and consequently together with (5.5.18) we get

$$\int_{K_{12}(\gamma)\backslash S(0,b)} \frac{|\psi_{12}|^2}{|x|^{2+\tau}} dx = \int_{K_{12}(\gamma)\backslash S(0,b)} \frac{|\psi_1|^2}{|x|^{2+\tau}} dx + \int_{K_{12}(\gamma)\backslash S(0,b)} \frac{|\psi_2|^2}{|x|^{2+\tau}} dx\,. \tag{5.5.19}$$

Inserting (5.5.17) and (5.5.19) into (5.5.12) yields

$$L_{12}[\psi_{12}] \geq \tilde{L}_{12}[\psi_2] + \int_{K_{12}(\gamma)} \left(|\nabla\psi_1|^2 - 2\frac{|\psi_1|^2}{|x|^{2+\tau}} - \varepsilon\frac{|\psi_1|^2}{|x|^2} \right) dx \tag{5.5.20}$$

where $\tilde{L}_{12}[\psi_2]$ is given in (5.5.4). Since $\operatorname{supp}\psi_1 \subset \{x \in \mathbb{R}^3 : |x| \geq b\}$ we can apply the radial Hardy Inequality and for $\varepsilon > 0$ small and $b > 0$ large enough we obtain

$$\int_{K_{12}(\gamma)} \left(|\nabla\psi_1|^2 - 2\frac{|\psi_1|^2}{|x|^{2+\tau}} - \varepsilon\frac{|\psi_1|^2}{|x|^2} \right) dx \geq 0\,.$$

This completes the proof of Lemma 5.5.2. ∎

Proof of Lemma 5.5.4

We aim to estimate

$$\tilde{L}_{12}[\psi_2] = \int_{K_{12}(\gamma)} \left(|\nabla\psi_2|^2 + \sum_{\alpha\in I} V_\alpha |\psi_2|^2 \mathbb{1}_{K_{12}(\tilde{\gamma})} - 2\frac{|\psi_2|^2}{|x|^{2+\tau}} \right) dx$$
$$- \varepsilon \int_{K_{12}(\gamma,\tilde{\gamma})} \frac{|P_\perp \psi_2|^2}{|(x_1,x_2)|^2} dx\,.$$

Due to Lemma B.2.2 there exists a constant $\tilde{C} > 0$ such that on on $K_{12}(\gamma) \setminus S(0,b)$

$$|V_{13} + V_{23}| \le \tilde{C}|x|^{-2-\delta}\,. \tag{5.5.21}$$

Then, using (5.5.21) together with $\tau < \delta$ yields

$$\tilde{L}_{12}[\psi_2] \ge \int_{K_{12}(\gamma)} \left(|\nabla\psi_2|^2 + V_{12}|\psi_2|^2 \mathbb{1}_{K_{12}(\tilde{\gamma})} - 3\frac{|\psi_2|^2}{|x|^{2+\tau}} \right) dx$$
$$- \varepsilon \int_{K_{12}(\gamma,\tilde{\gamma})} \frac{|P_\perp \psi_2|^2}{|(x_1,x_2)|^2} dx\,. \tag{5.5.22}$$

We rewrite (5.5.22) as

$$\tilde{L}_{12}[\psi_2] \ge \int_{K_{12}(\gamma)} \left(|\nabla_{12}\psi_2|^2 + V_{12}|\psi_2|^2 \mathbb{1}_{K_{12}(\tilde{\gamma})} \right) dx$$
$$+ \int_{K_{12}(\gamma)} \left|\partial_{x_3}\psi_2\right|^2 dx - 3\int_{K_{12}(\gamma)} \frac{|\psi_2|^2}{|x|^{2+\tau}} dx - \varepsilon \int_{K_{12}(\gamma,\tilde{\gamma})} \frac{|P_\perp \psi_2|^2}{|(x_1,x_2)|^2} dx\,. \tag{5.5.23}$$

We start with the first integral on the right–hand side of (5.5.23). With the definition of $\tilde{\psi}_2$ in Section 5.5.1 we have

$$\int_{K_{12}(\gamma)} |\nabla_{12}\psi_2|^2 dx = \int_{\mathbb{R}^3} \left|\nabla_{12}\tilde{\psi}_2\right|^2 dx\,. \tag{5.5.24}$$

The function $\tilde{\psi}_2$ and ψ_2 coincide inside of $K_{12}(\gamma)$ and consequently for the term involving V_{12} in (5.5.23) we have

$$\int_{K_{12}(\gamma)} V_{12}|\psi_2|^2 \mathbb{1}_{K_{12}(\tilde{\gamma})} dx$$
$$= \int_{\mathbb{R}^3} V_{12}\left|\tilde{\psi}_2\right|^2 dx - \int_{K_{12}(\gamma,\tilde{\gamma})} V_{12}|\psi_2|^2 dx - \int_{\mathbb{R}^3\setminus K_{12}(\gamma)} V_{12}\left|\tilde{\psi}_2\right|^2 dx\,. \tag{5.5.25}$$

Outside of $K_{12}(\tilde{\gamma})$ holds $|V_{12}| \le \tilde{C}|x|^{-3-\delta}$ for some $\tilde{C} > 0$. Consequently for $b > 0$ large enough

$$\left|\int_{K_{12}(\gamma,\tilde{\gamma})} V_{12}|\psi_2|^2 dx\right| \le \int_{K_{12}(\gamma,\tilde{\gamma})} |\psi_2(x)|^2 |x|^{-2-\tau} dx \tag{5.5.26}$$

and

$$\left|\int_{\mathbb{R}^3\setminus K_{12}(\gamma)} V_{12}\left|\tilde{\psi}_2\right|^2 dx\right| \leq \int_{\mathbb{R}^3\setminus K_{12}(\gamma)} \left|\tilde{\psi}_2(x)\right|^2 |x|^{-2-\tau} dx\,. \tag{5.5.27}$$

Combining (5.5.24), (5.5.25), (5.5.26) and (5.5.27) we find

$$\begin{aligned}\int_{K_{12}(\gamma)} |\nabla_{12}\psi_2|^2 + V_{12}|\psi_2|^2 dx \geq &\int_{\mathbb{R}^3} \left(\left|\nabla_{12}\tilde{\psi}_2\right|^2 + V_{12}\left|\tilde{\psi}_2\right|^2\right) dx \\ &- \int_{\mathbb{R}^3\setminus K_{12}(\gamma)} \frac{\left|\tilde{\psi}_2(x)\right|^2}{|x|^{2+\tau}} dx - \int_{K_{12}(\gamma,\tilde{\gamma})} \frac{|\psi_2|^2}{|x|^{2+\tau}} dx\,.\end{aligned} \tag{5.5.28}$$

By expressing $\tilde{\psi}_2$ in terms of $\Phi\varphi_0$ and F (see (5.5.8)), using $h_{12}\varphi_0 = 0$ and assertion (2) of Lemma 5.4.1 yields

$$\int_{\mathbb{R}^3} \left(\left|\nabla_{12}\tilde{\psi}_2\right|^2 + V_{12}\left|\tilde{\psi}_2\right|^2\right) dx \geq \mu\|\nabla_{12}F\|^2\,. \tag{5.5.29}$$

Inserting (5.5.29) into (5.5.28) gives

$$\begin{aligned}&\int_{K_{12}(\gamma)} |\nabla_{12}\psi_2|^2 + V_{12}|\psi_2|^2 dx \\ &\quad\geq \mu\|\nabla_{12}F\|^2 - \int_{\mathbb{R}^3\setminus K_{12}(\gamma)} \left|\tilde{\psi}_2(x)\right|^2 |x|^{-2-\tau} dx - \int_{K_{12}(\gamma,\tilde{\gamma})} |\psi_2|^2 |x|^{-2-\tau} dx\,.\end{aligned} \tag{5.5.30}$$

Next, we show that

$$\int_{\mathbb{R}^3\setminus K_{12}(\gamma)} \left|\tilde{\psi}_2(x)\right|^2 |x|^{-2-\tau} dx$$

can be estimated by an integral over the surface $\partial K_{12}(\gamma)$. We introduce polar coordinates

$$\begin{aligned} x_1 &= \rho\sin(\varphi), \\ x_2 &= \rho\cos(\varphi) \end{aligned} \tag{5.5.31}$$

with $\varphi \in [0, 2\pi)$ and $\rho \in [0, \infty)$. In this choice of coordinates the set $K_{12}(\gamma)$ is determined by $\rho \leq \kappa|x_3|$ for some $\kappa > 0$ depending on γ (see Figure 5.3). Then

$$\int_{\mathbb{R}^3\setminus K_{12}(\gamma)} \frac{\left|\tilde{\psi}_2(x)\right|^2}{|x|^{2+\tau}} dx = \int_{-\infty}^{\infty}\int_{\kappa|x_3|}^{\infty} \frac{\int_0^{2\pi}\left|\tilde{\psi}_2(\rho,\varphi,x_3)\right|^2 d\varphi}{\rho^{2+\tau}} \rho\, d\rho\, dx_3\,. \tag{5.5.32}$$

Outside of the conical set $K_{12}(\gamma)$ the function $\tilde{\psi}_2$ is equal to its value on the boundary and consequently substituting $\tilde{\psi}_2(\rho,\varphi,x_3)$ with $\tilde{\psi}_2(\kappa|x_3|,\varphi,x_3)$ in (5.5.33) and solving the integral over ρ yields

$$\begin{aligned}\int_{\mathbb{R}^3\setminus K_{12}(\gamma)} \frac{\left|\tilde{\psi}_2(x)\right|^2}{|x|^{2+\tau}}dx &= \int_{-\infty}^{\infty}\int_{\kappa|x_3|}^{\infty} \frac{\int_0^{2\pi}\left|\tilde{\psi}_2(\kappa|x_3|,\varphi,x_3)\right|^2 d\varphi}{\rho^{2+\tau}}\rho d\rho dx_3 \\ &= (\kappa^\tau\tau)^{-1}\int_{-\infty}^{\infty}\frac{\int_0^{2\pi}\left|\tilde{\psi}_2(\kappa|x_3|,\varphi,x_3)\right|^2 d\varphi}{|x_3|^{1+\tau}}|x_3|dx_3\,.\end{aligned} \tag{5.5.33}$$

Regarding the set $\partial K_{23}(\gamma)$ the surface measure $d\sigma$ equals $|x_3|dx_3d\varphi$ up to a constant depending

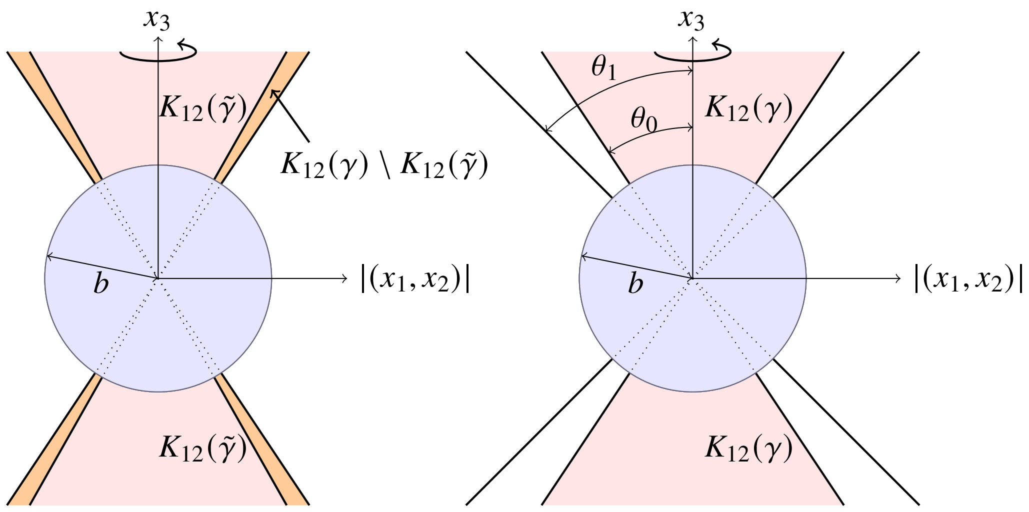

FIGURE 5.3: Left–hand side: sketch of the sets $K_{12}(\gamma)$ and $K_{12}(\tilde{\gamma})$ used in the proof of Lemma 5.3.1.
Right–hand side: sketch of the sets $K_{12}(\gamma)$ and $K_{12}(\gamma_1)$ where the angles θ_0 and θ_1 are defined as $\theta_0 = \arcsin(\gamma)$ and $\theta_1 = \arcsin(\gamma_1)$ and used in Lemma 5.3.3.

on γ and the function $P_\perp\tilde{\psi}_2 = 0$ such that $\tilde{\psi}_2 = P_0\psi$ on this surface. For $(x_1,x_2,x_3) \in \partial K_{12}(\gamma)$ we have $|x_3| = (1-\gamma^2)^{1/2}|x|$ and therefore there exists some $C_1 > 0$ that depends on γ and δ but is independent of ψ such that

$$\int_{\mathbb{R}^3\setminus K_{12}(\gamma)} \frac{\left|\tilde{\psi}_2(x)\right|^2}{|x|^{2+\tau}}dx \le C_1\int_{\partial K_{12}(\gamma)}\frac{|P_0\psi|^2}{|x|^{1+\tau}}d\sigma\,. \tag{5.5.34}$$

Combining (5.5.34) and (5.5.30) we arrive at

$$\begin{aligned}\int_{K_{12}(\gamma)} |\nabla_{12}\psi_2|^2 + V_{12}|\psi_2|^2 dx \ge \mu\|\nabla_{12}F\|^2 - C_1\int_{\partial K_{12}(\gamma)}\frac{|(P_0\psi)(x)|^2}{|x|^{1+\tau}}d\sigma \\ - \int_{K_{12}(\gamma,\tilde{\gamma})}\frac{|\psi_2|^2}{|x|^{2+\tau}}dx\,.\end{aligned} \tag{5.5.35}$$

Substituting (5.5.35) into (5.5.23) yields

$$\begin{aligned}\tilde{L}_{12}[\psi_2] \geq &\mu\|\nabla_{12}F\|^2 - C_1 \int_{\partial K_{12}(\gamma)} \frac{|P_0\psi|^2}{|x|^{1+\tau}} d\sigma \\ &+ \int_{K_{12}(\gamma)} \left(\left|\partial_{x_3}\psi_2\right|^2 - 4\frac{|\psi_2|^2}{|x|^{2+\tau}}\right) dx - \varepsilon \int_{K_{12}(\gamma,\tilde{\gamma})} \frac{|P_\perp\psi_2|^2}{|(x_1,x_2)|^2} dx\,.\end{aligned} \tag{5.5.36}$$

We proceed by studying the term

$$\begin{aligned}\int_{K_{12}(\gamma)} \left(\left|\partial_{x_3}\psi_2\right|^2 dx - 4\frac{|\psi_2|^2}{|x|^{2+\tau}}\right) dx = &\int_{K_{12}(\gamma)} \left(\left|\partial_{x_3}(P_0\psi_2)\right|^2 - 4\frac{|P_0\psi_2|^2}{|x|^{2+\tau}}\right) dx \\ &+ \int_{K_{12}(\gamma)} \left(\frac{1}{2}\left|\partial_{x_3}(P_\perp\psi_2)\right|^2 - 4\frac{|P_\perp\psi_2|^2}{|x|^{2+\tau}}\right) dx \\ &+ \int_{K_{12}(\gamma)} \frac{1}{2}\left|\partial_{x_3}(P_\perp\psi_2)\right|^2 dx\,.\end{aligned} \tag{5.5.37}$$

Using $P_\perp\psi_2 = 0$ on $\partial K_{12}(\gamma)$ and decreasing the integral by replacing $|x|$ with $|x_3|$ together with the one–dimensional Hardy Inequality (see Lemma B.1.1) yields for $b > 0$ large enough

$$\int_{K_{12}(\gamma)} \left(\frac{1}{2}\left|\partial_{x_3}(P_\perp\psi_2)\right|^2 - 4\frac{|P_\perp\psi_2|^2}{|x_3|^{2+\tau}}\right) dx \geq 0\,. \tag{5.5.38}$$

Combining (5.5.37) and (5.5.38) yields

$$\begin{aligned}\int_{K_{12}(\gamma)} \left(\left|\partial_{x_3}\psi_2\right|^2 dx - 4\frac{|\psi_2|^2}{|x|^{2+\tau}}\right) dx \geq &\int_{K_{12}(\gamma)} \left(\left|\partial_{x_3}(P_0\psi_2)\right|^2 - 4\frac{|P_0\psi_2(x)|^2}{|x_3|^{2+\tau}}\right) dx \\ &+ \frac{1}{2}\int_{K_{12}(\gamma)} \left|\partial_{x_3}(P_\perp\psi_2)\right|^2 dx\,.\end{aligned} \tag{5.5.39}$$

Next, we estimate the integral involving $P_0\psi_2$ in (5.5.39). The one–dimensional Hardy Inequality can not be applied directly, as $P_0\psi_2$ does not vanish on the boundary $\partial K_{12}(\gamma)$. So, we use the following construction instead.

Let G be defined as a continuous function in $K_{12}(\gamma) \setminus S(0,b)$ that coincides with $P_0\psi_2$ on the boundary $\partial K_{12}(\gamma)$ and is independent of x_3 within $K_{12}(\gamma)$. We define Γ in $K_{12}(\gamma) \setminus S(0,b)$ as

$$\Gamma \coloneqq P_0\psi_2 - G$$

such that Γ vanishes on $\partial K_{12}(\gamma)$. Then

$$\int_{K_{12}(\gamma)} \left|\partial_{x_3}(P_0\psi_2)\right|^2 dx = \int_{K_{12}(\gamma)} \left|\partial_{x_3}\Gamma\right|^2 dx \tag{5.5.40}$$

and

$$\begin{aligned}\int_{K_{12}(\gamma)} \frac{|P_0\psi_2|^2}{|x_3|^{2+\tau}}dx &= \int_{K_{12}(\gamma)} \frac{|\Gamma + G|^2}{|x_3|^{2+\tau}}dx \\ &\leq 2\int_{K_{12}(\gamma)} \frac{|\Gamma|^2}{|x_3|^{2+\tau}}dx + 2\int_{K_{12}(\gamma)} \frac{|G|^2}{|x_3|^{2+\tau}}dx\,.\end{aligned} \tag{5.5.41}$$

Combining (5.5.40) and (5.5.41) we find

$$\begin{aligned}\int_{K_{12}(\gamma)} \left(\left|\partial_{x_3}(P_0\psi_2)\right|^2 - 4\frac{|P_0\psi_2(x)|^2}{|x_3|^{2+\tau}}\right)dx \geq \int_{K_{12}(\gamma)} \left(\left|\partial_{x_3}\Gamma\right|^2 - 8\frac{|\Gamma|^2}{|x_3|^{2+\tau}}\right)dx \\ - \int_{K_{12}(\gamma)} 8\frac{|G|^2}{|x_3|^{2+\tau}}dx\,.\end{aligned}$$

Since ψ and consequently Γ vanishes for $|x_3| < b/2$ we can apply the one–dimensional Hardy inequality (see Lemma B.1.1), which yields for $\tau > 0$ and $b > 0$ large enough

$$\int_{K_{12}(\gamma)} \left|\partial_{x_3}\Gamma\right|^2 dx - 8\int_{K_{12}(\gamma)} \frac{|\Gamma|^2}{|x_3|^{2+\tau}}dx \geq 0\,. \tag{5.5.42}$$

This yields

$$\int_{K_{12}(\gamma)} \left(\left|\partial_{x_3}(P_0\psi_2)\right|^2 dx - 4\frac{|P_0\psi_2(x)|^2}{|x|^{2+\tau}}\right)dx \geq -8\int_{K_{12}(\gamma)} \frac{|G|^2}{|x_3|^{2+\tau}}dx\,. \tag{5.5.43}$$

Next, we show that the integral on the right–hand side of equation (5.5.43) can be estimated by an integral over $\partial K_{12}(\gamma)$. The function G is independent of x_3 in $K_{12}(\gamma)$, therefore using polar coordinates as in (5.5.31) we find

$$\begin{aligned}\int_{K_{12}(\gamma)} \frac{|G(x)|^2}{|x_3|^{2+\tau}}dx &= \int_0^\infty \int_{|x_3|\geq\kappa^{-1}\rho} \frac{\int_0^{2\pi} |G(\rho,\varphi,x_3)|^2 d\varphi}{|x_3|^{2+\tau}} dx_3\rho d\rho \\ &= \int_0^\infty \int_{|x_3|\geq\kappa^{-1}\rho} \frac{\int_0^{2\pi} \left|G(\rho,\varphi,\kappa^{-1}\rho)\right|^2 d\varphi}{|x_3|^{2+\tau}} dx_3\rho d\rho \\ &= (\kappa^{1+\tau}(1+\tau))^{-1}\int_0^\infty \frac{\int_0^{2\pi} \left|G(\rho,\varphi,\kappa^{-1}\rho)\right|^2 d\varphi}{\rho^{1+\tau}}\rho d\rho\,.\end{aligned}$$

Due to the definition of G and since $\rho = \gamma|x|$ on $\partial K_{12}(x)$ there exists a constant $C_2 > 0$ that depends on γ and δ but is independent of ψ such that

$$\int_{K_{12}(\gamma)} \frac{|G|^2}{|x_3|^{2+\tau}}dx = C_2\int_{\partial K_{12}(\gamma)} \frac{|P_0\psi|^2}{|x|^{1+\tau}}d\sigma\,. \tag{5.5.44}$$

Substituting the relation (5.5.44) into (5.5.43) it follows from (5.5.39) that

$$\int_{K_{12}(\gamma)} \left(\left|\partial_{x_3}\psi_2\right|^2 dx - 4\frac{|\psi_2|^2}{|x|^{2+\tau}} \right) dx \geq -8C_2 \int_{\partial K_{12}(\gamma)} \frac{|P_0\psi|^2}{|x|^{1+\tau}} d\sigma + \frac{1}{2}\int_{K_{12}(\gamma)} \left|\partial_{x_3}(P_\perp\psi_2)\right|^2 dx\,. \tag{5.5.45}$$

We insert (5.5.45) into (5.5.36) and define $C \coloneqq C_1 + 8C_2$, such that

$$\begin{aligned}\tilde{L}_{12}[\psi_2] \geq& \mu\|\nabla_{12}F\|^2 + \frac{1}{2}\int_{K_{12}(\gamma)} \left|\partial_{x_3}(P_\perp\psi_2)\right|^2 dx - \varepsilon\int_{K_{12}(\gamma,\tilde{\gamma})} \frac{|P_\perp\psi_2|^2}{|(x_1,x_2)|^2} dx \\ &- C\int_{\partial K_\alpha(\gamma)} \frac{|P_0\psi|^2}{|x|^{1+\tau}} d\sigma,\end{aligned}$$

which completes the proof of Lemma 5.5.4. ∎

Proof of Lemma 5.5.6

To prove the lemma it suffices to show that for any $\mu > 0$ and $\varepsilon \in (0, \mu/8)$ there exists a $\lambda \in (0, 1/2)$ such that for all $b > 0$ (depending on $\mu, \varepsilon, \lambda$) large enough, the following inequality holds:

$$\mu\|\nabla_{12}F\|^2 + \lambda\int_{K_{12}(\gamma)} \left|\partial_{x_3}(P_\perp\psi_2)\right|^2 dx - \varepsilon\int_{K_{12}(\gamma,\tilde{\gamma})} \frac{|P_\perp\psi_2|^2}{|(x_1,x_2)|^2} dx \geq 0\,. \tag{5.5.46}$$

We start with the second term on the left–hand side of (5.5.46). The function $P_\perp\psi_2$ vanishes for $|x_3| = 0$ and therefore by the one–dimensional Hardy Inequality (Lemma B.1.1)

$$\int_{K_{12}(\gamma)} \left|\partial_{x_3}(P_\perp\psi_2)\right|^2 dx \geq \frac{1}{4}\int_{K_{12}(\gamma)} \frac{|P_\perp\psi_2|^2}{|x_3|^2} dx\,. \tag{5.5.47}$$

Since $\psi_2 = \Phi\varphi_0 + F$ on $K_{12}(\gamma)$ and $(a+b)^2 \geq a^2/2 - b^2$ we can estimate the right–hand side of (5.5.47) by

$$\int_{K_{12}(\gamma)} \frac{|P_\perp\psi_2|^2}{|x_3|^2} dx \geq \frac{1}{2}\int_{K_{12}(\gamma)} |\Phi|^2\frac{|P_\perp\varphi_0|^2}{|x_3|^2} dx - \int_{K_{12}(\gamma)} \frac{|P_\perp F|^2}{|x_3|^2} dx\,. \tag{5.5.48}$$

Using that

$$|(x_1,x_2)|^2 \leq \frac{\gamma^2}{1-\gamma^2}x_3^2, \quad \forall x \in K_{12}(\gamma).$$

and substituting this into the right–hand side of (5.5.48) we find

$$\int_{K_{12}(\gamma)} \frac{|P_\perp\psi_2|^2}{|x_3|^2} dx \geq \frac{1}{2}\int_{K_{12}(\gamma)} |\Phi|^2\frac{|P_\perp\varphi_0|^2}{|x_3|^2} dx - \frac{\gamma^2}{1-\gamma^2}\int_{K_{12}(\gamma)} \frac{|P_\perp F|^2}{|(x_1,x_2)|^2} dx\,. \tag{5.5.49}$$

Combining (5.5.47) and (5.5.49) and assuming

$$\lambda < \frac{1-\gamma^2}{2\gamma^2}\mu$$

we arrive at

$$\begin{aligned}\lambda \int_{K_{12}(\gamma)} \left|\partial_{x_3}(P_\perp \psi_2)\right|^2 dx \\ \geq & \frac{\lambda}{8}\int_{K_{12}(\gamma)} |\Phi|^2 \frac{|P_\perp \varphi_0|^2}{|x_3|^2} dx - \frac{\lambda}{4}\frac{\gamma^2}{1-\gamma^2}\int_{K_{12}(\gamma)} \frac{|P_\perp F|^2}{|(x_1,x_2)|^2} dx \\ \geq & \frac{\lambda}{8}\int_{K_{12}(\gamma)} |\Phi|^2 \frac{|P_\perp \varphi_0|^2}{|x_3|^2} dx - \frac{\mu}{8}\int_{K_{12}(\gamma)} \frac{|P_\perp F|^2}{|(x_1,x_2)|^2} dx\,.\end{aligned} \tag{5.5.50}$$

Using $\varepsilon \in (0, \mu/8)$ we find that last term on the left–hand side of (5.5.46) can be estimated as

$$\begin{aligned}\varepsilon \int_{K_{12}(\gamma,\tilde{\gamma})} \frac{|P_\perp \psi_2|^2}{|(x_1,x_2)|^2} dx \\ \leq 2\varepsilon & \int_{K_{12}(\gamma,\tilde{\gamma})} |\Phi|^2 \frac{|P_\perp \varphi_0|^2}{|(x_1,x_2)|^2} dx + 2\varepsilon \int_{K_{12}(\gamma,\tilde{\gamma})} \frac{|P_\perp F|^2}{|(x_1,x_2)|^2} dx \\ \leq 2\varepsilon & \int_{K_{12}(\gamma,\tilde{\gamma})} |\Phi|^2 \frac{|P_\perp \varphi_0|^2}{|(x_1,x_2)|^2} dx + \frac{\mu}{4} \int_{K_{12}(\gamma,\tilde{\gamma})} \frac{|P_\perp F|^2}{|(x_1,x_2)|^2} dx\,.\end{aligned} \tag{5.5.51}$$

Inserting (5.5.50) and (5.5.51) into (5.5.46) we find

$$\begin{aligned}\mu\|\nabla_{12}F\|^2 + \lambda \int_{K_{12}(\gamma)} \left|\partial_{x_3}(P_\perp \psi_2)\right|^2 dx - \varepsilon \int_{K_{12}(\gamma,\tilde{\gamma})} \frac{|P_\perp \psi_2|^2}{|(x_1,x_2)|^2} dx \\ \geq \frac{\lambda}{8}\int_{K_{12}(\gamma)} |\Phi|^2 \frac{|P_\perp \varphi_0|^2}{|x_3|^2} dx - 2\varepsilon \int_{K_{12}(\gamma,\tilde{\gamma})} |\Phi|^2 \frac{|P_\perp \varphi_0|^2}{|(x_1,x_2)|^2} dx \\ + \mu\|\nabla_{12}F\|^2 - \frac{3}{8}\mu \int_{K_{12}(\gamma)} \frac{|P_\perp F|^2}{|(x_1,x_2)|^2} dx\,.\end{aligned} \tag{5.5.52}$$

Furthermore, due to the symmetry of $P_\perp F$ (see (5.4.6)) we have

$$\|\nabla_{12}F\|^2 = \|\nabla_{12}(P_0 F)\|^2 + \|\nabla_{12}(P_\perp F)\|^2 \geq \|\nabla_{12}(P_\perp F)\|^2 \geq 4\int_{\mathbb{R}^3} \frac{|P_\perp F|^2}{|(x_1,x_2)|^2} dx\,.$$

Consequently, for the terms in that last line of (5.5.52) we find

$$\mu\|\nabla_{12}F\|^2 - \frac{3}{8}\mu \int_{K_{12}(\gamma)} \frac{|P_\perp F|^2}{|(x_1,x_2)|^2} dx \geq 0\,.$$

To complete the proof of the lemma it remains to show for fixed λ and ε we can choose $b > 0$ large enough such that

$$\frac{\lambda}{8}\int_{K_{12}(\gamma)}|\Phi|^2\frac{|P_\perp\varphi_0|^2}{|x_3|^2}dx - 2\varepsilon\int_{K_{12}(\gamma,\tilde{\gamma})}|\Phi|^2\frac{|P_\perp\varphi_0|^2}{|(x_1,x_2)|^2}dx \geq 0\,. \tag{5.5.53}$$

The first integral in (5.5.53) is taken over the region $K_{12}(\gamma)$, while the second integral, which is negative, is taken over $K_{12}(\gamma,\tilde{\gamma})$, a subset of $K_{12}(\gamma)$. We will show that (5.5.53) follows from this observation and the decay properties of $P_\perp\varphi_0$ proved in Lemma 5.4.3.
It holds

$$\frac{\tilde{\gamma}^2}{1-\tilde{\gamma}^2}x_3^2 \leq |(x_1,x_2)|^2, \quad \forall x \in K_{12}(\gamma,\tilde{\gamma}), \tag{5.5.54}$$

and

$$\tilde{\gamma}b/2 \leq \tilde{\gamma}|x| \leq |(x_1,x_2)|, \quad \forall x \in K_{12}(\gamma,\tilde{\gamma}) \cap \operatorname{supp}(\psi)\,. \tag{5.5.55}$$

Using (5.5.54) and (5.5.55) and applying Lemma 5.4.3 there exists some $\nu > 0$ and a constant $c(\tilde{\gamma},\nu) > 0$ such that for the second integral in (5.5.53)

$$\begin{aligned}
&\int_{K_{12}(\gamma,\tilde{\gamma})}|\Phi|^2\frac{|P_\perp\varphi_0|^2}{|(x_1,x_2)|^2}dx \\
&= \int_{K_{12}(\gamma,\tilde{\gamma})}|\Phi|^2\frac{|P_\perp\varphi_0|^2}{|(x_1,x_2)|^2}\frac{(1+|(x_1,x_2)|)^\nu}{(1+|(x_1,x_2)|)^\nu}dx \\
&\leq \frac{1}{(1+\tilde{\gamma}b/2)^\nu}\frac{1-\tilde{\gamma}^2}{\tilde{\gamma}^2}\int_{K_{12}(\gamma,\tilde{\gamma})}\frac{|\Phi|^2}{|x_3|^2}\,(1+|(x_1,x_2)|)^\nu\,|P_\perp\varphi_0|^2 d(x_1,x_2)dx_3 \\
&= \frac{c(\tilde{\gamma},\nu)}{b^\nu}\int_{b/2}^{\infty}\frac{|\Phi|^2}{|x_3|^2}dx_3\,.
\end{aligned} \tag{5.5.56}$$

On the other hand for the first term in (5.5.53) we have for $b > 0$ large enough

$$\int_{K_{12}(\gamma)}|\Phi|^2\frac{|P_\perp\varphi_0|^2}{|x_3|^2}dx \geq \frac{\|P_\perp\varphi_0\|^2_{L^2(\mathbb{R}^2)}}{2}\int_{b/2}^{\infty}\frac{|\Phi|^2}{|x_3|^2}dx_3\,. \tag{5.5.57}$$

Combining (5.5.56) and (5.5.57) proves (5.5.53), which completes the proof of Lemma 5.5.6 and as discussed in 5.5.1 this completes also the proof of Lemma 5.3.1. ∎

5.5.3 Proof of Lemma 5.3.2

We aim to estimate

$$L_{23}[\psi_{23}] = \int_{K_{23}(\gamma)}\left(|\nabla\psi_{23}|^2 + \sum_{\beta\in I}V_\beta|\psi_{23}|^2\right)dx - \int_{K_{23}(\gamma)\setminus S(0,b)}\frac{|\psi_{23}|^2}{|x|^{2+\tau}}dx\,. \tag{5.5.58}$$

The potentials V_{1j} satisfy $\left|V_{1j}\right| \leq \tilde{C}|x|^{-3-\delta}$ for $j \in \{2,3\}$ and some $\tilde{C} > 0$ on $K_{23}(\gamma)$ due to Lemma B.2.2. Consequently, for $b > 0$ sufficiently large

$$L_{23}[\psi_{23}] \geq \int_{K_{23}(\gamma)} \left(|\nabla\psi_{23}|^2 + V_{23}|\psi_{23}|^2\right) dx - 2\int_{K_{23}(\gamma)\setminus S(0,b)} \frac{|\psi_{23}|^2}{|x|^{2+\tau}} dx, \tag{5.5.59}$$

which is equivalent to

$$\begin{aligned} L_{23}[\psi_{23}] \geq &\int_{K_{23}(\gamma)} \left(\left|\partial_{x_2}\psi_{23}\right|^2 + \left|\partial_{x_3}\psi_{23}\right|^2 + V_{23}|\psi_{23}|^2\right) dx \\ &+ \int_{K_{23}(\gamma)} \left|\partial_{x_1}\psi_{23}\right|^2 - 2\int_{K_{23}(\gamma)\setminus S(0,b)} \frac{|\psi_{23}|^2}{|x|^{2+\tau}} dx\,. \end{aligned} \tag{5.5.60}$$

Next, we estimate the first term on the right–hand side of equation (5.5.60), which corresponds to a part of the quadratic form of the operator h_{23} defined in (5.2.3). Note that the operator h_{23} is translation invariant. We introduce new coordinates (q,ξ), which correspond to the relative distance and position of the center of mass of the subsystem (23) with

$$q := \frac{1}{\sqrt{M_{23}}}(\sqrt{m_3}x_2 - \sqrt{m_2}x_3)\,,$$

$$\xi := \frac{1}{\sqrt{M_{23}}}(\sqrt{m_2}x_2 + \sqrt{m_3}x_3),$$

where $M_{23} := m_2 + m_3$. Note that $q^2 + \xi^2 = x_2^2 + x_3^2$. Direct computations show that in (q,ξ)–coordinates the operator h_{23} takes the form

$$h_{23} = -\partial_q^2 - \partial_\xi^2 + V_{23}\left(\left(\frac{|q|^2}{\mu_{23}} + (a_2 - a_3)^2\right)^{1/2}\right)$$

where the reduced mass μ_{23} of particles (23) is given by

$$\mu_{23} := \frac{m_2 m_3}{M_{23}}\,.$$

The set $K_{23}(\gamma)$ in (x_1,q,ξ)–coordinates is given by

$$\begin{aligned} K_{23}(\gamma) &= \left\{(x_1,q,\xi) \in \mathbb{R}^3 : |q| \leq \gamma\sqrt{\mu_{23}}\left(x_1^2 + q^2 + \xi^2\right)^{1/2}\right\} \\ &= \left\{(x_1,q,\xi) \in \mathbb{R}^3 : |q| \leq \kappa_0\left(x_1^2 + \xi^2\right)^{1/2}\right\} \end{aligned} \tag{5.5.61}$$

with

$$\kappa_0 := \left(\frac{\gamma^2\mu_{23}}{1-\gamma^2\mu_{23}}\right)^{1/2}\,. \tag{5.5.62}$$

The functional $L_{23}[\psi_{23}]$ can be written as

$$L_{23}[\psi_{23}] \geq \left(\frac{M_{23}}{\mu_{23}}\right)^{1/2} \Bigg[\int_{K_{23}(\gamma)} \left|\partial_q \psi_{23}\right|^2 + V_{23}|\psi_{23}|^2 d(x_1,q,\xi) + \int_{K_{23}(\gamma)} \left|\nabla_{(x_1,\xi)}\psi_{23}\right|^2 d(x_1,q,\xi) - 2\int_{K_{23}(\gamma)\setminus S(0,b)} \frac{|\psi_{23}|^2}{|(x_1,q,\xi))|^{2+\tau}} d(x_1,q,\xi) \Bigg] \tag{5.5.63}$$

where $(M_{23}/\mu_{23})^{1/2}$ is the Jacobian determinant of the transformation to the new set of coordinates (x_1,q,ξ). In abuse of notation, we denote ψ_{23} expressed in coordinates (x_1,q,ξ) by the same letter. We estimate (5.5.63) in two steps. As the first step, we show that

Lemma 5.5.8.

$$\int_{K_{23}(\gamma)} \left(\left|\partial_q \psi_{23}\right|^2 + V_{23}|\psi_{23}|^2\right) d(x_1,q,\xi) \geq -C \int_{\partial K_{23}(\gamma)} \frac{|\psi_{23}|^2}{|x|^{1+\delta}} d\sigma \tag{5.5.64}$$

for some $C > 0$ independent of ψ.

As a second step, we show the following lemma.

Lemma 5.5.9. *Define*

$$\mathcal{N}[\psi_{23}] := \int_{K_{23}(\gamma)} \left|\nabla_{(x_1,\xi)}\psi_{23}\right|^2 d(x_1,q,\xi) - 2\int_{K_{23}(\gamma)\setminus S(0,b)} \frac{|\psi_{23}|^2}{|(x_1,q,\xi))|^{2+\tau}} d(x_1,q,\xi)$$

then

$$\mathcal{N}[\psi_{23}] \geq -C \int_{\partial K_{23}(\gamma)} \frac{|\psi_{23}|^2}{|x|^{1+\tau}} d\sigma \tag{5.5.65}$$

for some constant $C > 0$ independent of ψ.

Proof of Lemma 5.5.8

We rewrite the first integral on the right–hand side of (5.5.63) as

$$\int_{K_{23}(\gamma)} \left(\left|\partial_q \psi_{23}\right|^2 + V_{23}|\psi_{23}|^2\right) d(x_1,q,\xi) = \int_{\mathbb{R}^2} \int_{-\kappa_0|(x_1,\xi)|}^{\kappa_0|(x_1,\xi)|} \left|\partial_q \psi_{23}\right|^2 + V_{23}|\psi_{23}|^2 dq\, d(x_1,\xi)\,. \tag{5.5.66}$$

Note that due to the positivity of operator h_{23} also holds

$$-\partial_q^2 + V_{23}\left(\left(\frac{|q|^2}{\mu_{23}} + (a_2-a_3)^2\right)^{1/2}\right) \geq 0\,.$$

Since the potential V_{23} satisfies

$$\left|V_{23}\left(\left(\frac{|q|^2}{\mu_{23}}+(a_2-a_3)^2\right)^{1/2}\right)\right| \leq \tilde{C}|q|^{2+\delta}$$

for some constant $\tilde{C}>0$ if q is sufficiently large, applying [13, Lemma 6.2] (for convenience of the reader, we proof it in Appendix B) there exists $C>0$ that depends on δ but is independent of ψ such that

$$\begin{aligned}\int_{-\kappa_0|(x_1,\xi)|}^{\kappa_0|(x_1,\xi)|} &\left|\partial_q\psi_{23}\right|^2+V_{23}|\psi_{23}|^2 dq \\ &\geq -C\frac{|\psi_{23}(x_1,\kappa_0|(x_1,\xi)|,\xi)|^2+|\psi_{23}(x_1,-\kappa_0|(x_1,\xi)|,\xi)|^2}{|(x_1,\xi)|^{1+\delta}}\,.\end{aligned} \tag{5.5.67}$$

Combining (5.5.66) and (5.5.67) we find

$$\begin{aligned}\int_{K_{23}(\gamma)} &\left(\left|\partial_q\psi_{23}\right|^2+V_{23}|\psi_{23}|^2\right)d(x_1,q,\xi) \\ &\geq -C\int_{\mathbb{R}^2}\frac{|\psi_{23}(x_1,\kappa_0|(x_1,\xi)|,\xi)|^2+|\psi_{23}(x_1,-\kappa_0|(x_1,\xi)|,\xi)|^2}{|(x_1,\xi)|^{1+\delta}}d(x_1,\xi)\,.\end{aligned} \tag{5.5.68}$$

The points $(x_1,\pm\kappa_0|(x_1,\xi)|,\xi)$ belong to the surface $\partial K_{23}(\gamma)$. Direct computations show that for the surface measure $d\sigma$ associated with the set $\partial K_{23}(\gamma)$ satisfies the relation

$$d\sigma=\kappa_0 d(x_1,\xi), \tag{5.5.69}$$

with κ_0 defined in (5.5.62). Consequently from (5.5.68) we find

$$\int_{K_{23}(\gamma)}\left(\left|\partial_q\psi_{23}\right|^2+V_{23}|\psi_{23}|^2\right)d(x_1,q,\xi) \geq -C\int_{\partial K_{23}(\gamma)}\frac{|\psi_{23}|^2}{|(x_1,\xi)|^{1+\delta}}d\sigma \tag{5.5.70}$$

for a possible different constant $C>0$. Using that on $\partial K_{23}(\gamma)$

$$|x|^2=|(x_1,\xi)|^2+q^2=(1+\kappa_0^2)|(x_1,\xi)|^2$$

completes the proof of Lemma 5.5.8. ∎

Proof of Lemma 5.5.9

This lemma mainly follows the ideas of [13, Lemma 6.7]. We introduce polar coordinates in the (x_1,ξ)–plane as

$$\rho:=\sqrt{x_1^2+\xi^2},\quad \varphi:=\arctan(x_1/\xi)\,.$$

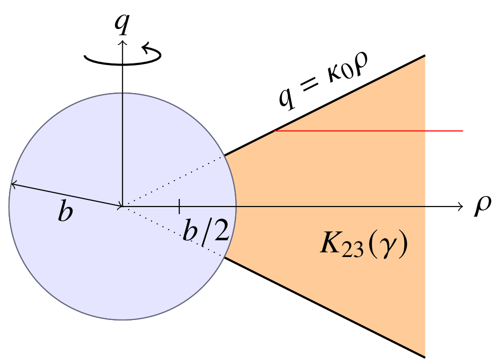

FIGURE 5.4: Sketch of the set $K_{23}(\gamma)$. In the circular blue area, the function ψ vanishes. For fixed $q \in \mathbb{R}$, the horizontal red line indicates the path of integration used in Lemma 5.5.9.

The set $\partial K_{23}(\gamma)$ corresponds to points with

$$|q| = \kappa_0 \rho,$$

where κ_0 was defined in (5.5.62). For each fixed $q \in \mathbb{R}$ let

$$\overline{\psi}(q) := \int_0^{2\pi} \psi_{23}(q, \kappa_0^{-1}|q|, \varphi) \frac{d\varphi}{2\pi} \quad \text{and} \quad \overline{\psi}_1(q, \rho, \varphi) := \overline{\psi}(q) \cdot \mathbb{1}(\rho, \varphi)\,.$$

Let $\mathscr{F} := \psi_{23} - \overline{\psi}_1$. We write $\nabla_{(\rho,\varphi)}$ for the gradient in polar coordinates in the (x_1, ξ)–plane. Then $\nabla_{(\rho,\varphi)}\overline{\psi}_1 \equiv 0$ and consequently

$$\begin{aligned} &\int_{K_{23}(\gamma)} \left|\nabla_{(x_1,\xi)}\psi_{23}\right|^2 d(x_1, q, \xi) \\ &\qquad = \int_{K_{23}(\gamma)} \left|\nabla_{(\rho,\varphi)}\psi_{23}\right|^2 d(q, \rho, \varphi) = \int_{K_{23}(\gamma)} \left|\nabla_{(\rho,\varphi)}\mathscr{F}\right|^2 d(q, \rho, \varphi), \end{aligned} \tag{5.5.71}$$

where $d(x_1, q, \xi) = d(q, \rho, \varphi) = \rho\, dq d\rho d\varphi$. Inserting (5.5.71) into the right–hand side of (5.5.65) we arrive at

$$\mathcal{N}[\psi_{23}] = \int_{K_{23}(\gamma)} \left|\nabla_{(\rho,\varphi)}\mathscr{F}\right|^2 d(q, \rho, \varphi) - 2 \int_{K_{23}(\gamma)\setminus S(0,b)} \frac{|\psi_{23}|^2}{|(x_1, q, \xi)|^{2+\tau}} d(x_1, q, \xi)\,. \tag{5.5.72}$$

Transforming the second integral on the right–hand side of (5.5.72) to polar coordinates, we get

$$\mathcal{N}[\psi_{23}] = \int_{K_{23}(\gamma)} \left|\nabla_{(\rho,\varphi)}\mathscr{F}\right|^2 d(q, \rho, \varphi) - 2 \int_{K_{23}(\gamma)\setminus S(0,b)} \frac{|\psi_{23}|^2}{|(q, \rho)|^{2+\tau}} d(q, \rho, \varphi)\,. \tag{5.5.73}$$

Since $\mathscr{F} = \psi_{23} - \overline{\psi}_1$ and $(a+b)^2 \leq 2a^2 + 2b^2$ it holds

$$\begin{aligned}&\int_{K_{23}(\gamma)\setminus S(0,b)} \frac{|\psi_{23}|^2}{|(q,\rho)|^{2+\tau}} d(q,\rho,\varphi)\\ &\leq 2\int_{K_{23}(\gamma)\setminus S(0,b)} \frac{|\mathscr{F}|^2}{|(q,\rho)|^{2+\tau}} d(q,\rho,\varphi) + 2\int_{K_{23}(\gamma)\setminus S(0,b)} \frac{|\overline{\psi}_1|^2}{|(q,\rho)|^{2+\tau}} d(q,\rho,\varphi)\,.\end{aligned} \tag{5.5.74}$$

Combining (5.5.73) and (5.5.74) yields

$$\begin{aligned}\mathcal{N}[\psi_{23}] \geq &\int_{K_{23}(\gamma)} \left|\nabla_{(\rho,\varphi)}\mathscr{F}\right|^2 d(q,\rho,\varphi) - 4\int_{K_{23}(\gamma)\setminus S(0,b)} \frac{|\mathscr{F}|^2}{|(q,\rho)|^{2+\tau}} d(q,\rho,\varphi)\\ &- 4\int_{K_{23}(\gamma)\setminus S(0,b)} \frac{|\overline{\psi}_1|^2}{|(q,\rho)|^{2+\tau}} d(q,\rho,\varphi)\,.\end{aligned} \tag{5.5.75}$$

Next, we show that the sum of the first two integrals on the right–hand side of (5.5.75) is positive. The function $\psi_{23} = 0$ for $|x| < b$ and consequently for

$$\rho_0 := \max\{\kappa_0^{-1}|q|, b/2\}$$

we have

$$\int_{K_{23}(\gamma)} \left|\nabla_{(\rho,\varphi)}\mathscr{F}\right|^2 d(q,\rho,\varphi) = \int_{-\infty}^{\infty}\int_{\rho_0}^{\infty}\int_0^{2\pi} \left|\nabla_{(\rho,\varphi)}\mathscr{F}(q,\rho,\varphi)\right|^2 d(\rho,\varphi)dq\,. \tag{5.5.76}$$

For $\rho = \rho_0$, the projection of $\mathscr{F}$ onto functions with zero angular momentum in the (x_1,ξ)–plane vanishes. As a result, the following two–dimensional Hardy inequality (see Lemma B.1.2) holds for almost all $q \in \mathbb{R}$:

$$\int_{\rho_0}^{\infty}\int_0^{2\pi} \left|\nabla_{(\rho,\varphi)}\mathscr{F}(q,\rho,\varphi)\right|^2 d(\rho,\varphi) \geq \frac{1}{4}\int_{\rho_0}^{\infty}\int_0^{2\pi} \frac{|\mathscr{F}(q,\rho,\varphi)|^2}{\rho^2\left(1+\ln^2(\rho)\right)} d(\rho,\varphi),$$

where we assume $\rho_0 > 1$ for sufficiently large $b > 0$. Inserting (5.5.3) into the right–hand side of (5.5.76) gives

$$\int_{K_{23}(\gamma)} \left|\nabla_{(\rho,\varphi)}\mathscr{F}\right|^2 d(q,\rho,\varphi) \geq \frac{1}{4}\int_{K_{23}(\gamma)} \frac{|\mathscr{F}|^2}{\rho^2\left(1+\ln^2(\rho)\right)} d(q,\rho,\varphi)\,. \tag{5.5.77}$$

Since $\rho > b/2$ on $K_{23}(\gamma) \cap \operatorname{supp}\psi_{23}$ the positivity of the sum of the first two terms on the right–hand side of (5.5.75) follows from (5.5.77) for $b > 0$ sufficiently large. We arrive at

$$\mathcal{N}[\psi_{23}] \geq -4\int_{K_{23}(\gamma)\setminus S(0,b)} \frac{|\overline{\psi}_1|^2}{|(q,\rho)|^{2+\tau}} d(q,\rho,\varphi)\,. \tag{5.5.78}$$

It remains to show that the integral on the right–hand side of (5.5.78) can be estimated by an integral over $\partial K_{23}(\gamma)$. By direct computation

$$\int_{K_{23}(\gamma)\setminus S(0,b)} \frac{\left|\overline{\psi}_1(q,\rho,\varphi)\right|^2}{|(q,\rho)|^{2+\tau}} d(q,\rho,\varphi) = 2\pi \int_{-\infty}^{\infty}\int_{\rho_0}^{\infty} \frac{\left|\overline{\psi}_1(q,\rho,\varphi)\right|^2}{|(q,\rho)|^{2+\tau}} \rho d\rho dq\,. \tag{5.5.79}$$

Using the definition of $\overline{\psi}_1$ and Schwarz Inequality

$$2\pi \int_{-\infty}^{\infty}\int_{\rho_0}^{\infty} \frac{\left|\overline{\psi}_1(q)\right|^2}{|(q,\rho)|^{2+\tau}} \rho d\rho dq \le \int_{-\infty}^{\infty}\int_{\rho_0}^{\infty} \frac{\int_0^{2\pi}\left|\psi_{23}(q,\kappa_0^{-1}|q|,\varphi)\right|^2 d\varphi}{|(q,\rho)|^{2+\tau}} \rho d\rho dq\,. \tag{5.5.80}$$

Combining (5.5.79) and (5.5.80) we arrive at

$$\begin{aligned} &\int_{K_{23}(\gamma)\setminus S(0,b)} \frac{\left|\overline{\psi}_1\right|^2}{|(q,\rho)|^{2+\tau}} d(q,\rho,\varphi) \\ &\qquad \le \int_{-\infty}^{\infty}\int_0^{2\pi} \left|\psi_{23}(q,\kappa_0^{-1}|q|,\varphi)\right|^2 d\varphi \int_{\rho_0}^{\infty} \frac{1}{|(q,\rho)|^{2+\tau}} \rho d\rho dq\,. \end{aligned}$$

Using $|(q,\rho)| > \rho$ and $\rho_0 > \kappa_0^{-1}|q|$, yields by solving the integral over ρ that there exists a constant $C > 0$, which depends on τ and κ_0 but is independent of ψ, such that

$$\int_{K_{23}(\gamma)\setminus S(0,b)} \frac{|\overline{\psi}_1|^2}{|(q,\rho)|^{2+\tau}}\, d(q,\rho,\varphi) \le C \int_{-\infty}^{\infty}\int_0^{2\pi} \frac{|\psi_{23}(q,\kappa_0^{-1}|q|,\varphi)|^2}{|q|^{1+\tau}}\, q\, dq\, d\varphi. \tag{5.5.81}$$

The points $(q,\kappa_0^{-1}|q|,\varphi)$ with $q \in \mathbb{R}$ and $\varphi \in [0,2\pi)$ correspond to points on the surface $\partial K_{23}(\gamma)$. Consequently, by substituting (5.5.81) into (5.5.78), we obtain for another constant $C > 0$ that depends on κ_0 and τ but is independent of ψ:

$$\mathcal{N}[\psi_{23}] \ge -C \int_{\partial K_{23}(\gamma)} \frac{|\psi|^2}{|x|^{1+\tau}}\, d\sigma, \tag{5.5.82}$$

where we used that $\psi_{23} = \psi$ on $\partial K_{23}(\gamma)$. This completes the proof of Lemma 5.5.9, and as discussed in 5.5.3, this also completes the proof of Lemma 5.3.2. ∎

5.5.4 Proof of Lemma 5.3.3

We prove Lemma 5.3.3 for $\alpha = (12)$. The proof for $\alpha = (13)$ is similar. We introduce spherical coordinates as follows:

$$\begin{aligned} x_1 &= |x|\sin(\varphi)\sin(\theta), \\ x_2 &= |x|\cos(\varphi)\sin(\theta), \\ x_3 &= |x|\cos(\theta), \end{aligned} \tag{5.5.83}$$

where $\varphi \in [0, 2\pi)$, $\theta \in [0, \pi]$, and $|x| \in [0, \infty)$. The boundary $\partial K_{12}(\gamma)$ is then described by $(|x|, \pm\theta_0, \varphi)$, where $\theta_0 = \arcsin(\gamma)$ and $\theta_0 \in [0, \pi]$ (see Figure 5.3).
Let $P_0[(12)]$ be the projection onto radially symmetric functions in the (x_1, x_2)–plane introduced in Lemma 5.3.1, then

$$\int_{\partial K_{12}(\gamma)} \frac{|(P_0[(12)]\psi)(x)|^2}{|x|^{1+\delta}}\, d\sigma \le \int_{\partial K_{12}(\gamma)} \frac{|\psi(x)|^2}{|x|^{1+\delta}}\, d\sigma \tag{5.5.84}$$

where the surface measure $d\sigma$ associated with $\partial K_{12}(\gamma)$ in the spherical coordinattes (5.5.83) is given by

$$d\sigma = |\sin\theta_0||x|d|x|d\varphi\,. \tag{5.5.85}$$

By applying the one–dimensional trace theorem in the θ variable (see, [31, Theorem 1, p. 272]) for every fixed $|x| > b/2$, $\varphi \in [0, 2\pi)$, there is a constant $C > 0$ that depends on θ_0 and $\theta_1 := \arcsin(\gamma_1)$ but is independent of $|x|$ and φ such that

$$\frac{|\psi(|x|, \theta_0, \varphi)|^2}{|x|^{1+\delta}} \le C \int_{\theta_0}^{\theta_1} \frac{|\psi(|x|, \theta, \varphi)|^2 + |(\partial_\theta\psi)(|x|, \theta, \varphi)|^2}{|x|^{1+\delta}} d\theta. \tag{5.5.86}$$

Integrating (5.5.86) with respect to $d\sigma$ in (5.5.85) yields

$$\begin{aligned} &\int_0^{2\pi}\int_{b/2}^{\infty} |\psi(|x|, \theta_0, \varphi)|^2 |\sin\theta_0||x|d|x|d\varphi \\ &\le C|\sin\theta_0| \int_0^{2\pi}\int_{\theta_0}^{\theta_1}\int_{b/2}^{\infty} \frac{|\psi(|x|, \theta, \varphi)|^2 + |(\partial_\theta\psi)(|x|, \theta, \varphi)|^2}{|x|^{1+\delta}} |x|d|x|d\theta d\varphi. \end{aligned} \tag{5.5.87}$$

where we have also used that $\psi(|x|, \theta, \varphi) = 0$ for $|x| < b/2$. Similar we get

$$\begin{aligned} &\int_0^{2\pi}\int_{b/2}^{\infty} |\psi(|x|, -\theta_0, \varphi)|^2 |\cos\theta||x|d|x|d\varphi \\ &\le C|\sin\theta_0| \int_0^{2\pi}\int_{-\theta_1}^{-\theta_0}\int_{b/2}^{\infty} \frac{|\psi(|x|, \theta, \varphi)|^2 + |(\partial_\theta\psi)(|x|, \theta, \varphi)|^2}{|x|^{1+\delta}} |x|d|x|d\theta d\varphi. \end{aligned} \tag{5.5.88}$$

For $K_{12}(\gamma, \gamma_1) = K_{12}(\gamma_1) \setminus K_{12}(\gamma)$ by combining (5.5.87) and (5.5.88) we find

$$\begin{aligned} &\int_{\partial K_{12}(\gamma)} \frac{|\psi(x)|^2}{|x|^{1+\delta}}\, d\sigma \\ &\le C|\sin\theta_0| \int_{K_{12}(\gamma,\gamma_1)} \frac{|\psi(|x|, \theta, \varphi)|^2 + |(\partial_\theta\psi)(|x|, \theta, \varphi)|^2}{|x|^{1+\delta}} |x|d|x|d\theta d\varphi\,. \end{aligned} \tag{5.5.89}$$

Using $dx = \sin(\theta)|x|^2 d|x| d\theta d\varphi$ and $\sin(\theta_0) \le |\sin(\theta)|$ on $K_{12}(\gamma, \gamma_1)$ we arrive at

$$\begin{aligned}&\int_{\partial K_{12}(\gamma)} \frac{|\psi(x)|^2}{|x|^{1+\delta}}\, d\sigma \\ &\le C \int_{K_{12}(\gamma,\gamma_1)} \frac{|\psi(|x|,\theta,\varphi)|^2}{|x|^{2+\delta}} dx + C \int_{K_{12}(\gamma,\gamma_1)} \frac{|(\partial_\theta \psi)(|x|,\theta,\varphi)|^2}{|x|^{2+\delta}} dx\,.\end{aligned} \tag{5.5.90}$$

Since $\psi(x) = 0$ for $|x| \le b/2$ we conclude from (5.5.90)

$$\begin{aligned}&\int_{\partial K_{12}(\gamma)} \frac{|\psi(x)|^2}{|x|^{1+\delta}}\, d\sigma \\ &\le \frac{C}{(b/2)^\delta} \left(\int_{K_{12}(\gamma,\gamma_1)} \frac{|\psi(|x|,\theta,\varphi)|^2}{|x|^2} dx + \int_{K_{12}(\gamma,\gamma_1)} \frac{|(\partial_\theta \psi)(|x|,\theta,\varphi)|^2}{|x|^2} dx \right).\end{aligned} \tag{5.5.91}$$

Applying the radial Hardy Inequality to the first term on the right–hand side of (5.5.91) yields

$$\begin{aligned}&\int_{\partial K_{12}(\gamma)} \frac{|\psi(x)|^2}{|x|^{1+\delta}}\, d\sigma \\ &\le \frac{C}{(b/2)^\delta} \left(\int_{K_{12}(\gamma,\gamma_1)} \frac{1}{4} \left|\partial_{|x|} \psi(|x|,\theta,\varphi)\right|^2 dx + \int_{K_{12}(\gamma,\gamma_1)} \frac{|(\partial_\theta \psi)(|x|,\theta,\varphi)|^2}{|x|^2} dx \right).\end{aligned} \tag{5.5.92}$$

Expressing the gradient in spherical coordinates, we conclude from (5.5.92) that

$$\int_{\partial K_{12}(\gamma)} \frac{|\psi(x)|^2}{|x|^{1+\delta}}\, d\sigma \le \frac{C}{(b/2)^\delta} \|\nabla \psi\|^2_{L^2(K_{12}(\gamma,\gamma_1))}, \tag{5.5.93}$$

which completes the proof of Lemma 5.3.3 ∎

5.5.5 Proof of Lemma 5.3.4

In the set of coordinates (x_1, q, ξ) introduced in 5.5.3 the set $\partial K_{23}(\gamma)$ is determined by

$$|q| = \kappa_0 (x_1^2 + \xi^2)^{1/2}$$

with κ_0 defined in (5.5.62). We introduce spherical coordinates as follows:

$$\begin{aligned} x_1 &= |x| \sin(\varphi) \cos(\vartheta), \\ \xi &= |x| \cos(\varphi) \cos(\vartheta), \\ q &= |x| \sin(\vartheta), \end{aligned} \tag{5.5.94}$$

where we used that the coordinates (x_1, q, ξ) fulfill $|x| = |(x_1, q, \xi)|$ (see Lemma B.2.4). In this set of coordinates $\vartheta_0 := \arctan(\kappa_0)$ corresponds to the opening angle of the conical set

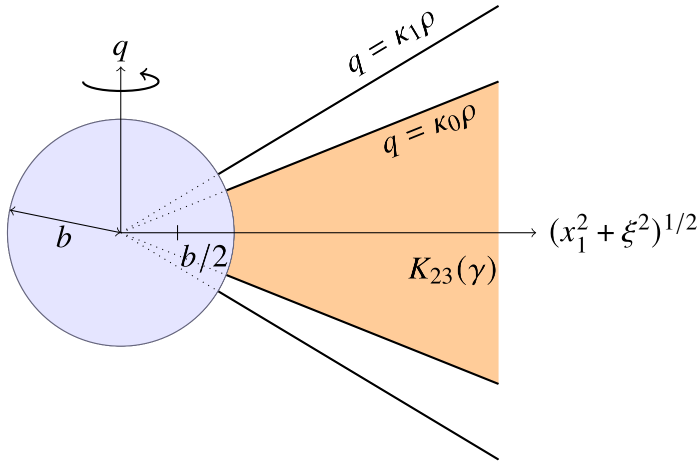

FIGURE 5.5: Sketch of the sets $K_{23}(\gamma)$ and $K_{23}(\gamma_1)$ and their relation to the constants κ_0 and κ_1. This construction is used in Lemma 5.3.4.

$K_{23}(\gamma)$. Let $\vartheta_1 \coloneqq \arctan \kappa_1$ with

$$\kappa_1 \coloneqq \left(\frac{\gamma_1^2 \mu_{23}}{1 - \gamma_1^2 \mu_{23}} \right)^{1/2}, \tag{5.5.95}$$

then $\vartheta_1 > \vartheta_0$ corresponds to the opening angle of the conical set $K_{23}(\gamma_1)$ (see Figure 5.5). Analogous to Lemma 5.3.3 by application of the one–dimensional trace theorem in the variable ϑ and the radial Hardy Inequality proves Lemma 5.3.4. ∎

Chapter 6

Conspiracy of Potential Wells and Absence of Efimov Effect in Dimension Four.

6.1 Introduction

We study the double–well operator

$$H_R := P^2 + V_1(x) + V_2(x - R), \quad P = -i\nabla_x \quad \text{on } L^2(\mathbb{R}^d) \tag{6.1.1}$$

for fixed $R \in \mathbb{R}^d$ and short–range potentials V_1, V_2 in dimension $d \geq 3$. This operator appears in the Born–Oppenheimer approximation for quantum three–body systems. This approximation is for instance used in the study of molecules. Beyond Coulomb interactions, it is also known that for short-range potentials, i.e., potentials that asymptotically decay faster than $|x|^{-2}$, the Born-Oppenheimer approximation and the operator H_R plays an important role in the understanding of the *Efimov effect* (see, e.g., [89], [66], [34] and [113]).

Remark 6.1.1. *In Section 1.5.2, and in particular in* (1.5.15)*, we provide a heuristic derivation of the operator* (6.1.1)*. In previous sections, we used the convention* $T = P^2/2$ *for the kinetic energy operator. Here, by assuming all involved particles in* (1.5.15) *have mass one, the prefactor* $1/2$ *in the kinetic energy becomes* 1*. Consequently, the choice in* (6.1.1) *is the natural one for the present discussion.*

The Efimov effect, first predicted by Efimov in [28], describes an unexpected phenomenon where three particles can form an infinite number of bound states, even if none of the two-particle subsystems are bound, provided at least two subsystems have a so–called *virtual level* (see Definition 1.4.1).
The Efimov effect exhibits several remarkable features. One of these is its so–called universality property. That is, the asymptotic behavior of the number of bound states below the essential spectrum does not depend on the microscopic details of the involved potentials.
We study the asymptotic limit of the ground state energy $E(R) := \inf \sigma(H_R)$ of the operator H_R in the parameter R in the case where the operators $h_1 := P^2 + V_1 \geq 0$ and $h_2 := P^2 + V_2 \geq 0$ do not have bound states but have virtual–levels.

For $d = 3$, it has been proven by Klaus and Simon in [66][Theorem 4] for strictly negative potentials that

$$|R|^2 E(R) \to -\alpha^2, \quad \text{as } |R| \to \infty,$$

where $\alpha > 0$ is the unique solution of $\exp(-\alpha) = \alpha$. Under some additional assumptions on the potentials, it was shown in [91, Theorem 4.3] by Pinchover that if $d \geq 5$, there exists $C \geq 0$ with

$$-C|R|^{2-d} \leq E(R) \leq -C^{-1}|R|^{2-d}$$

whenever $|R|$ is large enough. For dimensions $d \geq 5$ the existence of a virtual level of h_j with $j \in \{1, 2\}$ forces h_j to have zero as an eigenvalue. However, if $d = 3$ the operators h_j, do not necessarily have a zero–energy solution in $L^2(\mathbb{R}^3)$ but a *resonance* at zero (see Remark 1.4.2 and Remark 3.2.4).

The most challenging case is $d = 4$. The difference to dimension $d = 3$ is, that if the zero–energy solution is not in $L^2(\mathbb{R}^4)$ then its decay rate at infinity is critically slow, meaning that it barely misses being in $L^2(\mathbb{R}^4)$. We refer to Theorem 3.2.2 and the discussion thereafter for more details.

Assuming that the potentials are compactly supported and have additional smoothness, Pinchover showed in [90, Theorem 2.3] for $d = 4$, that there exists $C > 0$ such that

$$-C|R|^{-2} \leq E(R) \leq -C^{-1}|R|^{-2}\log(|R|)^{-1}$$

whenever $|R|$ is large enough. However, the lower bound in Pinchover's result *does not* match the upper bound. In this work, we establish a matching lower bound. Specifically, we prove that

$$-C|R|^{-2}\log(|R|)^{-1} \leq E(R)$$

for some $C > 0$ in Section 6.2 as Theorem 6.2.4. Using similar ideas as in the proof of Theorem 6.2.4, we provide in Section 6.3 a fully variational proof of the absence of the Efimov effect in dimension $d = 4$.

6.2 Conspiracy of Potential Wells in Dimension Four

6.2.1 Notation and Main Result

We study the double-well operator

$$H_R = P^2 + V_1(x) + V_2(x - R)$$

on $L^2(\mathbb{R}^4)$ for $R \in \mathbb{R}^4$ and potentials $V_1, V_2 \in L^2_{\text{loc}}(\mathbb{R}^4) \cap K_4$ where K_4 the Kato class defined in Definition 1.2.8. Then following [105, Lemma A.2.2] the potential V_j is infinitesimally form small with respect to P^2. We assume that V_j for $j \in \{1, 2\}$ is short-range, i.e. there are constants $C, \delta, \rho > 0$ such that

$$\left|V_j(x)\right| \leq C|x|^{-2-\delta}, \quad j \in \{1, 2\}. \tag{6.2.1}$$

for any $|x| > \rho$.

Remark 6.2.1. *With some changes below, one can instead assume the (weak) short–range property in* (3.2.2)*, which allows the potential to have local singularities outside of compact sets.*

We denote by $\sigma(H_R)$ the spectrum of H_R. We adopt the standard notation as, for instance, used in [13] and denote one-particle Schrödinger operators with a single potential well, such as $h_j := P^2 + V_j$ for $j \in \{1, 2\}$, using lowercase letters.

Definition 6.2.2 (= Definition 1.4.1)**.** *The operator $h = P^2 + V$ has a virtual level at zero if $H \geq 0$ and there exists $\varepsilon_1 \in (0, 1)$ such that for any $\varepsilon \in (0, \varepsilon_1)$*

$$\inf \sigma_{\text{ess}}(h - \varepsilon P^2) = 0 \quad \text{and} \quad \inf \sigma(h - \varepsilon P^2) < 0\,. \tag{6.2.2}$$

Remark 6.2.3. *In Definition 1.4.1 we have used a different mass convention where the kinetic energy is $P^2/2$. Throughout this section $h = P^2 + V$, see Remark 6.1.1.*

Theorem 6.2.4. *Let H_R on $L^2(\mathbb{R}^4)$ be defined as in* (6.1.1) *with short–range potentials $V_j \in L^2_{\text{loc}}(\mathbb{R}^4) \cap K_4$, such that $h_j = P^2 + V_j \geq 0$ has a virtual level for $j \in \{1, 2\}$. Then there exists $C > 0$ such that for any $R \in \mathbb{R}^4$*

$$E(R) := \inf \sigma(H_R) \geq -C|R|^{-2} \log(|R|)^{-1}\,. \tag{6.2.3}$$

We prove Theorem 6.2.4 in Section 6.2.2. First, we collect some properties of zero-energy resonances. Let

$$\dot{H}^1(\mathbb{R}^4) = \{u \in L^2(\mathbb{R}^4, |x|^{-2}dx) : \nabla u \in L^2(\mathbb{R}^4)\}$$

be the homogeneous Sobolev space equipped with the norm

$$\|u\|_{\dot{H}^1(\mathbb{R}^4)} := \left(\int_{\mathbb{R}^4} |\nabla u|^2 dx\right)^{1/2}\,.$$

These homogeneous Sobolev spaces have already been introduced by Birman in [22] (See [36, Chapter 2] for an overview). For any short–range potential $V \in L^2_{\text{loc}}(\mathbb{R}^4) \cap K_4$ we can apply Theorem 1.4.11 and Theorem 1.4.12. Consequently, if the operator $h := P^2 + V$ has a virtual level, then there exists $\varphi \in \dot{H}^1(\mathbb{R}^4)$, $\varphi \neq 0$ such that

$$h\varphi = 0 \tag{6.2.4}$$

in the sense that

$$\int_{\mathbb{R}^4} \nabla\psi\overline{\nabla\varphi}dx + \int_{\mathbb{R}^4} V\psi\overline{\varphi}dx = 0, \quad \forall\psi \in \dot{H}^1(\mathbb{R}^4). \tag{6.2.5}$$

Furthermore, there exists a constant $\mu > 0$, such that for every function $g \in \dot{H}^1(\mathbb{R}^4)$ with $\langle\nabla g, \nabla\varphi\rangle = 0$ we have

$$\langle g, hg\rangle \geq \mu\|\nabla g\|_2^2\,. \tag{6.2.6}$$

For $V \in K_4$ we have proven in Section 3.2 as Theorem 3.2.2 that then

$$\varphi(x) = -\frac{1}{2\pi}\frac{\langle V, \varphi\rangle}{1+|x|^2} + u(x) \tag{6.2.7}$$

for some $u \in L^2(\mathbb{R}^4)$.

6.2.2 Ground State Energy Estimate

In the proof of Theorem 6.2.4, we will use the following modification of [120, Lemma 5.1].

Lemma 6.2.5. *For any* $\varepsilon, b > 0$ *there exist* $0 < a < b$ *and continuous functions* $u, v : \mathbb{R} \to [0,1]$ *with piecewise continuous derivatives, such that* $u^2 + v^2 = 1$*,*

$$v(x) = \begin{cases} 1, & |x| \geq b \\ 0, & |x| \leq a \end{cases}, \quad u(x) = \begin{cases} 1, & |x| \leq a \\ 0, & |x| \geq b \end{cases},$$

and

$$|u'(x)|^2 + |v'(x)|^2 \leq \frac{\varepsilon}{|x|^2}\mathbb{1}_{\{a \leq |x| \leq b\}}.$$

Moreover, a can be chosen such that

$$e^{-(1+2/\varepsilon)} \leq \frac{a}{b} \leq e^{-2/\varepsilon}. \tag{6.2.8}$$

Proof. For the reader's convenience, we prove this lemma in the Appendix C as Lemma C.1.1. ■

Equipped with Lemma 6.2.5 we now give proof of the main Theorem 6.2.4.

Proof of Theorem 6.2.4. Let $\psi \in H^1(\mathbb{R}^4)$ with $\|\psi\|_2 = 1$. For fixed $R \in \mathbb{R}^4$ the quadratic form corresponding to the operator H_R in (6.1.1) is given by

$$L[\psi] := \int_{\mathbb{R}^4} |\nabla\psi|^2 dx + \int_{\mathbb{R}^4} \big(V_1(x) + V_2(x-R)\big)|\psi|^2 dx. \tag{6.2.9}$$

Theorem 6.2.4 follows directly if there exists a constant $C > 0$ independent of Ψ and R with

$$L[\psi] \geq -C|R|^{-2}\log(|R|)^{-1}. \tag{6.2.10}$$

The parameter $|R| > 0$ separates the potentials V_1 and V_2 into distinct regions of $\mathbb{R}^4$. We aim to localize L in regions where either one or both potentials are small. To this end, we define, for $s \in (0,1)$, the following sets:

$$\begin{aligned} B_1(s) &:= \{x \in \mathbb{R}^4 \mid |x| \leq s|R|\}, \\ B_2(s) &:= \{x \in \mathbb{R}^4 \mid |x-R| \leq s|R|\}, \\ \Omega(s) &:= \mathbb{R}^4 \setminus (B_1(s) \cup B_2(s)). \end{aligned}$$

By the short-range condition of V_j for $j \in \{1,2\}$, the potential V_2 is small on $B_1(s)$ for large $|R|$, while the potential V_1 is small on $B_2(s)$. On the set $\Omega(s)$, both potentials are small. Assume $b < 1/3$ such that $B_1(b) \cap B_2(b) = \emptyset$, then for any $\varepsilon > 0$ we choose $a > 0$ and functions $u, v : \mathbb{R} \to [0,1]$ according to Lemma 6.2.5. Define

$$\chi_1 := u\left(\frac{|x|}{|R|}\right), \quad \chi_2 := u\left(\frac{|x-R|}{|R|}\right), \text{ and } \chi_0 := \left(1 - \chi_1^2 - \chi_2^2\right)^{1/2},$$

then $\{\chi_0, \chi_1, \chi_2\}$ is a quadratic partition of unity with

$$\sum_{k=0}^{2} |\nabla \chi_k|^2 \leq \begin{cases} \varepsilon |x|^{-2}, & x \in B_1(b) \setminus B_1(a) \\ \varepsilon |x-R|^{-2}, & x \in B_2(b) \setminus B_2(a) \\ 0, & x \in \Omega(b) \cup B_1(a) \cup B_2(a) \end{cases}.$$

Let $A_k(b,a) := B_k(b) \setminus B_k(a)$ for $k \in \{1,2\}$ and then by application of the IMS localization formula (1.3.1) we find

$$\begin{aligned} L[\psi] &= \sum_{k=0}^{2} L[\chi_k \psi] - \sum_{k=0}^{2} \int_{\mathbb{R}^4} |\nabla \chi_k|^2 |\psi|^2 dx \\ &\geq \left(\sum_{k=0}^{2} L[\chi_k \psi]\right) - \varepsilon \int_{A_1(b,a)} \frac{|\psi|^2}{|x|^2} dx - \varepsilon \int_{A_2(b,a)} \frac{|\psi|^2}{|x-R|^2} dx \,. \end{aligned} \tag{6.2.11}$$

Define for any $f \in H^1$

$$\begin{aligned} L_1[f] &:= L[f] - \varepsilon \int_{A_1(b,a)} \frac{|f|^2}{|x|^2} dx, \\ L_2[f] &:= L[f] - \varepsilon \int_{A_2(b,a)} \frac{|f|^2}{|x-R|^2} dx \,. \end{aligned} \tag{6.2.12}$$

Then by inserting (6.2.12) into (6.2.11) we arrive at

$$L[\psi] \geq L[\chi_0 \psi] + L_1[\chi_1 \psi] + L_2[\chi_2 \psi] \,. \tag{6.2.13}$$

We prove Theorem 6.2.4 in two steps. In the first step, we show $L[\chi_0 \psi] \geq 0$ for $|R|$ large enough, and in the second step, we show that there exists $C > 0$ such that

$$L_j[\psi] \geq -C \frac{|\psi|^2}{|R|^2 \log(|R|)}, \quad j \in \{1,2\} \tag{6.2.14}$$

for $|R|$ large enough, which then completes the proof of Theorem 6.2.4. We begin with

Step 1:

We show for $|R|$ sufficiently large

$$L[\chi_0\psi] = \int_{\mathbb{R}^4} |\nabla (\chi_0\psi)|^2 dx + \int_{\mathbb{R}^4} (V_1(x) + V_2(x-R)) |\chi_0\psi|^2 dx \geq 0 \,. \tag{6.2.15}$$

By construction $\mathrm{supp}(\chi_0\psi) \subset \Omega(a)$. The potentials V_1 and $V_2(\cdot - R)$ are short-range such that for $|R| > 0$ large enough and $x \in \Omega(a)$

$$V_1(x) \leq |x|^{-2-\delta} \quad \text{and} \quad V_2(x-R) \leq |x-R|^{-2-\delta} \,. \tag{6.2.16}$$

Inserting (6.2.16) into (6.2.15) we arrive at

$$L[\chi_0\psi] \geq \int_{\mathbb{R}^4} |\nabla (\chi_0\psi)|^2 dx - \int_{\Omega(a)} \left(|x|^{-2-\delta} + |x-R|^{-2-\delta}\right) |\chi_0\psi|^2 dx \,. \tag{6.2.17}$$

Using that $\nabla \left[(\chi_0\psi)\,(x-R)\right] = \left[\nabla (\chi_0\psi)\right](x-R)$ together with the Hardy inequality in dimension four yields

$$\begin{aligned} \int_{\mathbb{R}^4} |\nabla (\chi_0\psi)|^2 dx &= \frac{1}{2} \int_{\mathbb{R}^4} |\nabla (\chi_0\psi)\,(x)|^2 dx + \frac{1}{2} \int_{\mathbb{R}^4} |\nabla \left[(\chi_0\psi)\,(x-R)\right]|^2 dx \\ &\geq \frac{1}{2} \int_{\mathbb{R}^4} \frac{|\chi_0\psi|^2}{|x|^2} dx + \frac{1}{2} \int_{\mathbb{R}^4} \frac{|\chi_0\psi|^2}{|x-R|^2} dx \,. \end{aligned} \tag{6.2.18}$$

Inserting (6.2.18) into (6.2.17) we arrive at

$$\begin{aligned} L[\chi_0\psi] \geq{} & \frac{1}{2} \int_{\mathbb{R}^4} \left(|x|^{-2} + |x-R|^{-2}\right) |\chi_0\psi|^2 dx \\ & - \int_{\Omega(a)} \left(|x|^{-2-\delta} + |x-R|^{-2-\delta}\right) |\chi_0\psi|^2 dx \,. \end{aligned} \tag{6.2.19}$$

Since $\delta > 0$, $|x| > a|R|$ and $|x-R| > a|R|$ on $\Omega(a)$ we find

$$\begin{aligned} & \int_{\Omega(a)} \left(|x|^{-2-\delta} + |x-R|^{-2-\delta}\right) |\chi_0\psi|^2 dx \\ & \qquad \leq \left(\frac{1}{a|R|}\right)^{\delta} \int_{\mathbb{R}^4} \left(|x|^{-2} + |x-R|^{-2}\right) |\chi_0\psi|^2 dx \,. \end{aligned} \tag{6.2.20}$$

Consequently by combining (6.2.20) and (6.2.19) we find $L[\chi_0\psi] \geq 0$.

Step 2:

We prove (6.2.14) for $j = 1$. The proof for $j = 2$ is similar. We aim to estimate

$$L_1[\chi_1\psi] = \int_{\mathbb{R}^4} |\nabla(\chi_1\psi)|^2 dx + \int_{\mathbb{R}^4} V_1(x)|\chi_1\psi|^2 dx + \int_{\mathbb{R}^4} V_2(x-R)|\chi_1\psi|^2 dx \\ - \varepsilon \int_{A_1(b,a)} \frac{|\chi_1\psi|^2}{|x|^2} dx\,.$$

We begin with estimating the term involving V_2. Since $b < 1/3$ and $\operatorname{supp}(\chi_1\psi) \subset B_1(b)$ we have for any $x \in \operatorname{supp}(\chi_1\psi)$ that $|x - R| > |R|/2$. Consequently the potential $V_2(\cdot - R)$ fulfills (6.2.1). Thus for $|R|$ sufficiently large

$$|V_2(|x-R|)| \le \frac{1}{|x-R|^{2+\delta}} \le \frac{2^{2+\delta}}{|R|^{2+\delta}} \le \frac{1}{|R|^{2+\delta/2}}\,.$$

Consequently, the term involving V_2 is negligible as it decays faster than the right-hand side of (6.2.14). It remains to estimate

$$\hat{L}[\chi_1\psi] \coloneqq \int_{\mathbb{R}^4} |\nabla(\chi_1\psi)|^2 dx + \int_{\mathbb{R}^4} V_1(x)|\chi_1\psi|^2 dx - \varepsilon \int_{A_1(b,a)} \frac{|\chi_1\psi|^2}{|x|^2} dx\,. \qquad (6.2.21)$$

We begin with the first two integrals on the right–hand side of (6.2.21). The operator $h_1 = P^2 + V_1$ has a virtual level at zero. As explained in Section 6.2.1 this implies the existence of a solution $\varphi_1 \in \dot{H}^1(\mathbb{R}^4)$ with $h_1\varphi_1 = 0$. We choose φ_1 to be normalized such that $\|\varphi_1\|_{\dot{H}^1(\mathbb{R}^4)} = 1$. Next, we project $\chi_1\psi$ onto φ_1 in the sense of $\dot{H}^1(\mathbb{R}^4)$ by introducing

$$\theta_R \coloneqq \langle \nabla\varphi_1, \nabla(\chi_1\psi)\rangle \quad \text{and} \quad g \coloneqq \chi_1\psi - \theta_R\varphi_1\,. \qquad (6.2.22)$$

Then

$$\langle \nabla\varphi_1, \nabla g\rangle = 0\,.$$

Due to the definition of θ_R and g in (6.2.22) we have

$$\int_{\mathbb{R}^4} |\nabla(\chi_1\psi)|^2 dx + \int_{\mathbb{R}^4} V_1|\chi_1\psi|^2 dx = \int_{\mathbb{R}^4} |\nabla g|^2 dx + \int_{\mathbb{R}^4} V_1|g|^2 dx \\ + 2\theta_R \operatorname{Re} \int_{\mathbb{R}^4} \left(\nabla g \overline{\nabla\varphi_1} + V_1 g \overline{\varphi_1}\right) dx\,. \qquad (6.2.23)$$

Since φ_1 is the zero–energy solution as explained in (6.2.5) it follows

$$\operatorname{Re} \int_{\mathbb{R}^4} \left(\nabla g \overline{\nabla\varphi_1} + V_1 g \overline{\varphi_1}\right) dx = 0$$

and therefore

$$\int_{\mathbb{R}^4} |\nabla(\chi_1\psi)|^2 dx + \int_{\mathbb{R}^4} V_1|\chi_1\psi|^2 dx = \int_{\mathbb{R}^4} |\nabla g|^2 dx + \int_{\mathbb{R}^4} V_1|g|^2 dx\,. \tag{6.2.24}$$

As discussed in Section 6.2.1, since $\langle \nabla\varphi_1, \nabla g\rangle = 0$, there exists a constant $\mu > 0$ such that

$$\int_{\mathbb{R}^4} |\nabla g|^2 dx + \int_{\mathbb{R}^4} V_1|g|^2 dx \geq \mu\|\nabla g\|_2^2\,. \tag{6.2.25}$$

Inserting (6.2.25) into the right–hand side of (6.2.24) yields

$$\int_{\mathbb{R}^4} |\nabla(\chi_1\psi)|^2 dx + \int_{\mathbb{R}^4} V_1(x)|\chi_1\psi|^2 dx \geq \mu\|\nabla g\|_2^2\,. \tag{6.2.26}$$

Combining (6.2.26) and (6.2.21) we find

$$\hat{L}[\chi_1\psi] \geq \mu\|\nabla g\|_2^2 - \varepsilon\int_{A_1(b,a)} \frac{|\chi_1\psi|^2}{|x|^2} dx\,. \tag{6.2.27}$$

Inserting $\chi_1\psi = \theta_R\varphi_1 + g$ into the right–hand side of (6.2.27) yields

$$\begin{aligned} \hat{L}[\chi_1\psi] &\geq \mu\|\nabla g\|_2^2 - \varepsilon\int_{A_1(b,a)} \frac{|\theta_R\varphi_1 + g|^2}{|x|^2} dx \\ &\geq \mu\|\nabla g\|_2^2 - 2\varepsilon\int_{A_1(b,a)} \frac{|\theta_R\varphi_1|^2}{|x|^2} - 2\varepsilon\int_{A_1(b,a)} \frac{|g|^2}{|x|^2} dx\,. \end{aligned} \tag{6.2.28}$$

To prove (6.2.14) it suffices to show that for given $\mu > 0$ and $\varepsilon \in (0, \mu/4)$ for $|R| > 0$ sufficiently large there exists a $c_0 > 0$ depending on μ, ε only such that

$$\mu\|\nabla g\|_2^2 - 2\varepsilon\int_{A_1(b,a)} \frac{|\theta_R\varphi_1|^2}{|x|^2} - 2\varepsilon\int_{A_1(b,a)} \frac{|g|^2}{|x|^2} dx \geq -\frac{c_0}{|R|^2\log(|R|)}\,. \tag{6.2.29}$$

Using $\varepsilon \in (0, \mu/4)$ together with $A_1(b, a) \subset \mathbb{R}^4$ and applying Hardy Inequality in dimension four we have

$$2\varepsilon\int_{A_1(b,a)} \frac{|g|^2}{|x|^2} dx \leq \frac{\mu}{2}\int_{\mathbb{R}^4} \frac{|g|^2}{|x|^2} dx \leq \frac{\mu}{2}\|\nabla g\|_2^2\,. \tag{6.2.30}$$

and consequently

$$\frac{\mu}{2}\|\nabla g\|_2^2 - 2\varepsilon\int_{A_1(b,a)} \frac{|g|^2}{|x|^2} dx \geq 0\,. \tag{6.2.31}$$

Inserting (6.2.31) into the right–hand side of (6.2.28) we arrive at

$$\hat{L}[\chi_1\psi] \geq \frac{\mu}{2}\|\nabla g\|_2^2 - 2\varepsilon\theta_R^2\int_{A_1(b,a)} \frac{|\varphi_1|^2}{|x|^2} dx\,. \tag{6.2.32}$$

Next, estimate the last term on the right-hand side of (6.2.32) for which the integral is taken over the set $A_1(b,a) = \{x \in \mathbb{R}^4 : a|R| \leq |x| \leq b|R|\}$. Using that φ_1 is the resonance function, which decays as $|x|^{-2}$ for $|x|$ large enough as explained in Section 6.2.1, we can determine the behavior of this integral in $|R|$. In particular there exist $c > 0$ and $u \in L^2(\mathbb{R}^4)$ such that

$$\varphi_1(x) = \frac{-c}{|x|^2} + u(x)\,. \tag{6.2.33}$$

Then for $|R|$ large enough there exists $c_1 > 0$ with

$$\begin{aligned} \int_{A_1(b,a)} \frac{|\varphi_1|^2}{|x|^2} dx &\leq \frac{2}{a^2|R|^2} \int_{A_1(b,a)} \left(\frac{c^2}{|x|^4} + |u|^2 \right) dx \\ &\leq \frac{2}{a^2|R|^2} \left(c^2 \ln\left(\frac{b}{a}\right) + \|u\|_2^2 \right) \\ &\leq \frac{c_1}{|R|^2}\,. \end{aligned} \tag{6.2.34}$$

Here $c_1 > 0$ may depend a and b but is independent of R. Inserting (6.2.34) into (6.2.32) we arrive at

$$\hat{L}[\chi_1\psi] \geq \frac{\mu}{2}\|\nabla g\|_2^2 - 2\varepsilon c_1 \frac{\theta_R^2}{|R|^2}\,. \tag{6.2.35}$$

Next, we estimate the behavior of θ_R for large $|R|$. Recall that we chose $\|\psi\|_2 = 1$ and hence

$$1 = \|\psi\|_2^2 \geq \int_{|x|\leq a|R|} |\chi_1\psi|^2 dx = \int_{|x|\leq a|R|} |\theta_R\varphi_1 + g|^2 dx \tag{6.2.36}$$

and using $(a+b)^2 \geq a^2/2 - b^2$ we arrive at

$$\frac{\theta_R^2}{2} \int_{|x|\leq a|R|} |\varphi_1|^2 dx \leq 1 + \int_{|x|\leq a|R|} |g|^2 dx\,. \tag{6.2.37}$$

Applying the Hardy Inequality in dimension four, we find

$$\int_{|x|\leq a|R|} |g|^2 dx \leq a|R|^2 \int_{\mathbb{R}^4} \frac{|g|^2}{|x|^2} dx \leq a|R|^2 \|\nabla g\|_2^2\,. \tag{6.2.38}$$

Combining (6.2.37) and (6.2.38) we find

$$\theta_R^2 \leq 2\left(1 + a|R|^2\|\nabla g\|_2^2\right)\left(\int_{|x|\leq a|R|} |\varphi_1|^2 dx\right)^{-1}\,. \tag{6.2.39}$$

We continue by estimating the integral on the right–hand side of (6.2.39). Using (6.2.33) and $\varphi_1 \in L^2_{\text{loc}}(\mathbb{R}^4)$ there exist $c_2, c_3 > 0$ such that

$$\begin{aligned}\int_{|x|\leq a|R|} |\varphi_1|^2 dx &= \int_{|x|\leq 1} |\varphi_1|^2 dx + \int_{1\leq |x|\leq a|R|} |\varphi_1|^2 dx \\ &\geq c_2 + \frac{c^2}{2}\int_{1\leq|x|\leq a|R|} |x|^{-4} dx - \|u\|_2^2 \\ &\geq c_3 \log(|R|)\end{aligned} \tag{6.2.40}$$

where $c_3 > 0$ depends on $a > 0$ only. Combining (6.2.39) and (6.2.40) yields

$$\theta_R^2 \leq 2c_3^{-1}\log(|R|)^{-1} + 2c_3^{-1} a|R|^2 \log(|R|)^{-1}\|\nabla g\|_2^2 . \tag{6.2.41}$$

Inserting (6.2.41) into (6.2.35) we arrive at

$$\hat{L}[\chi_1\psi] \geq \frac{\mu}{2}\|\nabla g\|_2^2 - \frac{aC}{\log(|R|)}\|\nabla g\|_2^2 - \frac{C}{|R|^2\log(|R|)} \tag{6.2.42}$$

with $C = 4\varepsilon c_1 c_3^{-1}$ a positive constant independent of R. Consequently, for $|R| > 0$ large enough, the sum of the first two terms in the right–hand side of (6.2.42) is positive, which proves (6.2.14) and therefore completes the proof of Theorem 6.2.4. ∎

6.3 Absence of Efimov Effect in Dimension Four

6.3.1 Basic Definitions and Notation

We consider three bosons in dimension $d = 4$ at the positions $(x_1, x_2, x_3) \in \mathbb{R}^{3\times 4}$ with masses m_i for $i \in \{1, 2, 3\}$. The Schrödinger operator on $L^2(\mathbb{R}^{3\times 4})$ for this system is

$$\mathcal{H} = \sum_{i=1}^{3} \frac{-1}{2m_i} P_{x_i}^2 + \sum_{1\leq i<j\leq 3} V_{ij}(x_i - x_j) . \tag{6.3.1}$$

We assume that the potentials $V_{ij} \in L^2_{\text{loc}}(\mathbb{R}^4) \cap K_4$ are short-range. The operator $\mathcal{H}$ is invariant under simultaneous translation of (x_1, x_2, x_3) in $\mathbb{R}^4$. By standard arguments

$$\mathcal{H} = \left[T_0 + \sum_{1\leq i<j\leq 3} V_{ij}\right] \otimes \mathbb{1} + \mathbb{1} \otimes \frac{-1}{2M}\Delta_R$$

where $M = \sum_{i=1}^3 m_i$ and T_0 is the Laplace-Beltrami operator on $L^2(R_0)$ where

$$R_0 := \left\{(x_1, x_2, x_3) \in \mathbb{R}^{3d} : \sum_{i=1}^{3} m_i x_i = 0\right\}$$

and $\frac{-1}{2M}\Delta_R$ is the operator associated with the kinetic energy of the relative motion of the center of mass. We define

$$H := T_0 + \sum_{1\le i<j\le 3} V_{ij} \tag{6.3.2}$$

which is an operator on $L^2(R_0)$ where R_0 is an eight-dimensional subspace of $\mathbb{R}^{3\times 4}$.
Denote by $\sigma_{\mathrm{ess}}(H)$ the essential and by $\sigma_{\mathrm{disc}}(H)$ the discrete spectrum of H. Our main result is

Theorem 6.3.1. *Let H be the operator defined in* (6.3.2) *with V_{ij} short-range for any $(ij) \in \{(12),(13),(23)\}$. Assume that $\sigma_{\mathrm{ess}}(H) = [0,\infty)$. Then $\sigma_{\mathrm{disc}}(H)$ is at most finite.*

Remark 6.3.2. *Due to the HVZ theorem $\sigma_{\mathrm{ess}}(H) \ge 0$ is equivalent to the fact that all two-particle subsystems do not have a bound state below their essential spectrum. Theorem 6.2.4 does not impose any condition on the existence or absence of virtual levels in the two-particle subsystems. In particular, it shows that the Efimov effect [28] in dimension four does not exist.*

We use the common aberration for labeling pairs of particles as $\alpha = (ij) \in I$, where $I := \{(12),(13),(23)\}$. The remaining particle is then labeled by $k \in \{1,2,3\} \setminus \{i,j\}$. We introduce the coordinates $(q_\alpha, \xi_\alpha, R)$ with

$$q_{(ij)} := \left(2\mu_{ij}\right)^{1/2}(x_i - x_j), \quad \xi_{(ij)} := \left(2\nu_{ij}\right)^{1/2}\left(\frac{m_i x_i + m_j x_j}{m_i + m_j} - x_k\right), \tag{6.3.3}$$

Here

$$\mu_{ij} := \frac{m_i m_j}{m_i + m_j}, \quad \nu_{ij} := \frac{(m_i + m_j)m_k}{M}, \quad k \in \{1,2,3\} \setminus \{i,j\}\,. \tag{6.3.4}$$

denote the reduced masses. Given the positions, $x_i \in R_0$, $i \in \{1,2,3\}$ of the particles and fixed $\alpha \in I$ direct computations show

$$\sum_{i=1}^{3} m_i |x_i|^2 = |q_\alpha|^2 + |\xi_\alpha|^2, \quad \alpha \in I\,. \tag{6.3.5}$$

In this new set of coordinates, the operator T_0 takes the form

$$T_0 = -\Delta_{q_\alpha} - \Delta_{\xi_\alpha} \quad \text{on } L^2(\mathbb{R}^8), \tag{6.3.6}$$

and

$$h_\alpha := -\Delta_{q_\alpha} + V_\alpha, \quad \text{on } L^2(\mathbb{R}^4), \tag{6.3.7}$$

denotes the two-particle Schrödinger operator of the particle pair α. As we mentioned, due to the HVZ theorem under the conditions of 6.3.1, we have $h_\alpha \ge 0$.

6.3.2 On the Discrete Spectrum of H

To prove that the discrete spectrum $\sigma_{\text{disc}}(H)$ is at most finite, it suffices to find a finite-dimensional space $\mathcal{M} \subset L^2(R_0)$ such that for any $\psi \in L^2(R_0)$ orthogonal to $\mathcal{M}$

$$\langle \psi, H\psi \rangle \geq 0.$$

As it was shown by Zhislin [129] such a space $\mathcal{M}$ exists if there are constants $b, \beta > 0$ with

$$\mathcal{L}[\psi] := \langle \psi, H\psi \rangle - \int_{|x| \in [b,2b]} \frac{|\psi|^2}{|x|^\beta} dx \geq 0$$

for every $\psi \in C_0^1(\mathbb{R}^4)$ with $\operatorname{supp}\psi \subset \{x \in R_0 : |x| > b\}$. Let $\alpha \in I$, for $\gamma > 0$ and $\tilde{\gamma} \in (0, \gamma)$ we define

$$\mathcal{K}_\alpha(\gamma) := \{x \in R_0 : |q_\alpha| < \gamma|\xi_\alpha|\}, \quad \mathcal{K}_{ij}(\gamma, \tilde{\gamma}) := \mathcal{K}_\alpha(\gamma) \setminus \mathcal{K}_\alpha(\tilde{\gamma})\,.$$

The set $\mathcal{K}_\alpha(\gamma)$ represents a conical region in R_0 where the distance between particles in α is small relative to their distances from the third particle. In Appendix C, we show that the sets $\mathcal{K}_{ij}(\gamma)$ are mutually disjoint for sufficiently small $\gamma > 0$. We will henceforth assume this condition throughout the following proof.

Proof of Theorem 6.3.2. Everywhere below we assume that $\psi \in C_0^1(R_0)$ with

$$\operatorname{supp}(\psi) \subset \{x \in R_0 : |x| > b\},$$

where $b > 0$ is large and will be chosen later.
Following [120, Lemma 5.1]for given $\varepsilon > 0$ and $\gamma > 0$ there exists a continuous differential function u and $\tilde{\gamma} \in (0, \gamma)$ such that

$$u_\alpha(x) := u\left(\frac{|q_\alpha|}{|\xi_\alpha|}\right), \quad \forall x \in R_0 \quad \text{such that} \quad u_\alpha(x) = \begin{cases} 1 & x \in \mathcal{K}_\alpha(\tilde{\gamma}) \\ 0 & x \notin \mathcal{K}_\alpha(\gamma) \end{cases}$$

and with $v_\alpha := (1 - u_\alpha^2)^{1/2}$ such that the next inequality holds

$$|\nabla u_\alpha|^2 + |\nabla v_\alpha|^2 \leq \varepsilon \left(|x|^{-2}|v_\alpha|^2 + |q_\alpha|^{-2}|u_\alpha|^2\right), \quad x \in \mathcal{K}_\alpha(\tilde{\gamma}, \gamma)\,. \tag{6.3.8}$$

Let $\mathcal{V} := \left(1 - \sum_{\alpha \in I} u_\alpha^2\right)^{1/2}$ then since the sets $\mathcal{K}_\alpha(\gamma)$ for $\alpha \in I$ are disjoint we have $\mathcal{V} = v_\alpha$ on $\operatorname{supp}(\nabla v_\alpha)$ and the family of functions $\{\mathcal{V}, U_{12}, U_{13}, U_{23}\}$ forms a quadratic partition of unity. Let

$$\psi_\alpha := \psi u_\alpha, \quad \psi_0 := \psi \mathcal{V}\,.$$

Applying (6.3.8) and the IMS localization formula gives

$$\mathcal{L}[\psi] \geq \mathcal{L}_0[\psi_0] + \sum_{\alpha \in I} \mathcal{L}_\alpha[\psi_\alpha]$$

where

$$
\begin{aligned}
\mathcal{L}_\alpha[\psi_\alpha] &:= \langle \psi_\alpha, H\psi_\alpha\rangle - \varepsilon \int_{\mathcal{K}_\alpha(\gamma,\tilde{\gamma})} \frac{|\psi_\alpha|^2}{|q_\alpha|^2}\, dx - \int_{|x|\in[b,2b]} \frac{|\psi_\alpha|^2}{|x|^\beta} dx, \quad \forall \alpha \in I, \\
\mathcal{L}_0[\psi_0] &:= \langle \psi_0, H\psi_0\rangle - \varepsilon \int_{\mathcal{K}_\alpha(\gamma,\tilde{\gamma})} \frac{|\psi_0|^2}{|x|^2}\, dx - \int_{|x|\in[b,2b]} \frac{|\psi_0|^2}{|x|^\beta} dx\,.
\end{aligned} \tag{6.3.9}
$$

Remark 6.3.3. *In $x = 0$, the functions u_α, v_α are not continuous and consequently not differentiable. Since* $\operatorname{supp}\psi \subset \{x \in R_0 : |x| > b\}$ *this is irrelevant.*
The parameter $\beta > 0$ can be chosen freely. We fix $\beta = 2 + \tau$ for some $\tau \in (0, \delta)$, where $\delta > 0$ is the parameter in definition of the potentials.

We prove the theorem in two steps. First, we show $\mathcal{L}_0[\psi_0] \geq 0$ and in a second step we show $\mathcal{L}_\alpha[\psi_\alpha] \geq 0$ for any $\alpha \in I$, and for and $\varepsilon, \gamma > 0$ small and $b > 0$ depending on ε, γ sufficiently large. Following [120, Lemma 5.1] we can always make $\varepsilon > 0$ small by choosing $\tilde{\gamma}$ small.

Step 1:

We show

$$
\mathcal{L}_0[\psi_0] := \left\langle \psi_0, T_0 + \sum_{1\leq i<j\leq 3} V_{ij}\psi_0 \right\rangle - \varepsilon \int_{\mathcal{K}_\alpha(\gamma,\tilde{\gamma})} \frac{|\psi_0|^2}{|x|^2}\, dx - \int_{|x|\in[b,2b]} \frac{|\psi_0|^2}{|x|^{2+\tau}} dx \geq 0\,. \tag{6.3.10}
$$

For $b > 0$ large enough, we can combine the last two terms on the right–hand side of (6.3.10), arriving at

$$
\mathcal{L}_0[\psi_0] \geq \left\langle \psi_0, T_0 + \sum_{\alpha\in I} V_\alpha\psi_0 \right\rangle - 2\varepsilon \int_{|x|>b} \frac{|\psi_0|^2}{|x|^2}\, dx\,. \tag{6.3.11}
$$

For $b > 0$ large enough on $\operatorname{supp}\psi_0$ each of the potentials V_α fulfill $|V_\alpha| < \varepsilon|x|^{-2}$ and consequently

$$
\mathcal{L}_0[\psi_0] \geq \langle \psi_0, T_0\psi_0\rangle - 3\varepsilon \int_{|x|>b} \frac{|\psi_0|^2}{|x|^2}\, dx\,. \tag{6.3.12}
$$

The operator T_0 is the Laplace–Beltrami operator on $L^2(R_0)$. The non–negativity of the right–hand side of (6.3.12) follows directly from the radial Hardy Inequality whenever $\varepsilon > 0$ is small enough.

Step 2:

With the coordinates (q_α, ξ_α) defined in (6.3.3) and the representation of H in (6.3.6) it is

$$
\begin{aligned}
\langle \psi_\alpha, H\psi_\alpha\rangle = &\int_{\mathcal{K}_\alpha(\gamma)} \left|\nabla_{q_\alpha}\psi_\alpha\right|^2 d(q_\alpha, \xi_\alpha) + \int_{\mathcal{K}_\alpha(\gamma)} \left|\nabla_{\xi_\alpha}\psi_\alpha\right|^2 d(q_\alpha, \xi_\alpha) \\
&+ \int_{\mathcal{K}_\alpha(\gamma)} \sum_{\sigma\in I} V_\sigma |\psi_\alpha|^2 d(q_\alpha, \xi_\alpha)\,.
\end{aligned} \tag{6.3.13}
$$

Any of the potential V_σ, with $\sigma \in I$ fulfill (6.2.1) and consequently there exists a constants $C, \delta, A > 0$ such, that

$$|V_\sigma(x)| \le C|x|^{-2-\delta} \tag{6.3.14}$$

for any $x \in R_0$ with $|x| > A$. For $b > 0$ large enough on $\operatorname{supp}\psi_\alpha \subset \mathcal{K}_\alpha(\gamma) \cap \{x \in R_0 : |x| > b\}$ the potential V_σ with $\sigma \ne \alpha$ fulfils (6.3.14) and consequently we can estimate the last term in (6.3.13) as

$$\begin{aligned}\langle\psi_\alpha, H\psi_\alpha\rangle \ge &\int_{\mathcal{K}_\alpha(\gamma)} \left|\nabla_{q_\alpha}\psi_\alpha\right|^2 d(q_\alpha,\xi_\alpha) + \int_{\mathcal{K}_\alpha(\gamma)} \left|\nabla_{\xi_\alpha}\psi_\alpha\right|^2 d(q_\alpha,\xi_\alpha) \\ &+ \int_{\mathcal{K}_\alpha(\gamma)} V_\alpha|\psi_\alpha|^2 d(q_\alpha,\xi_\alpha) \; - 2C\int_{\mathcal{K}_\alpha(\gamma)} \frac{|\psi_\alpha|^2}{|x|^{2+\delta}}dx\,.\end{aligned} \tag{6.3.15}$$

Inserting (6.3.15) into $\mathcal{L}_\alpha[\psi_\alpha]$ defined in (6.3.9) we arrive at

$$\begin{aligned}\mathcal{L}_\alpha[\psi_\alpha] \ge &\int_{\mathcal{K}_\alpha(\gamma)} \left(\left|\nabla_{q_\alpha}\psi_\alpha\right|^2 + V_\alpha|\psi_\alpha|^2\right) d(q_\alpha,\xi_\alpha) + \int_{\mathcal{K}_\alpha(\gamma)} \left|\nabla_{\xi_\alpha}\psi_\alpha\right|^2 d(q_\alpha,\xi_\alpha) \\ &- \varepsilon\int_{\mathcal{K}_\alpha(\gamma,\tilde\gamma)} \frac{|\psi_\alpha|^2}{|q_\alpha|^2} + \mathcal{E}[\psi_\alpha],\end{aligned} \tag{6.3.16}$$

where

$$\mathcal{E}[\psi_\alpha] \coloneqq \int_{\mathcal{K}_\alpha(\gamma)} \left|\nabla_{\xi_\alpha}\psi_\alpha\right|^2 d(q_\alpha,\xi_\alpha) - 2C\int_{\mathcal{K}_\alpha(\gamma)} \frac{|\psi_\alpha|^2}{|x|^{2+\delta}}dx - \int_{|x|\in[b,2b]} \frac{|\psi_\alpha|^2}{|x|^\beta}dx\,.$$

Next, we show $\mathcal{E}[\psi_\alpha] \ge 0$ for $b > 0$ large enoug. Recal that $\beta = 2 + \tau$ for some $\tau \in (0, \delta)$. Since ψ_α is supported outside of $\{x \in R_0 : |x| > b\}$

$$\mathcal{E}[\psi_\alpha] \ge \int_{\mathcal{K}_\alpha(\gamma)} \left|\nabla_{\xi_\alpha}\psi_\alpha\right|^2 d(q_\alpha,\xi_\alpha) - 2\int_{\mathcal{K}_\alpha(\gamma)} \frac{|\psi_\alpha|^2}{|x|^{2+\tau}}dx\,. \tag{6.3.17}$$

Using (6.3.5) and consequently $|x| \ge C|\xi_\alpha|$ for some $C > 0$ depending on the masses only together with the Hardy Inequality in dimension four yields $\mathcal{E}[\psi_\alpha] \ge 0$ for $b > 0$ sufficiently large. Consequently, we arrive at

$$\begin{aligned}\mathcal{L}_\alpha[\psi_\alpha] \ge &\int_{\mathcal{K}_\alpha(\gamma)} \left(\left|\nabla_{q_\alpha}\psi_\alpha\right|^2 + V_\alpha|\psi_\alpha|^2\right) d(q_\alpha,\xi_\alpha) + \int_{\mathcal{K}_\alpha(\gamma)} \left|\nabla_{\xi_\alpha}\psi_\alpha\right|^2 d(q_\alpha,\xi_\alpha) \\ &- \varepsilon\int_{\mathcal{K}_\alpha(\gamma,\tilde\gamma)} \frac{|\psi_\alpha|^2}{|q_\alpha|^2} d(q_\alpha,\xi_\alpha)\,.\end{aligned} \tag{6.3.18}$$

We introduce several new functions first to prove the positivity of the right-hand side of (6.3.18). The operator h_α defined in (6.3.7) can have a virtual level at zero. For fixed $\xi_\alpha \in \mathbb{R}^4$ the function $\psi_\alpha(\cdot, \xi_\alpha) \in C^\infty(\mathbb{R}^4)$ is compactly supported with

$$\operatorname{supp}\psi_\alpha(\cdot,\xi_\alpha) \subset \{q_\alpha \in \mathbb{R}^4 : |q_\alpha| < \kappa|\xi_\alpha|\}\,.$$

Let $\varphi \in \dot{H}^1(\mathbb{R}^4)$ be the corresponding solution with $h_\alpha \varphi = 0$ if it exists. Let $f : \mathbb{R}^4 \to \mathbb{C}$ be the projection of $\psi_\alpha(\cdot, \xi_\alpha)$n onto $\varphi \in \dot{H}^1(\mathbb{R}^4)$ such, that for any $\xi_\alpha \in \mathbb{R}^4$

$$f(\xi_\alpha) \coloneqq \langle \varphi, \psi_\alpha(\cdot, \xi_\alpha) \rangle_{\dot{H}^1(dq_\alpha)} \|\varphi\|^{-2}_{\dot{H}^1(dq_\alpha)}$$

and let $g : R_0 \to \mathbb{C}$ defined by the relation

$$\psi_\alpha(q_\alpha, \xi_\alpha) = \varphi(q_\alpha) f(\xi_\alpha) + g(q_\alpha, \xi_\alpha) . \tag{6.3.19}$$

Then, by construction g satisfies

$$\langle \nabla_{q_\alpha} \varphi, \nabla_{q_\alpha} g(\cdot, \xi_\alpha) \rangle_{L^2(\mathbb{R}^4)} = 0, \quad \forall \xi_\alpha \in \mathbb{R}^4 .$$

If the operator h_α does not have a virtual level, we assume $f \equiv 0$ such that $\psi_\alpha = g$.
Next, we estimate the first integral on the right-hand side of (6.3.18). Inserting (6.3.19) into

$$\int_{\mathcal{K}_\alpha(\gamma)} \left(\left| \nabla_{q_\alpha} \psi_\alpha \right|^2 + V_\alpha |\psi_\alpha|^2 \right) d(q_\alpha, \xi_\alpha)$$

and applying (6.2.6) there exist a constant $\mu > 0$ depending on the masses but independent of ψ such that

$$\int_{\mathcal{K}_\alpha(\gamma)} \left(\left| \nabla_{q_\alpha} \psi_\alpha \right|^2 + V_\alpha |\psi_\alpha|^2 \right) d(q_\alpha, \xi_\alpha) \geq \mu \left\| \nabla_{q_\alpha} g \right\|^2 . \tag{6.3.20}$$

Combining (6.3.18) and (6.3.20) we arrive at

$$\mathcal{L}_\alpha[\psi_\alpha] \geq \mu \left\| \nabla_{q_\alpha} g \right\|^2 + \int_{\mathcal{K}_\alpha(\gamma)} \left| \nabla_{\xi_\alpha} \psi_\alpha \right|^2 d(q_\alpha, \xi_\alpha) - \varepsilon \int_{\mathcal{K}_\alpha(\gamma, \tilde{\gamma})} \frac{|\psi_\alpha|^2}{|q_\alpha|^2} d(q_\alpha, \xi_\alpha) . \tag{6.3.21}$$

Next, We estimate the second term on the right-hand side of (6.3.21). By the Hardy inequality in dimension four and since $\psi_\alpha = f\varphi + g$

$$\begin{aligned} \int_{\mathcal{K}_\alpha(\gamma)} \left| \nabla_{\xi_\alpha} \psi_\alpha \right|^2 d(q_\alpha, \xi_\alpha) &\geq \int_{\mathcal{K}_\alpha(\gamma)} \frac{|\psi_\alpha|^2}{|\xi_\alpha|^2} d(q_\alpha, \xi_\alpha) \\ &\geq \frac{1}{2} \int_{\mathcal{K}_\alpha(\gamma)} |f|^2 \frac{|\varphi|^2}{|\xi_\alpha|^2} d(q_\alpha, \xi_\alpha) - \int_{\mathcal{K}_\alpha(\gamma)} \frac{|g|^2}{|\xi_\alpha|^2} d(q_\alpha, \xi_\alpha) . \end{aligned} \tag{6.3.22}$$

For the last integral in the right–hand side of (6.3.21), we find

$$\begin{aligned} &\int_{\mathcal{K}_\alpha(\gamma, \tilde{\gamma})} \frac{|\psi_\alpha|^2}{|q_\alpha|^2} d(q_\alpha, \xi_\alpha) \\ &\qquad \leq 2 \int_{\mathcal{K}_\alpha(\gamma, \tilde{\gamma})} |f|^2 \frac{|\varphi|^2}{|q_\alpha|^2} d(q_\alpha, \xi_\alpha) + 2 \int_{\mathcal{K}_\alpha(\gamma, \tilde{\gamma})} \frac{|g|^2}{|q_\alpha|^2} d(q_\alpha, \xi_\alpha) . \end{aligned} \tag{6.3.23}$$

Consequently by inserting (6.3.22) and (6.3.23) into (6.3.21) we arrive at

$$\mathcal{L}_\alpha[\psi_\alpha] \geq \mathcal{N}_1[\psi_\alpha] + \mathcal{N}_2[\psi_\alpha]\,,$$

where

$$\mathcal{N}_1[\psi_\alpha] \coloneqq \mu\left\|\nabla_{q_\alpha} g\right\|^2 - \int_{\mathcal{K}_\alpha(\gamma)} \frac{|g|^2}{|\xi_\alpha|^2} d(q_\alpha, \xi_\alpha) - 2\varepsilon \int_{\mathcal{K}_\alpha(\gamma,\tilde{\gamma})} \frac{|g|^2}{|q_\alpha|^2} d(q_\alpha, \xi_\alpha), \tag{6.3.24}$$

and

$$\mathcal{N}_2[\psi_\alpha] \coloneqq \frac{1}{2}\int_{\mathcal{K}_\alpha(\gamma)} |f|^2 \frac{|\varphi|^2}{|\xi_\alpha|^2} d(q_\alpha, \xi_\alpha) - 2\varepsilon \int_{\mathcal{K}_\alpha(\gamma,\tilde{\gamma})} |f|^2 \frac{|\varphi|^2}{|q_\alpha|^2} d(q_\alpha, \xi_\alpha)\,. \tag{6.3.25}$$

The theorem follows if we can show for any $\mu > 0$ and $\varepsilon \in (0, \mu/4)$ that $\mathcal{N}_1[\psi_\alpha] \geq 0$ and $\mathcal{N}_2[\psi_\alpha] \geq 0$ for $b > 0$ sufficiently large.

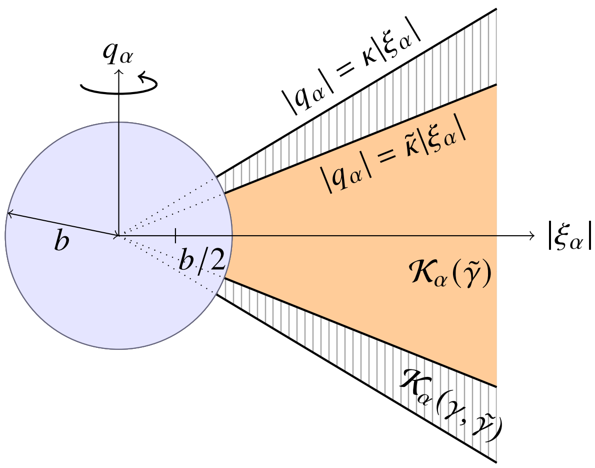

FIGURE 6.1: Sketch of the sets $\mathcal{K}_\alpha(\gamma)$ and $\mathcal{K}_\alpha(\gamma, \tilde{\gamma})$.

We begin with $\mathcal{N}_1[\psi_\alpha]$. For any $x \in \mathcal{K}_\alpha(\gamma)$ it holds $|q_\alpha| < \kappa|\xi_\alpha|$ where $\kappa \coloneqq \gamma(1-\gamma^2)^{1/2}$ and consequently for the second term on the right-hand side of (6.3.24) we find together with the Hardy Inequality

$$\int_{\mathcal{K}_\alpha(\gamma)} \frac{|g|^2}{|\xi_\alpha|^2} d(q_\alpha, \xi_\alpha) \leq \kappa^2 \int_{\mathcal{K}_\alpha(\gamma)} \frac{|g|^2}{|q_\alpha|^2} d(q_\alpha, \xi_\alpha) \leq \kappa^2 \left\|\nabla_{q_\alpha} g\right\|^2. \tag{6.3.26}$$

Substituting (6.3.26) into (6.3.24) for $\kappa^2 < \mu/2$ we arrive at

$$\mathcal{N}_1[\psi_\alpha] \geq \frac{\mu}{2}\left\|\nabla_{q_\alpha} g\right\|^2 - 2\varepsilon \int_{\mathcal{K}_\alpha(\gamma,\tilde{\gamma})} \frac{|g|^2}{|q_\alpha|^2} d(q_\alpha, \xi_\alpha)\,.$$

Using $\varepsilon < \mu/4$ together with the Hardy Inequality yields $\mathcal{N}_1[\psi_\alpha] \geq 0$.

Next, we show that $\mathcal{N}_2[\psi_\alpha]$ is positive. For any $x \in \mathcal{K}_\alpha(\gamma, \tilde{\gamma})$ it holds $|q_\alpha| < \tilde{\kappa}|\xi_\alpha|$ where $\tilde{\kappa} := \tilde{\gamma}(1-\tilde{\gamma}^2)^{1/2}$ and consequently for the second integral on the right–hand side of (6.3.25) holds

$$2\varepsilon \int_{\mathcal{K}_\alpha(\gamma,\tilde{\gamma})} |f|^2 \frac{|\varphi|^2}{|q_\alpha|^2} d(q_\alpha, \xi_\alpha) \leq 2\varepsilon\tilde{\kappa}^{-2} \int_{\mathcal{K}_\alpha(\gamma,\tilde{\gamma})} |f|^2 \frac{|\varphi|^2}{|\xi_\alpha|^2} d(q_\alpha, \xi_\alpha) . \tag{6.3.27}$$

Inserting (6.3.27) int (6.3.25) yields

$$\mathcal{N}_2[\psi_\alpha] \geq \frac{1}{2} \int_{\mathcal{K}_\alpha(\gamma)} |f|^2 \frac{|\varphi|^2}{|\xi_\alpha|^2} d(q_\alpha, \xi_\alpha) - 2\varepsilon\tilde{\kappa}^{-2} \int_{\mathcal{K}_\alpha(\gamma,\tilde{\gamma})} |f|^2 \frac{|\varphi|^2}{|\xi_\alpha|^2} d(q_\alpha, \xi_\alpha) . \tag{6.3.28}$$

Note that the second integral on the right–hand side of (6.3.28) is taken over $\mathcal{K}_\alpha(\gamma, \tilde{\gamma})$, which is a subset of $\mathcal{K}_\alpha(\gamma)$. We show that for $b > 0$ large enough, the first integral on the right–hand side of (6.3.28) dominates the second integral.
The function f is constant in q_α and consequently, by Fubini's Theorem and the geometry of the set $\mathcal{K}_\alpha(\gamma)$ (see Figure 6.1), we find for the first integral on the right–hand side of (6.3.28)

$$\frac{1}{2} \int_{\mathcal{K}_\alpha(\gamma)} |f|^2 \frac{|\varphi|^2}{|\xi_\alpha|^2} d(q_\alpha, \xi_\alpha) = \frac{1}{2} \int_{|\xi_\alpha|>b/2} \frac{|f(\xi_\alpha)|^2}{|\xi_\alpha|^2} \int_{|q_\alpha|<\kappa|\xi_\alpha|} |\varphi(q_\alpha)|^2 dq_\alpha d\xi_\alpha . \tag{6.3.29}$$

Using the decay property of φ in (6.2.7) there exists a constant $C > 0$ such that for almost any $\xi_\alpha \in \mathbb{R}^4$

$$\int_{|q_\alpha|<\kappa|\xi_\alpha|} |\varphi(q_\alpha)|^2 dq_\alpha \geq C \log\left(\kappa|\xi_\alpha|\right) . \tag{6.3.30}$$

Combining (6.3.29) and (6.3.30) shows

$$\frac{1}{2} \int_{\mathcal{K}_\alpha(\gamma)} |f|^2 \frac{|\varphi|^2}{|\xi_\alpha|^2} d(q_\alpha, \xi_\alpha) \geq \frac{C}{2} \int_{|\xi_\alpha|>b/2} \frac{|f(\xi_\alpha)|^2}{|\xi_\alpha|^2} |\log\left(\kappa|\xi_\alpha|\right)|^2 d\xi_\alpha . \tag{6.3.31}$$

We proceed similarly for the second integral on the right–hand side of (6.3.28). The set $\mathcal{K}_\alpha(\gamma, \tilde{\gamma})$ is determined by the relations $\tilde{\kappa}|\xi_\alpha| \leq |q_\alpha| \leq \kappa|\xi_\alpha| \leq$ (see Figure 6.1). Consequently

$$\int_{\mathcal{K}_\alpha(\gamma,\tilde{\gamma})} |f|^2 \frac{|\varphi|^2}{|\xi_\alpha|^2} d(q_\alpha, \xi_\alpha) = \int_{|\xi_\alpha|>b/2} \frac{|f(\xi_\alpha)|^2}{|\xi_\alpha|^2} \int_{|q_\alpha|\in(\tilde{\kappa}|\xi_\alpha|,\kappa|\xi_\alpha|)} |\varphi(q_\alpha)|^2 dq_\alpha d\xi_\alpha . \tag{6.3.32}$$

Using the decay property of φ in (6.2.7) there exists a constants $C_0, C_1 > 0$ such that for almost any $\xi_\alpha \in \mathbb{R}^4$

$$\int_{|q_\alpha|\in(\tilde{\kappa}|\xi_\alpha|,\kappa|\xi_\alpha|)} |\varphi(q_\alpha)|^2 dq_\alpha \leq C_0 + C_1 \log\left(\frac{\kappa}{\tilde{\kappa}}\right) =: C_2(\kappa, \tilde{\kappa}) . \tag{6.3.33}$$

Note that compared to (6.3.30) the expression in (6.3.33) is bounded for large $|\xi_\alpha|$. Combining (6.3.32) and (6.3.33) we find

$$\int_{\mathcal{K}_\alpha(\gamma,\tilde{\gamma})} |f|^2 \frac{|\varphi|^2}{|\xi_\alpha|^2} d(q_\alpha, \xi_\alpha) \leq C_2(\kappa, \tilde{\kappa}) \int_{|\xi_\alpha|>b/2} \frac{|f(\xi_\alpha)|^2}{|\xi_\alpha|^2} d\xi_\alpha \,. \tag{6.3.34}$$

Substituting (6.3.31) and (6.3.34) into (6.3.28) yields for $b > 0$ large enough

$$\mathcal{N}_2[\psi_\alpha] \geq \left(\frac{C}{2} \log(\kappa b) - 2\varepsilon \tilde{\kappa}^{-2} C_2(\kappa, \tilde{\kappa}) \right) \int_{|\xi_\alpha|>b/2} \frac{|f(\xi_\alpha)|^2}{|\xi_\alpha|^2} d\xi_\alpha \geq 0$$

for $b > 0$ large enough. This completes the proof of Theorem 6.3.1. ∎

Appendix A

A.1 Density Argument for $\alpha_{N,s}$

Lemma A.1.1. *Let* $\alpha_{N,s}$ *be defined as in equation* (4.5.1) *and* $A \subset \mathbb{R}^{3N}$ *be defined as*

$$A_0 = \{(x_1, x_2, \dots x_N) \in A : x_k \neq 0 \, \textit{for} \; 1 \leq k \leq N\}$$

then

$$\alpha_{N,s} = \inf \left\{ \frac{\sum_{\substack{1 \leq i,k \leq N \\ i \neq k}} \frac{|x_k|^s + |x_i|^s}{|x_i - x_k|}}{2(N-1) \sum_{k=1}^{N} |x_k|^{s-1}} : (x_1, x_2, \dots x_N) \in A_0 \right\} . \tag{A.1.1}$$

Proof. We define

$$F(x_1, x_2, \dots, x_N) \coloneqq \frac{\sum_{\substack{1 \leq i,k \leq N \\ i \neq k}} \frac{|x_k|^s + |x_i|^s}{|x_i - x_k|}}{2(N-1) \sum_{k=1}^{N} |x_k|^{s-1}} . \tag{A.1.2}$$

Note that F is continuous in A and A_0 is dense in A. Since any $(x_1, x_2, \dots, x_N) \in A$ consists of arbitrary but distinct point in $\mathbb{R}^3$ we may always assume that $|x_1| \leq |x_2| \leq \cdots \leq |x_N|$ by relabeling the indices. Since the vectors are distinct, only x_1 may vanish. The set A_0 is a subset of A and thus

$$\alpha_{N,s} \leq \inf\{F(x_1, x_2, \dots, x_N) : (x_1, x_2, \dots, x_N) \in A_0\} =: \zeta_{N,s} .$$

The claim follows if we can show $\zeta_{N,s} \leq \alpha_{N,s}$. We show for arbitrary $\varepsilon > 0$ that $\zeta_{N,s} \leq \alpha_{N,s} + \varepsilon$ and conclude the statement in the limit $\varepsilon \longrightarrow 0$. Let $\varepsilon > 0$ arbitrary, then by the definition of the infimum, there exists some $r_\varepsilon \in A$ such that $F(r_\varepsilon) \leq \alpha_{N,s} + \varepsilon/2$. If $r_\varepsilon \in A_0$ then $F(r_\varepsilon) \geq \zeta_{N,s}$ and the inequality follows directly. If $r_\varepsilon \in A \setminus A_0$ then $(r_\varepsilon)_1 = 0$. By continuity of F in r_ε we can find $u_\varepsilon \in A_0$ such that $|F(r_\varepsilon) - F(u_\varepsilon)| \leq \varepsilon/2$ and thus

$$\zeta_{N,s} \leq F(u_\varepsilon) \leq \alpha_{N,s} + \varepsilon .$$

Thus, we have shown $\zeta_{N,s} = \alpha_{N,s}$, and the statement follows immediately. ∎

A.2 Funk-Hecke Formula and Multipole Moments

Lemma A.2.1. *For any function $f \in L^1(-1,1)$ and any Legendre polynomial*

$$\frac{1}{4\pi}\int_{S^2} f(\xi\cdot\omega)P_l(\zeta\cdot\omega)d\omega = \lambda P_l(\xi\cdot\zeta) \tag{A.2.1}$$

for all $\xi, \zeta \in S^2$ where

$$\lambda = \frac{1}{2}\int_{-1}^{1} P_l(t)f(t)dt\,.$$

Proof. This is a direct consequence of the Funk–Hecke formula in three dimensions, see equation (2.66) just after Theorem 2.22 in Chapter 2.6 of [6]. ∎

Lemma A.2.2. *Let $\lambda > -2$,$a \in \mathbb{R}^3$ and $r, |a| > 0$, then*

$$\int_{S^2} |a + r\omega|^\lambda \frac{d\omega}{4\pi} = \frac{(|a|+r)^{\lambda+2} - (|a|-r)^{\lambda+2}}{2r|a|(\lambda+2)}\,.$$

Proof. Since the Legendre polynomial $P_0 = 1$ and $|a+r\omega|^2 = |a|^2 + r^2 + 2r|a|\widehat{a}\cdot\omega$ we see from Lemma A.2.1 that

$$\int_{S^2} |a+r\omega|^t\lambda\frac{d\omega}{4\pi} = \frac{1}{2}\int_{-1}^{1}(|a|^2 + r\omega + 2r|a|t)^{\lambda/2}\frac{d\omega}{4\pi} = \frac{(|a|+r)^{\lambda+2} - (|a|-r)^{\lambda+2}}{2r|a|(\lambda+2)}\,.$$

∎

Lemma A.2.3. *Let $s \geq -2$, $\zeta \in S^2$, $w \in \mathbb{R}^3 \setminus \{0\}$, and $r > 0$. Then*

$$\int_{S^2} |w+r\omega|^s \frac{d\omega}{4\pi} = \frac{(|w|+r)^{s+2} - ||w|-r|^{s+2}}{2r|w|(s+2)}$$

$$\int_{S^2} |w+r\omega|^s \langle\zeta,\omega\rangle\frac{d\omega}{4\pi} = c(r)\langle w,\zeta\rangle$$

$$\int_{S^2} |w+r\omega|^s P_l(\langle\hat{w},\omega\rangle)\frac{d\omega}{4\pi} = \frac{1}{2}\int_{-1}^{1}(w^2+r^2+2r|w|t)^{s/2}P_l(t)dt$$

where $c(r) \coloneqq \int_{-1}^{1}(1+r^2+2rt)^{s/2}t\,dt$ and $c_{k,n} \coloneqq (2n+1)\int_{-1}^{1} t^k P_n(t)\,dt$.

Proof. The zero-order moment is easy to compute and follows directly from Lemma A.2.2. Similar

$$\begin{aligned}\int_{S^2}\left|\hat{x}_j + r\omega\right|^s P_1(\langle\hat{a},\omega\rangle)\frac{d\omega}{4\pi} &= \int_{S^2}\left|\hat{x}_j + r\omega\right|^s\langle\hat{a},\omega\rangle\frac{d\omega}{4\pi}\\ &= \langle\hat{a}, \int_{S^2}\left|\hat{x}_j + r\omega\right|^s\omega\frac{d\omega}{4\pi}\rangle\\ &= \langle U^{-1}\hat{a}, \int_{S^2}\left|U^{-1}\hat{x}_j + r\omega\right|^s\omega\frac{d\omega}{4\pi}\rangle\end{aligned}$$

for any $U \in SO(3)$. Choose $U \in SO(3)$ such that $U^{-1}\hat{x}_j = \hat{e}_3$ then

$$\begin{aligned}\int_{S^2} \left|U^{-1}\hat{x}_j + r\omega\right|^s \omega \frac{d\omega}{4\pi} &= \int_{S^2} |\hat{e}_3 + r\omega|^s \omega \frac{d\omega}{4\pi} \\ &= 2\pi\hat{e}_3 \int_0^\pi (1 + r^2 + 2r\cos\theta)^{s/2} \cos\theta \frac{\sin\theta d\theta}{4\pi} \\ &= \frac{\hat{e}_3}{2} \int_{-1}^1 (1 + r^2 + 2rt)^{s/2} t dt =: \hat{e}_3 c(r)\end{aligned}$$

and thus

$$\int_{S^2} \left|\hat{x}_j + r\omega\right|^s P_1(\langle\hat{a}, \omega\rangle) \frac{d\omega}{4\pi} = c(r)\langle\hat{a}, U\hat{e}_3\rangle \tag{A.2.2}$$

for some $c(r) \geq 0$. To compute higher multipole moments, we need to extend $\left|\hat{x_j} + r\omega\right|^s$ in terms of Legendre polynomials. Note, that

$$\left|\hat{x}_j + r\omega\right|^s = \left(1 + r^2 + 2r\langle\hat{x_j}, \omega\rangle\right)^{s/2} = (1 + r^2)^{s/2} \left(1 + \frac{2r}{1 + r^2}\langle\hat{x}_j, \omega\rangle\right)^{s/2} \tag{A.2.3}$$

For convenience, we define

$$q := \frac{2r}{1 + r^2} .$$

By Newton's generalized binomial theorem, we can extend the right–hand side of (A.2.3)

$$(1 + r^2)^{s/2} \left(1 + \frac{2r}{1 + r^2}\langle\hat{x}_j, \omega\rangle\right)^{s/2} = (1 + r^2)^{s/2} \sum_{k=0}^{\infty} \binom{s/2}{k} q^k \left(\langle\hat{x}_j, \omega\rangle\right)^k \tag{A.2.4}$$

which converges absolutely since $q\langle\hat{x}_j, \omega\rangle \leq 1$ by assumption. If $s/2 \in \mathbb{N}$, then the generalized binomial coefficients are identical to the normal binomial coefficients with

$$\binom{s/2}{k} = 0, \quad k > s/2 \in \mathbb{N} . \tag{A.2.5}$$

Hence, the series above is only a finite sum in that case. If $s/2 \notin \mathbb{N}$ then for any $k \in \mathbb{N}_0$ the generalized binomial coefficients are defined as

$$\binom{s/2}{k} = \frac{\frac{s}{2}(\frac{s}{2} - 1) \cdots (\frac{s}{2} - (k - 1))}{k!} = \frac{\prod_{n=0}^{k-1}(\frac{s}{2} - n)}{k!} .$$

We extend monomials in terms of Legendre polynomials. From Rodrigou's Formula (see [1, Chapter 8]), one can derive the explicit representation

$$P_n(t) = 2^n \sum_{m=0}^{n} t^m \binom{n}{m} \binom{\frac{n+m-1}{2}}{n} .$$

Let

$$\begin{aligned} c_{k,n} &:= \frac{(2n+1)}{2} \int_{-1}^{1} t^k P_n(t)\, dt \\ &= (2n+1)2^{n-1} \sum_{m=0}^{n} \binom{n}{m} \binom{\frac{n+m-1}{2}}{n} \int_{-1}^{1} t^{k+m}\, dt \end{aligned} \tag{A.2.6}$$

then its clear that $c_{k,n} = 0$ for $n > k$. We differ the cases for which k is even and for which k is odd. When k is even, then $c_{k,n} = 0$ whenever n is odd, as one easily concludes from equation (A.2.6). Analogous when k is odd $c_{k,n} = 0$ whenever n is even. Hence for $n \le k$,

$$c_{k,n} = \begin{cases} (2n+1)2^{n-1} \sum_{m=0}^{n} \binom{n}{m} \binom{\frac{n+m-1}{2}}{n} \frac{2}{k+m+1}, & k+m \text{ is even,} \\ 0, & k+m \text{ is odd,} \\ 1, & k=m=0 \end{cases} . \tag{A.2.7}$$

By the orthogonality of Legendre Polynomials

$$\int_{-1}^{1} P_n(t) P_m(t)\, dt = \frac{2\delta_{mn}}{2n+1}$$

it then follows

$$t^k = \sum_{l=0}^{k} c_{k,l} P_l(t)\,. \tag{A.2.8}$$

By the usual definition of the double factorial, one can derive by elementary steps that

$$t^k = \sum_{l=k,k-2,\ldots} \frac{(2l+1)k!}{2^{(k-l)/2} \left(\frac{k-l}{2}\right)! (l+k+1)!!} P_k(t). \tag{A.2.9}$$

For even numbers of $k = 2n$ with $n \in \mathbb{N}_0$ this means

$$t^{2n} = \sum_{u=0}^{n} \frac{(4u+1)(2n)!}{2^{(n-u)}\, (n-u)!(2(n+u)+1)!!} P_{2u}(t). \tag{A.2.10}$$

and for odd numbers of $k = 2n+1$ with $n \in \mathbb{N}_0$ this is

$$t^{2n+1} = \sum_{u=0}^{n} \frac{(4u+3)(2n+1)!}{2^{(n-u)}\, (n-u)!(2(n+u)+3)!!} P_{2u+1}(t). \tag{A.2.11}$$

Combining the equation (A.2.8), (A.2.4) and (A.2.3) shows

$$\left|\hat{x}_j + r\omega\right|^s = (1+r^2)^{s/2} \sum_{k=0}^{\infty} \binom{s/2}{k} q^k \sum_{n=0}^{k} c_{k,n} P_n(\langle \hat{x}_j, \omega \rangle)\,. \tag{A.2.12}$$

Using this representation, we can compute the remaining multipole moments. For $l \geq 2$ we compute

$$\begin{aligned}
&\int_{S^2} \left|\hat{x}_j + r\omega\right|^s P_l(\langle \hat{a}, \omega\rangle) \frac{d\omega}{4\pi} \\
&= (1+r^2)^{s/2} \sum_{k=0}^{\infty} \binom{s/2}{k} q^k \sum_{n=0}^{k} c_{k,n} \int_{S^2} P_n(\langle \hat{x}_j, \omega\rangle) P_l(\langle \hat{a}, \omega\rangle) \frac{d\omega}{4\pi}.
\end{aligned} \tag{A.2.13}$$

The remaining integral follows from the orthogonality of Legendre Polynomials. By extending the Legendre Polynomials P_n into the spherical harmonics Y_{nm} one easily shows the following orthogonality relation for $a, b \in \mathbb{R}^3$ with $\|a\| = \|b\| = 1$,

$$\begin{aligned}
&\int_{S^2} P_l(\langle \omega, a\rangle) P_n(\langle \omega, b\rangle) \frac{d\omega}{\left|S^2\right|} \\
&= \sum_{m'=-l}^{l} \sum_{m=-n}^{n} \frac{4\pi}{2l+1} \frac{4\pi}{2n+1} \int_{S^2} Y^*_{lm}(\omega) Y_{nm'}(\omega) \frac{d\omega}{\left|S^2\right|} Y^*_{lm}(a) Y_{nm'}(b) \\
&= \sum_{m'=-l}^{l} \sum_{m=-n}^{n} \frac{4\pi}{2l+1} \frac{4\pi}{2n+1} \frac{\delta_{mm'}\delta_{ln}}{\left|S^2\right|} Y_{lm}(a) Y^*_{nm'}(b) \\
&= \frac{\delta_{ln}}{2l+1} P_l(\langle a, b\rangle).
\end{aligned} \tag{A.2.14}$$

Thus combining equation (A.2.14) and (A.2.13) shows for $l \geq 2$,

$$\begin{aligned}
&\int_{S^2} \left|\hat{x}_j + r\omega\right|^s P_l(\langle \hat{a}, \omega\rangle) \frac{d\omega}{4\pi} \\
&= (1+r^2)^{s/2} \sum_{k=2}^{\infty} \binom{s/2}{k} q^k \sum_{n=0}^{k} c_{k,n} \frac{\delta_{ln}}{2l+1} P_l(\langle \hat{a}, \hat{x}_j\rangle) \\
&= (1+r^2)^{s/2} \sum_{k=l}^{\infty} \binom{s/2}{k} \frac{q^k c_{k,l}}{2l+1} P_l(\langle \hat{a}, \hat{x}_j\rangle)
\end{aligned} \tag{A.2.15}$$

where the series still converges absolutely as mentioned after equation (A.2.4). Note that in the case $s = 2$, the expression vanishes due to equation (A.2.5). ∎

Lemma A.2.4. *For $s \in [2, 3]$, $k \in \mathbb{N}$ with $k \geq 2$ let*

$$A_k = \left|\binom{s/2}{k}\right| \sum_{l=2}^{k} \frac{c_{k,l}}{2l+1}$$

with $c_{k,l}$ defined in equation (A.2.6). *Then*

$$\sum_{k=4}^{\infty} A_k \leq \frac{s}{2}\left(\frac{s}{2}-1\right)\left(2-\frac{s}{2}\right)\frac{28}{625}\,.$$

Proof. Note that

$$\sum_{l=0}^{k} c_{k,l} = 1$$

due to its defining equation

$$t^k = \sum_{l=0}^{k} c_{k,l} P_l(t)\,.$$

by choosing $t = 1$ and noting $P_l(1) = 1$ for any $l \in \mathbb{N}$. Consequently

$$A_k \leq \frac{1}{5}\left|\binom{s/2}{k}\right| \sum_{l=2}^{k} c_{k,l} \leq \frac{1}{5}\left|\binom{s/2}{k}\right| \sum_{l=0}^{k} c_{k,l} = \frac{1}{5}\left|\binom{s/2}{k}\right|$$

where we used $c_{k,l} \geq 0$ (see their explicit form in (A.2.6)). For the generalized binomial coefficients, the inequality

$$\left|\binom{s/2}{k}\right| \leq \frac{\frac{s}{2}(\frac{s}{2}-1)}{k(k-1)} \leq \frac{s}{2}\left(\frac{s}{2}-1\right)\left(\frac{1}{k-1}-\frac{1}{k}\right)$$

holds for any $s \in [2,3]$ and $k \geq 2$, $k \in \mathbb{N}$. Thus for $n_0 \in \mathbb{N}$

$$\sum_{k=n_0}^{\infty} A_k \leq \sum_{k=n_0}^{N} A_k + \frac{s}{2}\left(\frac{s}{2}-1\right)\frac{1}{5(N-1)}$$

and consequently

$$\sum_{k=N}^{\infty} A_k < \frac{s}{2}\left(\frac{s}{2}-1\right)\left(2-\frac{s}{2}\right)\frac{2}{5(N-1)} =: \delta(N)$$

is arbitrary small for N large enough. Thus, we can estimate the series over A_k with arbitrary precision. Let $n_0 = 4$ then

$$\sum_{k=n_0}^{\infty} A_k \leq \sum_{k=4}^{2} NA_k + \delta(2N) = \sum_{k=2}^{N} A_{2k} + \sum_{k=2}^{N-1} A_{2k+1} + \delta(2N)\,.$$

With the explicit expression of $c_{k,l}$ in (A.2.10) we find

$$A_{2k} \leq \frac{s}{2}\left(\frac{s}{2}-1\right)\left(2-\frac{s}{2}\right)\sum_{l=1}^{k}\frac{(2k-2)!}{2^{k-l}(k-l)!(2(k+l)+1)!!}$$

and analogous with (A.2.11)

$$A_{2k-1} \leq \frac{s}{2}\left(\frac{s}{2}-1\right)\left(2-\frac{s}{2}\right)\sum_{l=1}^{k}\frac{(2k-1)!}{2^{k-l}(k-l)!(2(k+l)+3)!!} .$$

Choosing $N = 1000$ and computing those terms on a computer explicitly, we find

$$\sum_{k=4}^{1001} A_k \leq \frac{s}{2}\left(\frac{s}{2}-1\right)\left(2-\frac{s}{2}\right)(0.0242 + 0.0203) .$$

Adding the error estimate

$$\delta(2000) \leq \frac{s}{2}\left(\frac{s}{2}-1\right)\left(2-\frac{s}{2}\right) 0.0003$$

such that

$$\sum_{k=4}^{\infty} A_k \leq \frac{s}{2}\left(\frac{s}{2}-1\right)\left(2-\frac{s}{2}\right)\frac{448}{10000} .$$

∎

A.3 Explicit Constant in an Inequality due to Lieb

Lemma A.3.1. *For any $p \in [1,2]$ the constant C_p in equation* (4.6.11) *is given by*

$$C_p = \frac{3\sqrt{\pi}}{4}\frac{(4\pi)^{-p/3}}{p^{1+p/2}}\frac{\left(\frac{15\sqrt{\pi}}{8}\frac{\Gamma(3/p)}{\Gamma(7/2+3/p)}\right)^{p/2}\frac{\Gamma(3/p+1)}{\Gamma(3/p+7/2)}}{\left(\frac{\sqrt{\pi}}{4}\frac{\Gamma(3/p+1)}{\Gamma(3/p+5/2)}\right)^{1+5p/6}} \tag{A.3.1}$$

where Γ is the Gamma function defined by the improper integral

$$\Gamma(r) \coloneqq \int_0^\infty x^{r-1}e^{-x}dx .$$

Proof. We give only a sketch of the calculations. Following [72, p. 563] one needs to solve the following three integrals

$$\int_{\mathbb{R}^3} f_p(x)dx, \int_{\mathbb{R}^3} |x|^p f_p(x)dx \text{ and } \int_{\mathbb{R}^3} [f_p(x)]^{5/3}dx$$

for

$$f_p(x) \coloneqq \begin{cases} (1-|x|^p)^{\frac{3}{2}} & |x| \leq 1 \\ 0 & \text{elsewise} \end{cases} . \tag{A.3.2}$$

the first integral can be solved by a straightforward calculation, and the latter two can be solved by substituting $u = |x|^p$. The first integral reduces to

$$\int_0^1 r^2(1-r^p)^{3/2}\,dr = \frac{\sqrt{\pi}}{4}\frac{\Gamma(3/p+1)}{\Gamma(3/p+5/2)}\,.$$

After substituting, the second integral reduces to

$$\frac{1}{p}\int_0^1 u^{3/p}(1-u)^{3/2}du = \frac{3\sqrt{\pi}}{4p}\frac{\Gamma(3/p+1)}{\Gamma(3/p+7/2)}\,.$$

The third integral reduces to

$$\frac{1}{p}\int_0^1 u^{(3-p)/p}(1-u)^{5/2}du = \frac{15\sqrt{\pi}}{8p}\frac{\Gamma(3/p)}{\Gamma(3/p+7/2)}\,.$$

Combining these three integrals gives the desired constant. ∎

A.4 Estimate on Groundstate Energie of the Bohr Atom

The following Lemma is a well-known fact. We include it here for convenience.

Lemma A.4.1. *Given the operator in* (4.2.1) *(in atomic units) for N fermions with $u \in \mathbb{N}$ spin-degrees of freedom and nuclear charge Z then the ground state energy is bound by*

$$-E_{N,Z} \leq AZ^2N^{1/3}$$

with $A = \frac{1}{2}u^{2/3}3^{1/3}$.

Proof. The energy levels of hydrogen with nuclear charge Z

$$h := -\frac{1}{2}\Delta - \frac{Z}{|x|} \tag{A.4.1}$$

are

$$E_n = \frac{-Z^2}{n^2}Ry \tag{A.4.2}$$

where Ry is the Rydberg energy. In atomic units

$$Ry = \frac{m_e e^2}{2(4\pi\varepsilon_0)^2\hbar} = \frac{1}{2}\,. \tag{A.4.3}$$

Each of these energy levels is n^2-times degenerated. Note that the interelectronic repulsion is a positive contribution to the operator in (4.2.1) and thus

$$H_{N,Z} \geq \sum_{i=1}^{N}\left(-\frac{1}{2}\Delta_i - \frac{Z}{|x_i|}\right)\,. \tag{A.4.4}$$

The ground state of the right–hand side can be computed explicitly in terms of the energies in equation (A.4.2). Due to the fermionic symmetry, the particles occupy the energy levels starting from the lowest, counting the degeneration in the ground state. Let $E_0(N,Z)$ the ground-state energy of the right hand side of equation (A.4.4) and Denote by $L \in \mathbb{N}$ the last completely filled energy Level then there exists $c \in [0,1)$ such that

$$E_0(N,Z) = cu(L+1)^2 E_{L+1} + u\sum_{j=1}^{L} j^2 E_j = -uZ^2 R_y(c+L)\,.$$

Here we have used that due to the spin of the particles, each state can be u-times occupied. It remains to compare L with N.

$$\frac{N}{u} = c(L+1)^2 + \sum_{j=1}^{L} j^2 = c(L+1)^2 + \frac{L^3}{3} + \frac{L^2}{2} + \frac{L}{6}\,.$$

A straightforward calculation using $c \in [0,1]$ shows

$$(L+c)^3 \le \frac{3N}{u}\,.$$

We conclude

$$-E_{N,Z} \le -E_0(N,Z) \le uZ^2 R_y \left(\frac{3N}{u}\right)^{1/3} = \frac{1}{2} u^{2/3} 3^{1/3} Z^2 N^{1/3}\,.$$

∎

A.5 A Useful Elementary Inequality

Lemma A.5.1. *Let $r \neq 0$ and $p \ge 1$ then*

$$\begin{aligned}\frac{(1+r)^{p-1} - (1-r)^{p-1}}{2r(p+1)} &\ge \frac{(1+r)^p - (1-r)^p}{2rp} \\ &\ge \left(1 - \frac{p-1}{3} r^2\right) \frac{(1+r)^{p+1} - (1-r)^{p+1}}{2r(p+1)}\,.\end{aligned} \tag{A.5.1}$$

Proof. Since the inequalities in (A.5.1) are symmetric under changing r to $-r$, it is enough to prove them for $r > 0$. In this case (A.5.1) is equivalent to

$$\begin{aligned}\frac{(1+r)^{p+1} - (1-r)^{p+1}}{p+1} &\ge \frac{(1+r)^p - (1-r)^p}{p} \\ &\ge \left(1 - \frac{p-1}{3} r^2\right) \frac{(1+r)^{p+1} - (1-r)^{p+1}}{p+1}\,.\end{aligned} \tag{A.5.2}$$

The first bound,

$$h(r) := \frac{(1+r)^{p+1} - (1-r)^{p+1}}{(p+1)} \geq \frac{(1+r)^p - (1-r)^p}{p} =: k(r) \tag{A.5.3}$$

for $r \geq 0$ is easy to show. Since $h(0) = 0 = k(0)$ it follows as soon as $h'(r) \geq k'(r)$ for $r \geq 0$. This is equivalent to

$$(1+r)^p + (1-r)^p \geq (1+r)^{p-1} - (1-r)^{p-1} \quad \text{for } r \geq 0\,. \tag{A.5.4}$$

Expanding

$$\begin{aligned}(1+r)^p \pm (1-r)^p &= (1+r)^{p-1}(1+r) \pm (1-r)^{p-1}(1-r) \\ &= (1+r)^{p-1} \pm (1-r)^{p-1} + r\big((1+r)^{p-1} \mp (1-r)^{p-1}\big)\end{aligned} \tag{A.5.5}$$

in the left–hand–side of (A.5.4) we see that (A.5.4) is equivalent to

$$r\left((1+r)^{p-1} - (1-r)^{p-1}\right) \geq 0$$

which is true for $r \geq 0$ if $p \geq 1$. This proves the first bound in (A.5.2).
We prove the second inequality in (A.5.2) by determining $c \in \mathbb{R}$ such that

$$f_1(r) := \frac{(1+r)^p - (1-r)^p}{p} \geq \left(1 - cr^2\right) \frac{(1+r)^{p+1} - (1-r)^{p+1}}{(p+1)} =: g_1(r)\,, \tag{A.5.6}$$

for $r \geq 0$. At $r = 0$ we have $f_1(0) = g_1(0)$, so (A.5.6) is true for $r \geq 0$ as soon as $f_1'(r) \geq g_1'(r)$ for $r \geq 0$. This is equivalent to

$$\begin{aligned}(1+r)^{p-1} + (1-r)^{p-1} \geq (1-cr^2)\,((1+r)^p + (1-r)^p) \\ \cdot \frac{2cr\left((1+r)^{p+1} - (1-r)^{p+1}\right)}{p+1}\,.\end{aligned} \tag{A.5.7}$$

Using (A.5.5) this is equivalent to

$$\begin{aligned}f_2(r) := -\big((1+r)^{p-1} - (1-r)^{p-1}\big) + \frac{2c}{p+1}\left((1+r)^{p+1} - (1-r)^{p+1}\right) \\ + cr\,((1+r)^p + (1-r)^p) \geq 0 \quad \text{for } r \geq 0\,.\end{aligned} \tag{A.5.8}$$

Since $f_2(0) = 0$ we know that (A.5.8) holds as soon as $f_2'(r) \geq 0$ for $r \geq 0$. Now

$$\begin{aligned}f_2'(r) = -(p-1)\left((1+r)^{p-2} + (1-r)^{p-2}\right) + 3c\,((1+r)^p + (1-r)^p) \\ + cpr\left((1+r)^{p-1} - (1-r)^{p-1}\right)\end{aligned}$$

and using (A.5.5) twice, the second time with p replaced with $p-1$, we have

$$(1+r)^p \pm (1-r)^p = (1+r)^{p-2} \pm (1-r)^{p-2} + 2r\left((1+r)^{p-2} \mp (1-r)^{p-2}\right) \\ + r^2\left((1+r)^{p-2} \pm (1-r)^{p-2}\right) .$$

Hence, we see that

$$f_2'(r) = (3c - (p-1))\left((1-r)^{p-2} + (1+r)^{p-2}\right) \\ + (6+p)cr\left((1+r)^{p-2} - (1-r)^{p-2}\right) \\ + (3+p)cr^2\left((1+r)^{p-2} + (1-r)^{p-2}\right) \geq 0$$

for all $r \geq 0$ as soon as $c \geq (p-1)/3 \geq 0$. This proves the second inequality in (A.5.2) and finishes the proof of (A.5.1). ∎

A.6 Rescaling of the Hartree Energy

Lemma A.6.1. *Consider the Hartree energy, which is given by*

$$E^H_{N,Z} = \inf\left\{\mathcal{E}^H_Z(\psi) : \psi \in H^1(\mathbb{R}^3), \|\psi\|_2^2 = N\right\},$$

where

$$\mathcal{E}^H_Z(\psi) = \frac{1}{2}\int (\nabla\psi)^2 \,\mathrm{d}x - Z\int \frac{|\psi|^2}{|x|}\,\mathrm{d}x + \frac{1}{2}\iint \frac{|\psi(x)|^2|\psi(y)|^2}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y\,, \quad \psi \in H^1\,.$$

Then

$$E^H_{N,Z} = Z^3 e(N/Z)$$

where $e(\cdot)$ is defined as in (4.8.18) *namely*

$$e(t) = \inf\left\{\mathcal{E}^H_1(g) : g \in H^1(\mathbb{R}^3), \|g\|_2^2 = t\right\}, \textit{ for } t > 0 \textit{ and } e(0) := 0\,.$$

Proof. Let $\psi \in H^1$ with $\|\psi\|_2^2 = N$ and define

$$\psi(x) := s^{-1/2}\lambda^{-3/2} g(x/\lambda)\,.$$

By direct computations

$$\mathcal{E}^{\mathrm{H}}_Z(\psi) = s^{-1}\lambda^{-2}\left[\frac{1}{2}\int (\nabla g)^2\,\mathrm{d}x - Z\lambda\int\frac{|g|^2}{|x|}\,\mathrm{d}x + s^{-1}\lambda\frac{1}{2}\iint\frac{|g(x)|^2|g(y)|^2}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y\right].$$

Choose $s = \lambda = Z^{-1}$ then

$$\mathcal{E}_Z^{\mathrm{H}}(\psi) = Z^3 \left[\frac{1}{2} \int (\nabla g)^2 \,\mathrm{d}x - \int \frac{|g|^2}{|x|} \,\mathrm{d}x + \frac{1}{2} \iint \frac{|g(x)|^2 |g(y)|^2}{|x-y|} \,\mathrm{d}x \,\mathrm{d}y \right],$$

with

$$\|g\|_2^2 = s\|\psi\|_2^2 = \frac{N}{Z}.$$

By the definition of $E_{N,Z}^{\mathrm{H}}$ this proves

$$E_{N,Z}^{\mathrm{H}} = Z^3 \inf \left\{ \mathcal{E}_1^H(g) : g \in H^1(\mathbb{R}^3), \|g\|_2^2 = \frac{N}{Z} \right\}.$$

Comparing this with the definition of $e(\cdot)$ proves the statement. ∎

A.7 Excess Charge Problem in the Hartree Model

We apply the Benguria–Lieb–Nam argument directly to the Hartree Model similar to [20] to derive analytic bounds on the value t_{c} defined in Section 4.8. Since $N \le t_{\mathrm{c}} Z$ (see Remark 4.8), this directly proves new bounds on the maximal allowed excess charge in the Hartree model. In particular, we prove

Lemma A.7.1. *Let t_c be the minimizer according to* (4.8.19) *then*

$$t_c \le \inf_{s\in[1,2]} b(s) \left(\frac{11+s^2}{12} \right), \quad \textit{with} \quad b(s) = \left(\min_{0\le r\le 1} \frac{1+r^s}{1+r^{s-1}} \right)^{-1}.$$

Remark A.7.2. *Numerically, it was found $t_c \approx 1.21$ (see [18]), and up to our knowledge, the best analytic bound is $t_c \le 1.5211$ in [20]. We improve upon their result. Choose $s = 1.624$ then one easily checks $b(1.624) < 1.29$ and consequently*

$$t_c \le 1.29 \cdot \frac{11 + (1.624)^2}{12} \le 1.47.$$

Proof of A.7.1. Let f with $\|f\|_2^2 = N$ be the unique minimizer of the Hartree functional following [110, p. 166] then f is the unique positive solution to

$$\frac{-\Delta f}{2} = \Phi f \tag{A.7.1}$$

with

$$\Phi(x) = Z|x|^{-1} - (|f|^2 * |\cdot|^{-1})(x).$$

Let $s \in (1,2]$ and multiply (A.7.1) from the left by $|\cdot|^s f$ and integrate, then

$$\frac{1}{2}\langle |x|^s f, -\Delta f \rangle = Z\langle |x|^{s-1} f, f \rangle - \frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} |f(x)|^2 \frac{|x|^s + |y|^s}{|x-y|} |f(y)|^2 d(x,y). \tag{A.7.2}$$

The Hartree equation (A.7.1) is invariant under rotations, and consequently, f is rotationally symmetric. Thus, using Newton's theorem

$$\frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}|f(x)|^2\frac{|x|^s+|y|^s}{|x-y|}|f(y)|^2d(x,y)=\frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}|f(x)|^2\frac{|x|^s+|y|^s}{\max\{|x|,|y|\}}|f(y)|^2d(x,y)\,.$$

Therefore, with $r(x,y)=\frac{\min\{|x|,|y|\}}{\max\{|x|,|y|\}}$,

$$\begin{aligned}
&\frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}|f(x)|^2\frac{|x|^s+|y|^s}{\max\{|x|,|y|\}}|f(y)|^2d(x,y)\\
&=\frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}|f(x)|^2\frac{|x|^s+|y|^s}{\max\{|x|,|y|\}(|x|^{s-1}+|y|^{s-1})}|f(x)|^2(|x|^{s-1}+|y|^{s-1})|f(y)|^2d(x,y)\\
&=\frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{1+r(x,y)^s}{1+r(x,y)^{s-1}}|f(x)|^2(|x|^{s-1}+|y|^{s-1})|f(y)|^2\\
&\geq\min_{0\leq r\leq 1}\frac{1+r^s}{1+r^{s-1}}\int_{\mathbb{R}^3}|x|^{s-1}|f(y)|^2dx\|f\|_2^2=\frac{\|f\|_2^2}{b(s)}\langle|x|^{s-1}f,f\rangle,
\end{aligned}\tag{A.7.3}$$

with

$$b(s)^{-1}=\min_{0\leq r\leq 1}\frac{1+r^s}{1+r^{s-1}}$$

the same number as in Proposition 4.4.5. Combining (A.7.2) and (A.7.3) yields

$$\frac{\|f\|_2^2}{b(s)}\leq Z+\frac{\frac{1}{2}\langle|x|^sf,\Delta f\rangle}{\langle|x|^{s-1}f,f\rangle}\,.$$

By application of Lemma 4.8.8 (note that f is not normalized) we find

$$\frac{\|f\|_2^2}{b(s)}\leq Z+\frac{s^2-1}{8}\frac{\langle|x|^{-1}f,f\rangle}{\|f\|_2^2}$$

and by the Coulomb–Uncertainty principle (see (4.8.5))

$$\langle|x|^{-1}f,f\rangle\leq\|f\|_2\left(\langle f,-\Delta f\rangle\right)^{1/2}\,.$$

Similar to Lemma 4.8.4, we have the following virial theorem

$$\langle f,-\Delta f\rangle=-2E^H_{N,Z}$$

where $E^H_{N,Z}$ is the Hartree energy (see Lemma A.6.1). Summarizing the above, we have shown

$$\frac{\|f\|_2^2}{b(s)}\leq Z+\frac{s^2-1}{8}\|f\|_2^{-1}\left(-2E^H_{N,Z}\right)^{1/2}\,.$$

Using $E^H_{N,Z} = Z^3 e(N/Z)$ (see Lemma A.6.1) and $\|f\|_2^2 = N$ we arrive at

$$\frac{N}{b(s)} \leq Z + \frac{s^2-1}{8} N^{-1/2} \left(-2Z^3 e(N/Z)\right)^{1/2},$$

and after dividing by Z and multiplying by $b(s)$ this yields

$$\frac{N}{Z} \leq b(s) \left(1 + \frac{s^2-1}{8} \left(\frac{N}{Z}\right)^{-1/2} (-2e(N/Z))^{1/2}\right).$$

In the Hartree model its true that $\frac{N}{Z} \to t_c$ as $Z \to \infty$ and $e(\cdot)$ is continuous such that by taking the limit $Z \to \infty$

$$t_c \leq b(s) \left(1 + \frac{s^2-1}{8} \left(\frac{-e(t_c)}{t_c}\right)^{1/2}\right).$$

In Lemma 4.8.4 we have proven

$$e(t_c) \geq -\frac{2t_c}{9}.$$

and consequently, we arrive at

$$t_c \leq b(s) \left(1 + \frac{s^2-1}{12}\right).$$

For $s = 1$, this proves $t_c \leq 2$ as shown by Lieb, and for $s = 2$, this reduced to the inequality found in [20]. ∎

Appendix B

B.1 Hardy–Type Inequalities

In the work at hand, several types of Hardy Inequalities are used. We collect them here from different sources and refer to their proofs.
The one–dimensional Hardy Inequality, for which a proof can be found in [36, Theorem 2.65] is:

Lemma B.1.1. *Let* $u \in \dot{H}^1(\mathbb{R})$ *and assume* $\liminf_{r\to 0}|u(r)| = 0$*. Then*

$$\int_{\mathbb{R}} \frac{|u(r)|^2}{|r|^2}\, dr \leq 4 \int_{\mathbb{R}} |u'(r)|^2\, dr\,. \tag{B.1.1}$$

The following is the Hardy Inequality in dimension two, for which a proof can be found in [109] or derived from [36, Pop. 2.68]

Lemma B.1.2. *Let* $u \in \dot{H}^1(\mathbb{R}^2)$ *with*

$$\int_0^{2\pi} u(c,\varphi)d\varphi = 0,$$

where (ρ,φ) *are polar coordinates and* $c > 0$*. Then the following Hardy Inequality is true:*

$$\int_{\mathbb{R}^2} \frac{|u|^2}{|x|^2\left(1+\ln^2\left(\frac{|x|}{c}\right)\right)} dx \leq 4\int_{\mathbb{R}^2} |\nabla u|^2 dx\,.$$

The following is the radial Hardy Inequality on conical sets, which was proven in [83, §4].

Lemma B.1.3. *Let* $d \geq 2$ *and* $K \subset \mathbb{S}^{d-1}$ *a smooth domain and*

$$\Omega \coloneqq \{x = |x|\omega : \omega \in K\}\,.$$

Then for any $u \in \dot{H}^1(\Omega \setminus \{0\})$ *the following Hardy Inequality holds:*

$$\int_{\Omega} |u|^2|x|^{-2}dx \leq \left(\frac{2}{d-2}\right)^2 \int_{\Omega} |\nabla u|^2 dx\,.$$

B.2 Remarks on the Geometry of the Sets $K_\alpha(\gamma)$

Lemma B.2.1. *Let* $\alpha, \beta \in \{(12), (13), (23)\}$ *then*

$$K_\alpha(\gamma) \cap K_\beta(\gamma) = \{0\}$$

for $\alpha \neq \beta$ *if* $\gamma > 0$ *is small enough.*

Proof. We begin with the sets $K_{1j}(\gamma)$ for $j \in \{2, 3\}$. Assume that $x \in K_{12}(\gamma) \cap K_{13}(\gamma)$ and $x \neq 0$ then

$$|x|^2 \le (x_1^2 + x_2^2) + (x_1^2 + x_3^3) < 2\gamma^2|x|^2$$

which fails for γ small enough, which we assume henceforth. Consequently, we have

$$K_{12}(\gamma) \cap K_{13}(\gamma) = \{0\}$$

Next we assume that $x \in K_{12}(\gamma) \cap K_{23}(\gamma)$ and $x \neq 0$, then

$$x_1^2 + x_2^2 < \gamma^2|x|^2 ,$$
$$\left|\frac{x_2}{\sqrt{m_2}} - \frac{x_3}{\sqrt{m_3}}\right| < \gamma|x| .$$

Let $m := \min\{m_1, m_2, m_3\}$ and $M := \max\{m_1, m_2, m_3\}$ and recall the choice $\sqrt{m_i}y_i = x_i$ then

$$\begin{aligned} y_1^2 + y_2^2 &< \frac{\gamma^2}{m} M|y|^2 , \\ |y_2 - y_3| &< \gamma\sqrt{M}|y| . \end{aligned} \tag{B.2.1}$$

Note that the points $(y_2, 0)$, $(y_3, 0)$ and $(0, y_1)$ are the corners of a triangle in $\mathbb{R}^2$ and thus by the triangle inequality

$$\sqrt{y_1^2 + y_3^2} \le \sqrt{y_1^2 + y_2^2} + |y_2 - y_3| < \gamma\sqrt{M}\left(1 + m^{-1/2}\right)|y| . \tag{B.2.2}$$

Combining (B.2.1) and (B.2.2) there exists a constant $c(M, m) > 0$ independent of γ and $y \neq 0$ such that

$$|y|^2 \le (y_1^2 + y_2^2) + (y_1^2 + y_3^2) \le c(M, m)|\gamma|^2|y|^2$$

which fails for γ small enough and thus $K_{12}(\gamma) \cap K_{23}(\gamma) = \{0\}$. Repeating the same arguments for the set $K_{13}(\gamma) \cap K_{23}(\gamma)$ concludes the proof. ∎

Lemma B.2.2. *Let* $\alpha \in \{(12), (13), (23)\}$ *and let* $\gamma > 0$ *satisfy the condition* (B.2.1). *Assume that the potentials* V_α *satisfy* (5.2.2). *Then there exists* $C > 0$ *such that for any* $x \notin K_\alpha(\gamma)$ *with* $|x| > b$ *holds*

$$|V_\alpha(x)| \le C|x|^{-\nu_\alpha}, \tag{B.2.3}$$

where $\nu_{23} = 2 + \delta$ *and* $\nu_{12} = \nu_{13} = 3 + \delta$.

Remark B.2.3. *Lemma B.2.2 implies that for small $\gamma > 0$ condition* (B.2.3) *holds on $\Omega(\gamma)$ for any of the potentials if $|x| > b$ and $b > 0$ large enough. Consequently the condition* (B.2.3) *applies on any of the sets $K_\alpha(\gamma, \tilde{\gamma})$ defined in Section 5.3.1.*

Proof. We begin with $\alpha = (23)$. The potential V_{23} fulfills (5.2.2) and thus there exist constants $C, \delta > 0$ and $A > 0$ such that

$$|V_{23}(|\mathbf{r}_{23}|)| \leq C(1 + |\mathbf{r}_{23}|)^{-2-\delta}, \tag{B.2.4}$$

whenever $|\mathbf{r}_{23}| > A$. For $x \notin K_{23}(\gamma)$ we have

$$|\mathbf{r}_{23}| \geq \left| \frac{x_2}{\sqrt{m_2}} - \frac{x_3}{\sqrt{m_3}} \right| \geq \gamma |x| \,. \tag{B.2.5}$$

Consequently $|\mathbf{r}_{23}| > A$ for $|x| > b$ for $b > 0$ large enough. Combining (B.2.5) and (B.2.4) the statement for $\alpha = (23)$ follows directly.
Next, we prove the case $\alpha = (12)$. The proof for $\alpha = (13)$ is similar. The potential V_{12} fulfills (5.2.2) and thus there exist constants $C, \delta > 0$ and $A > 0$ such that

$$|V_{12}(|\mathbf{r}_{12}|)| \leq C(1 + |\mathbf{r}_{12}|)^{-3-\delta} \tag{B.2.6}$$

whenever $|\mathbf{r}_{12}| > A$. Assume $x \notin K_{12}(\gamma)$ then

$$\begin{aligned} |\mathbf{r}_{12}| &\geq \left(\frac{x_1^2}{m_1} + \frac{x_2^2}{m_2} - \cos(\zeta) 2 \frac{x_1 x_2}{\sqrt{m_1 m_2}} \right)^{1/2} \\ &\geq \left(\frac{x_1^2}{m_1} + \frac{x_2^2}{m_2} \right)^{1/2} (1 - \cos(\zeta))^{1/2} \\ &\geq \left(\min\left\{ \frac{1}{m_1}, \frac{1}{m_2} \right\} (1 - \cos(\zeta)) \right)^{1/2} |(x_1, x_2)| \\ &\geq \left(\min\left\{ \frac{1}{m_1}, \frac{1}{m_2} \right\} (1 - \cos(\zeta)) \gamma \right)^{1/2} |x| \,. \end{aligned} \tag{B.2.7}$$

where we have used that $2ab \leq a^2 + b^2$ from the first to the second line in (B.2.7). Since $\zeta \in (0, \pi/2]$, combining (B.2.7) and (B.2.6) completes the proof. ∎

Lemma B.2.4. *Let $(x_1, x_2, x_3) \in \mathbb{R}^3$ and let (q, ξ) be defined as,*

$$q = \frac{1}{\sqrt{M_{23}}} (\sqrt{m_3} x_2 - \sqrt{m_2} x_3) \,,$$

$$\xi = \frac{1}{\sqrt{M_{23}}} (\sqrt{m_2} x_2 + \sqrt{m_3} x_3),$$

where $M_{23} := m_2 + m_3$. Then

$$|x| = |(x_1, q, \xi)| \,. \tag{B.2.8}$$

The surface measure on the set $\partial K_{23}(\gamma)$ in this set of coordinates is given by

$$d\sigma = \kappa_0 d(x_1, \xi) \tag{B.2.9}$$

with

$$\kappa_0 = \left(\frac{\gamma^2 \mu_{23}}{1-\gamma^2\mu_{23}}\right)^{1/2}, \quad \mu_{23} = \frac{m_2 m_3}{m_2 + m_3}. \tag{B.2.10}$$

Proof. Direct computations show

$$\begin{aligned} q^2 + \xi^2 &= \frac{1}{M_{23}}(m_3 x_2^2 + m_2 x_3^2 - 2\sqrt{m_2 m_3} x_2 x_3) + \frac{1}{M_{23}}(m_2 x_2^2 + m_3 x_3^2 + 2\sqrt{m_2 m_3} x_2 x_3) \\ &= x_2^2 + x_3^2 . \end{aligned}$$

Consequently, (B.2.8) holds.
The set $\partial K_{23}(\gamma)$ is determined by

$$\left|\frac{x_2}{\sqrt{m_2}} - \frac{x_3}{\sqrt{m_3}}\right| = \gamma |x| . \tag{B.2.11}$$

Expressing x_2 and x_3 in (q, ξ)–varibales gives

$$x_2 = \left(\frac{m_2}{M_{23}}\right)^{1/2}\left(\xi + \left(\frac{m_3}{m_2}\right)^{1/2} q\right), \quad x_3 = \left(\frac{m_3}{M_{23}}\right)^{1/2}\left(\xi - \left(\frac{m_2}{m_3}\right)^{1/2} q\right). \tag{B.2.12}$$

Inserting (B.2.12) into (B.2.11) gives

$$\left|\frac{x_2}{\sqrt{m_2}} - \frac{x_3}{\sqrt{m_3}}\right| = (\mu_{23})^{-1/2}|q|, \tag{B.2.13}$$

for μ_{23} in (B.2.10).
Combining (B.2.11) and (B.2.13) shows that the surface $\partial K_{23}(\gamma)$ is determined by the relation

$$|q| = (\mu_{23})^{1/2}\gamma |(x_1, q, \xi)| . \tag{B.2.14}$$

Solving (B.2.14) for $|q|$ yields

$$|q| = \kappa_0 |(x_1, \xi)| \quad \text{where} \quad \kappa_0 = \left(\frac{\gamma^2\mu_{23}}{1-\gamma^2\mu_{23}}\right)^{1/2}. \tag{B.2.15}$$

Using (B.2.15) as parametrization of the surface $\partial K_{23}(\gamma)$ the relation for the surface element $d\sigma$ of $\partial K_{23}(\gamma)$ in (B.2.9) follows from direct computations. ∎

B.3 Estimate used in Lemma 5.4.3

Lemma B.3.1. *Let $\xi \in C^\infty([0,\infty))$ with $\xi(t) = 0$ for $t \le 1$ and $\xi(t) = 1$ for $t \ge 2$, such that $\xi(t) \le 1$ and $\xi'(t) \le 2$ for any $t \in [0,\infty)$. For any $\omega, \kappa, \beta > 0$ we define*

$$G(|x|) := \frac{|x|^\kappa}{1+\omega|x|^\kappa}\xi(|x|/\beta)\,.$$

Then

$$|\nabla G(x)| \le \kappa|x|^{-1}G(x), \textit{ for } |x| > 2\beta$$

and for

$$|\nabla G(x)| \le \beta^{\kappa-1}\left(2^{\kappa+1} + \kappa 2^{\kappa-1}\right), \ \textit{ for } |x| \in [\beta, 2\beta].$$

Proof. By construction

$$\xi\left(\frac{|x|}{\beta}\right) \equiv 1$$

for $|x| \ge 2\beta$ and consequently

$$|(\nabla G)(x)| = \left|\nabla\left(\frac{|x|^\kappa}{1+\omega|x|^\kappa}\right)\right| = \frac{\kappa|x|^{\kappa-1}}{(1+\omega|x|^\kappa)^2} \le \kappa|x|^{-1}G(x)\,.$$

For $|x| \in [\beta, 2\beta]$

$$\xi\left(\frac{|x|}{\beta}\right) \le 2,$$

then for $|x| \in [\beta, 2\beta]$

$$\begin{aligned}|(\nabla G)(x)| &\le \frac{2}{\beta}\frac{|x|^\kappa}{1+\omega|x|^\kappa} + \left|\nabla\left(\frac{|x|^\kappa}{1+\omega|x|^\kappa}\right)\right| \\ &\le 2^{\kappa+1}\beta^{\kappa-1} + \kappa 2^{\kappa-1}\beta^{\kappa-1} \\ &= \beta^{\kappa-1}\left(2^{\kappa+1} + \kappa 2^{\kappa-1}\right)\,.\end{aligned}$$

∎

B.4 Proof of Lemma 6.2 of [13]

Lemma B.4.1. *Let $h = -\partial_q^2 + V(q)$ on $L^2(\mathbb{R})$, such that $h \ge 0$. Assume that for every $\varepsilon > 0$ there exists a constant $C(\varepsilon) > 0$, such that*

$$\int_{\mathbb{R}} |V(q)||\psi(q)|^2 dq \le \varepsilon \int_{\mathbb{R}} |\psi'(q)|^2 dq + C(\varepsilon)\int_{\mathbb{R}} |\psi(q)|^2 dq \quad \forall \psi \in H^1(\mathbb{R})\,.$$

Assume there are constants $\tilde{C}, A, \delta > 0$ *such that*

$$|V(q)| \leq \tilde{C}|q|^{-2-\delta} \tag{B.4.1}$$

for any $q \in \mathbb{R}$ *with* $|q| > A$. *Then there exists a constant* $C > 0$, *such that for any* $L > 0$ *and any function* $\psi \in H^1(\mathbb{R})$

$$\mathcal{J}(\psi, L) := \int_{-L}^{L} \left(|\psi'(q)|^2 + V(q)|\psi(q)|^2\right) dq \geq -CL^{-1-\delta}\left(|\psi(L)|^2 + |\psi(-L)|^2\right) .$$

Proof. Let $L > A$, for $s > 0$ we define for $|q| \leq L + 2$

$$\psi_s(q) := \begin{cases} \psi(L)\frac{(L+s)-q}{s} & q \in (L, (L+s)) \\ \psi(q) & q \in [-L, L] \\ \psi(-L)\frac{(L+s)+q}{s} & q \in (-(L+s), -L) \end{cases}$$

and $\psi_s(q) = 0$ for $|q| > L + s$. Then $\psi_s \in H^1(\mathbb{R})$. By construction $\mathcal{J}(\psi, L) = \mathcal{J}(\psi_s, L)$ and since $h \geq 0$

$$\begin{aligned} \mathcal{J}(\psi, L) \geq &- \int_{L}^{\infty} \left(\left|\psi_s'(q)\right|^2 + |V(q)||\psi_s(q)|^2\right) dq \\ &- \int_{-\infty}^{-L} \left(\left|\psi_s'(q)\right|^2 + |V(q)||\psi_s(q)|^2\right) dq \,. \end{aligned} \tag{B.4.2}$$

We estimate the first integral on the right–hand side of (B.4.2). Using that ψ' and ψ are supported on $\{q \in \mathbb{R}, |q| \leq L + s\}$ yields

$$\begin{aligned} &\int_{L}^{\infty} \left(\left|\psi_s'(q)\right|^2 + |V(q)||\psi_s(q)|^2\right) dq \\ &\quad = \int_{L}^{L+s} \left|\psi_s'(q)\right|^2 dq + \int_{L}^{L+s} |V(q)||\psi_s(q)|^2 dq \,. \end{aligned} \tag{B.4.3}$$

The first term on the right–hand side of (B.4.3) vanishes in the limit $s \to \infty$ and for the second term we find

$$\int_{L}^{L+s} |V(q)||\psi_s(q)|^2 dq \leq |\psi(L)|^2 \int_{L}^{L+s} |V(q)| dq \,. \tag{B.4.4}$$

Applying (B.4.1) and solving the remaining integral on the right–hand side of (B.4.4) we find there exists a constant $C > 0$ depending on $\delta > 0$ but independent of L and s such that

$$\int_{L}^{L+s} |V(q)||\psi_s(q)|^2 dq \leq \frac{C}{L^{1+\delta}} |\psi(L)|^2 \,. \tag{B.4.5}$$

Using the same Arguments for the Integral over $(-\infty, -L]$ in (B.4.2) proves the statement in the limit $s \to \infty$. ∎

Appendix C

C.1 Partition Functions

The following estimate is a version of a result that was first shown in [120][Lemma 5.1] and used in several other papers.

Lemma C.1.1 (= Lemma 6.2.5)**.** *For any $\varepsilon, b > 0$ there exist $0 < a < b$ and continuous functions $u, v : \mathbb{R} \to [0,1]$ with piecewise continuous derivatives, such that $u^2 + v^2 = 1$,*

$$v(x) = \begin{cases} 1, & |x| \geq b \\ 0, & |x| \leq a \end{cases}, \quad u(x) = \begin{cases} 1, & |x| \leq a \\ 0, & |x| \geq b \end{cases}, \tag{C.1.1}$$

and

$$|u'(x)|^2 + |v'(x)|^2 \leq \frac{\varepsilon}{|x|^2} \mathbb{1}_{\{a \leq |x| \leq b\}}. \tag{C.1.2}$$

Moreover, a can be chosen such that

$$e^{-(1+2/\varepsilon)} \leq \frac{a}{b} \leq e^{-2/\varepsilon}. \tag{C.1.3}$$

Proof. Given $0 \leq v \leq 1$ we have $u = (1 - v^2)^{1/2}$. In particular, $u' = -(1 - v^2)^{-1/2} v v'$ and

$$u'^2 + v'^2 = \frac{v'^2}{1 - v^2} = \frac{v'^2}{(1 + v)(1 - v)} \leq \frac{v'^2}{1 - v}. \tag{C.1.4}$$

The denominator becomes zero when v approaches 1, i.e., in the limit $t \to 1-$, which must be compensated by a fast enough decay of the derivative of v as $t \to 1-$.
We make the ansatz $v(t) = 1$ for $t > 1$ and

$$v(t) = \left(1 - \varepsilon \int_t^1 (1 - s) \frac{ds}{s}\right)_+ \tag{C.1.5}$$

for $0 \leq t \leq 1$. Then $0 \leq v \leq 1$, is piecewise continuously differentiable and $v(t) = 0$ for $0 \leq t \leq a$, where a is determined by

$$\int_a^1 (1 - s) \frac{ds}{s} = \frac{1}{\varepsilon}. \tag{C.1.6}$$

Clearly, $v'(t) = \varepsilon(1-t)/t$ for $a < t < 1$ and $v'(t) = 0$ for $0 < t < a$ or $t > 1$. Thus

$$\frac{v'(t)^2}{1-v(t)} \le \frac{C\varepsilon}{t^2}\mathbb{1}_{\{a<t<1\}} \tag{C.1.7}$$

with

$$C = \sup_{0<t<1} \frac{(1-t)^2}{\int_t^1 (1-s)\,\frac{ds}{s}}\,. \tag{C.1.8}$$

Note that

$$\int_t^1 (1-s)\,\frac{ds}{s} = \int_t^1 (1-s)\big(\frac{1}{s}-1+1\big)\,ds = \int_t^1 (1-s)\big)\,ds + \int_t^1 (1-s)^2\,\frac{ds}{s} \tag{C.1.9}$$

$$= \frac{1}{2}(1-t)^2 + h(t)\,. \tag{C.1.10}$$

with $h(t) = \int_t^1 (1-s)^2\,\frac{ds}{s} \ge 0$ for $0 < t \le 1$. This immediately implies $C \le 2$. Moreover, since

$$0 \le \frac{1}{(1-t)^2}h(t) = \int_t^1 \frac{(1-s)^2}{(1-t)^2}\,\frac{ds}{s} \le \int_t^1 \frac{ds}{s} \to 0 \quad \text{as } t \to 0 \tag{C.1.11}$$

one sees that

$$C = \sup_{0<t<1} \frac{(1-t)^2}{\int_t^1 (1-s)\,\frac{ds}{s}} = \sup_{0<t<1} \frac{2}{1+\frac{2}{(1-t)^2}h(t)} = \lim_{t\to 1-} \frac{2}{1+\frac{2}{(1-t)^2}h(t)} = 2\,. \tag{C.1.12}$$

To get a bound on $0 < a < 1$, recall that it is determined by

$$\ln\Big(a^{-1}\Big) - (1-a) = \int_a^1 (1-s)\frac{ds}{s} = \varepsilon^{-1}\,. \tag{C.1.13}$$

Hence we have

$$\ln\Big(a^{-1}\Big) - 1 < \varepsilon^{-1} < \ln\Big(a^{-1}\Big) \tag{C.1.14}$$

from which $e^{-(1+1/\varepsilon)} \le a \le e^{-1/\varepsilon}$ follows. Replacing ε by $\varepsilon/2$ proves the Lemma for $b = 1$. For general $b > 0$, on scales the functions u and v by replacing them with $u(t/b)$ and $v(t/b)$. ∎

C.2 Remarks on the Geometry of the Sets $\mathcal{K}_\alpha(\gamma)$

The fact that the conical sets $\mathcal{K}_\alpha(\gamma)$, $\alpha \in I$ do not overlap outside of $\{x \in R_0 : |x| > b\}$ for $\gamma > 0$ small enough is well known and goes back to the work of M. A. Antonets, G. M. Zhislin, and I. A. Shereshevsky (see appendix of the Russian edition of [56]). We prove the following

Lemma C.2.1. *Let* $\alpha, \beta \in \{(12), (13), (23)\}$ *then there exits some* $\gamma_0 > 0$ *depending on the masses only such that for any* $\gamma < \gamma_0$ *and* $\alpha \neq \beta$

$$\mathcal{K}_\alpha(\gamma) \cap \mathcal{K}_\beta(\gamma) = \{0\} \,. \tag{C.2.1}$$

Proof. In the following, we denote by $\lesssim$ that the inequality holds up to a constant, possibly depending on $m_1, m_2, m_3 > 0$. It suffices to prove the statement for $\alpha = (12)$ and $\beta = (13)$. Since $x \in R_0$ and $m_1, m_2, m_3 > 0$, the points x_1, x_2, x_3 span a triangle such that the origin (the center of mass) is within the area of this triangle and consequently

$$\sum_{i=1}^{3} |x_i| \leq \sum_{(ij)\in I} \left| x_i - x_j \right| . \tag{C.2.2}$$

Due to the equivalence of norms in $\mathbb{R}^n$, it is

$$|x| = \left(\sum_{i=1}^{3} |x_i|^2 \right)^{1/2} \lesssim \sum_{(ij)\in I} \left| x_i - x_j \right| .$$

Assume now that $x \in \mathcal{K}_{12}(\gamma) \cap \mathcal{K}_{13}(\gamma)$ then by the definition of the sets $\mathcal{K}_\alpha(\gamma)$, $\alpha \in I$ and the triangle inequality

$$|x_2 - x_3| \leq (|x_1 - x_2| + |x_1 - x_3|) \lesssim \gamma(|\xi_{13}| + |\xi_{12}|) \,. \tag{C.2.3}$$

Combining (C.2.2) and (C.2.3) together with the definition of the sets $\mathcal{K}_\alpha(\gamma)$, $\alpha \in I$ we arrive at

$$|x|^2 \lesssim \gamma^2 \sum_{\alpha\in I} |\xi_\alpha|^2 \,. \tag{C.2.4}$$

Recall that by construction for any $\alpha \in I$

$$\sum_{i=1}^{3} m_i |x_i|^2 = |q_\alpha|^2 + |\xi_\alpha|^2, \quad \alpha \in I \,. \tag{C.2.5}$$

Using (C.2.5) we conclude from (C.2.4) that

$$|x|^2 \lesssim \gamma^2 |x|^2 \tag{C.2.6}$$

which only holds for $x = 0$ for $\gamma > 0$ small enough and consequently proves the statement of Lemma C.2.1. ∎

Appendix D

D.1 Existence of Resonance Solutions

We aim to prove Theorem 1.4.11. Before we give the proof, we state the following

Lemma D.1.1. *Let $A \subset \mathbb{R}^d$ with $|A| < \infty$, then the embedding $\dot{H}^1(A) \hookrightarrow L^p(A)$ is compact for all $1 \leq p < \frac{2d}{d-2}$.*

Proof. For instance, a proof for this can be found in [74, Theorem 8.6]. ∎

Recall, that for a positive potential V the form domain $Q(V)$ is the space of all functions $f \in L^2(\mathbb{R}^d)$ for which $\langle f, Vf\rangle = \|V^{1/2}f\|^2 < \infty$. Similarly we define $\dot{Q}(V)$ as the space of all functions $\psi \in \dot{H}^1(\mathbb{R}^d)$ for which $\langle \psi, V\psi\rangle < \infty$.

Theorem D.1.2 (= Theorem 1.4.11)**.** *Let $d \geq 3$, consider the potential $V : \mathbb{R}^d \to \mathbb{R}$ and define $V_+ = \max(0, V)$ and $V_- = \min(0, V)$. Suppose that the operator $H = P^2/2 + V$ (considered as quadratic form) has a virtual level at zero. Assume the following conditions:*

a) *$V_+ \in L^1_{\text{loc}}(\mathbb{R}^d)$,*
b) *V_- is infinitesimally form-bounded w.r.t. P^2,*
c) *There exists $\theta > 0$ such that the weighted potential $\widetilde{V}_- := (1 + |\cdot|)^{2+2\theta} V_-$ is form bounded w.r.t. P^2.*

Then there exists a non–vanishing function $\varphi_0 \in \dot{H}^1(\mathbb{R}^d) \cap \dot{Q}(V_+)$ satisfying

$$\frac{1}{2}\langle P\psi, P\varphi_0\rangle + \langle \psi, V\varphi_0\rangle = 0, \quad \forall \psi \in \dot{H}^1(\mathbb{R}^d) \cap \dot{Q}(V_+). \tag{D.1.1}$$

In particular,

$$\frac{1}{2}\langle P\varphi_0, P\varphi_0\rangle + \langle \varphi_0, V\varphi_0\rangle = 0\,. \tag{D.1.2}$$

We first state Lemmas D.1.3 and D.1.5 below, and prove Theorem D.1.2 with the help of the two lemmas. The proof of the Lemmas is given in Sections D.1.1 and D.1.2.

Lemma D.1.3. *Let $d \geq 3$. For some $\theta > 0$ define $\widetilde{\psi} = (1 + |\cdot|)^{-1-\theta}\psi$ for $\psi \in H^1(\mathbb{R}^d)$. Then we have $\widetilde{\psi} \in L^2(\mathbb{R}^d)$ and there exists a constant $C < \infty$ independent of ψ such that $\|P\widetilde{\psi}\| \leq C\|P\psi\|$.*
Moreover, if ψ has support in $B_R(0)^c = \{|x| \geq R\}$ for some $R > 0$, then $\|P\widetilde{\psi}\| \leq C(1 + R)^{-1-\theta}\|P\psi\|$ and $\|\widetilde{\psi}\| \leq (1 + R)^{-\theta}\|P\psi\|$.

Remark D.1.4. *Note that for wave function ψ we define the weighted function $\widetilde{\psi}$ different from the weighted potential $\widetilde{V} = (1 + |\cdot|)^{2+2\theta} V$. This is done to ensure, at least formally, $\langle \psi, V\psi \rangle = \langle \widetilde{\psi}, \widetilde{V}\widetilde{\psi} \rangle$. For notational convenience, we suppress the dependence of $\widetilde{\psi}$ and $\widetilde{V}$ on the parameter $\theta > 0$.*

Lemma D.1.5. *Let $d \geq 3$. For any sequence $(\psi_n)_{n\in\mathbb{N}} \subset \dot{H}^1(\mathbb{R}^d)$, which is normalized in the sense that $\|P\psi_n\| = 1$, and converges weakly to φ_0 in $\dot{H}^1(\mathbb{R}^d)$ we have*

a) $\langle \varphi_0, V_-\varphi_0 \rangle < \infty$,
b) $\lim\limits_{n\to\infty} \langle \psi_n, V_-\psi_n \rangle = \langle \varphi_0, V_-\varphi_0 \rangle$,
c) $\limsup_{n\to\infty} \langle \psi_n, V_-\psi_n \rangle \leq \langle \varphi_0, V_-\varphi_0 \rangle - 1$,
d) $\langle \varphi_0, V_+\varphi_0 \rangle \leq \liminf_{n\to\infty} \langle \psi_n, V_+\psi_n \rangle$.

Proof of Theorem D.1.2. Let $(\delta_n)_{n\in\mathbb{N}} \subset (0,1)$ be a sequence satisfying $\delta_n \downarrow 0$ as $n \to \infty$. Since H has a virtual level at zero, the perturbed operator

$$H_n := \frac{1-\delta_n}{2} P^2 + V$$

has a negative ground state energy $E_n < 0$ for all $n \in \mathbb{N}$.
For each fixed $n \in \mathbb{N}$, let $\psi_n \in H^1$ be the ground state of H_n corresponding to the ground state energy $E_n < 0$. Then, as $n \to \infty$, we have $E_n \uparrow 0$, hence

$$\frac{1-\delta_n}{2} \|P\psi_n\|^2 + \langle \psi_n, V_+\psi_n \rangle - \langle \psi_n, V_-\psi_n \rangle < E_n \|\psi_n\|^2 < 0.$$

for all $n \in \mathbb{N}$.
We normalize $\psi_n \in H^1$ by $\|\psi_n\|_{\dot{H}^1} = \|P\psi_n\| = 1$ for all $n \in \mathbb{N}$. Under this normalization, we obtain

$$\frac{1-\delta_n}{2} + \langle \psi_n, V_+\psi_n \rangle - \langle \psi_n, V_-\psi_n \rangle < 0 \tag{D.1.3}$$

for all $n \in \mathbb{N}$.
Since the sequence $(\psi_n)_{n\in\mathbb{N}} \subset \dot{H}^1(\mathbb{R}^d)$ is bounded, there exists a weakly convergent subsequence with weak limit $\varphi_0 \in \dot{H}^1(\mathbb{R}^d)$. We denote this subsequence also by $(\psi_n)_{n\in\mathbb{N}}$. Taking a further subsequence, if necessary, we can also assume that $(\psi_n)_{n\in\mathbb{N}}$ also converges pointwise almost everywhere. Using statements (a) and (b) of Lemma D.1.5 together with (D.1.3), we obtain

$$\frac{1}{2} + \liminf_{n\to\infty} \langle \psi_n, V_+\psi_n \rangle - \langle \varphi_0, V_-\varphi_0 \rangle \leq 0.$$

Using statement (d) of Lemma D.1.5 yields

$$\|P\varphi_0\|^2 + \langle \varphi_0, V\varphi_0 \rangle \leq \frac{1}{2} + \liminf_{n\to\infty} \langle \psi_n, V_+\psi_n \rangle - \langle \varphi_0, V_+\varphi_0 \rangle \leq 0. \tag{D.1.4}$$

To complete the proof, we must show that

$$\frac{1}{2}\|P\varphi_0\|^2 + \langle \varphi_0, V\varphi_0 \rangle \geq 0. \tag{D.1.5}$$

We now prove (D.1.5). Let $\eta \in C_0^\infty(\mathbb{R})$ such that $\eta(t) = 1$ for $t \le 1$, $\eta(t) = 0$ for $t \ge 2$, and $\|\partial_t \eta\|_\infty \le 2$. For a fixed $T > 0$, define $\xi_T : \mathbb{R}^d \to \mathbb{R}$ as

$$\xi_T(x) := \eta\left(\frac{|x|}{T}\right).$$

Then $\xi_T \varphi_0 \in H^1(\mathbb{R}^d)$. Since the operator $H = P^2 + V$ is self-adjoint and non-negative, we have

$$\frac{1}{2}\|P(\xi_T\varphi_0)\|^2 + \langle \xi_T\varphi_0, V\xi_T\varphi_0\rangle \ge 0. \tag{D.1.6}$$

Let $T_n = 2^n$ for all $n \in \mathbb{N}$, so that $T_n \to \infty$ as $n \to \infty$. Define $\xi_n := \xi_{T_n}$. Note that $\xi_n\varphi_0 \in L^2(\mathbb{R}^d)$. By the monotone convergence theorem, we then have

$$\lim_{n\to\infty} \langle \xi_n\varphi_0, V_\pm \xi_n\varphi_0\rangle = \langle \varphi_0, V_\pm\varphi_0\rangle.$$

It remains to show that $P(\xi_n\varphi_0)$ converges to $P\varphi_0$ in $L^2(\mathbb{R}^d)$. Note, that

$$P(\xi_n\varphi_0) = (P\xi_n)\varphi_0 + \xi_n P\varphi_0\,.$$

By the monotone convergence theorem, we have $\xi_n P\varphi_0 \to P\varphi_0$ in $L^2(\mathbb{R}^d)$. Thus, it suffices to show that $(P\xi_n)\varphi_0 \to 0$ in $L^2(\mathbb{R}^d)$. We compute

$$|P\xi_n|^2 \le 4T_n^{-2}\mathbb{1}_{\{T_n\le|x|\le 2T_n\}} \le |x|^{-2}\mathbb{1}_{\{T_n\le|x|\le 2T_n\}},$$

and by Hardy's inequality, we obtain

$$\begin{aligned}\sum_{n=0}^{\infty}\|(P\xi_n)\varphi_0\|^2 &\le \sum_{n=0}^{\infty}\langle\varphi_0, |x|^{-2}\mathbb{1}_{\{T_n\le|x|\le 2T_n\}}\varphi_0\rangle \\ &\le \langle \varphi_0, |x|^{-2}\varphi_0\rangle \lesssim \|P\varphi_0\|^2 \le 1.\end{aligned}$$

Since the series converges, we have $\|(P\xi_n)\varphi_0\| \to 0$ as $n \to \infty$. Taking the limit of (D.1.6) as $n \to \infty$, we conclude

$$\frac{1}{2}\|P\varphi_0\|^2 + \langle\varphi_0, V\varphi_0\rangle \ge 0.$$

Combining (D.1.5) and (D.1.4), we find

$$\langle \varphi_0, H\varphi_0\rangle = \frac{1}{2}\|P\varphi_0\|^2 + \langle\varphi_0, V\varphi_0\rangle = 0.$$

This shows that φ_0 is the minimizer of the associated Lagrange problem, thus completing the proof. We make this explicit below.
Let q_H be the quadratic form of the operator $H = \frac{1}{2}P^2 + V$, where V satisfies the conditions of Theorem D.1.2. For any $f \in \dot{H}^1(\mathbb{R}^d) \cap \dot{Q}(V_+)$ an explicit calculation shows that

$$q_H(\varphi_0 + tf, \varphi_0 + tf)$$

is a second order polynomial in $t \in \mathbb{R}$. Moreover, as just shown, $q_H(\varphi_0 + tf, \varphi_0 + tf) \geq 0$ for all $t \in \mathbb{R}$ and $q_H(\varphi_0, \varphi_0) = 0$. So, the polynomial has a minimum at $t = 0$. Thus, by an explicit calculation,

$$0 = \frac{d}{dt} q_H(\varphi_0 + tf, \varphi_0 + tf)\Big|_{t=0} = 2\,\mathrm{Re}\, q_H(\varphi_0, f).$$

By replacing f with if, we obtain $0 = \mathrm{Re}\, iq_H(\varphi_0, f) = \mathrm{Im}\, q_H(\varphi_0, f)$, which shows that $q_H(\varphi_0, f) = 0$ for all $f \in \dot{H}^1(\mathbb{R}^d) \cap \dot{Q}(V_+)$. Hence also $q_H(f, \varphi_0) = \overline{q_H(\varphi_0), f)} = 0$. ∎

D.1.1 Existence of Resonance Solutions Part II

Proof of Lemma D.1.3. By construction and Hardy's inequality, we have $\widetilde{\varphi}_0 \in L^2(\mathbb{R}^d)$.
By a direct computation, we have

$$\nabla\widetilde{\psi}(x) = -(1+\theta)(1+|x|)^{-2-\theta}\frac{x}{|x|}\psi(x) + (1+|x|)^{-1-\theta}\nabla\psi(x)\,.$$

Hence,

$$\begin{aligned}\|P\widetilde{\psi}\|^2 &= \langle\nabla\psi, (1+|x|)^{-2-2\theta}\nabla\psi\rangle + (1+\theta)^2\langle\psi, (1+|x|)^{-4-2\theta}\psi\rangle \\ &\quad - (1+\theta)\,\mathrm{Re}(\langle\nabla\psi, (1+|x|)^{-3-2\theta}\frac{x}{|x|}\psi\rangle)\,.\end{aligned}$$

Integrating by parts, one has

$$\begin{aligned}&\langle\nabla\psi, (1+|x|)^{-3-2\theta}\frac{x}{|x|}\psi\rangle = -\langle\psi, \nabla((1+|x|)^{-3-2\theta}\frac{x}{|x|}\psi)\rangle \\ &= (3+2\theta)\langle\psi, (1+|x|)^{-4-2\theta}\psi\rangle - \langle\psi, (1+|x|)^{-3-2\theta}\frac{d-1}{|x|}\psi\rangle - \langle\psi, (1+|x|)^{-3-2\theta}\frac{x}{|x|}\nabla\psi\rangle\end{aligned}$$

Thus,

$$2\,\mathrm{Re}(\langle\nabla\psi, (1+|x|)^{-3-2\theta}\frac{x}{|x|}\psi\rangle) = (3+2\theta)\langle\psi, (1+|x|)^{-4-2\theta}\psi\rangle - \langle\psi, (1+|x|)^{-3-2\theta}\frac{d-1}{|x|}\psi\rangle$$

which yields

$$\begin{aligned}\|P\widetilde{\psi}\|^2 &= \langle\nabla\psi, (1+|x|)^{-2-2\theta}\nabla\psi\rangle + (1+\theta)(d-1)\langle\psi, (1+|x|)^{-3-2\theta}|x|^{-1}\psi\rangle \\ &\quad - (1+\theta)(2+3\theta)\langle\psi, (1+|x|)^{-4-2\theta}\psi\rangle) \\ &\leq \langle\nabla\psi, (1+|x|)^{-2-2\theta}\nabla\psi\rangle + (1+\theta)(d-1)\langle\psi, (1+|x|)^{-2-2\theta}|x|^{-2}\psi\rangle\,. \end{aligned} \tag{D.1.7}$$

Using Hardy's inequality, we obtain

$$\langle\psi, (1+|x|)^{-2-2\theta}|x|^{-2}\psi\rangle \lesssim \|P\psi\|^2\,,$$

moreover, if $\operatorname{supp}(\psi) \subset B_R(0)^c$, we have

$$\langle \psi, (1+|x|)^{-2-2\theta}|x|^{-2}\psi \rangle \leq (1+R)^{-2-2\theta}\langle \psi, |x|^{-2}\psi \rangle \lesssim (1+R)^{-2-2\theta}\|P\psi\|^2 .$$

Together with (D.1.7) this proves the second and third claim of the lemma.
The last claim follows from

$$\left\|\widetilde{\psi}\right\| \leq (1+R)^{-\theta}\left\|(1+|\cdot|)^{-2}\psi\right\| \lesssim (1+R)^{-\theta}\|P\psi\| .$$

∎

D.1.2 Existence of Resonance Solutions Part III

Proof of Lemma D.1.5. Claim (c) follows immediately from the second claim and the bound (D.1.3).
We begin by proving *statement (a)*. Define

$$\widetilde{\varphi}_0 \coloneqq (1+|x|)^{-1-\theta}\varphi_0.$$

By assumption, the potential $\widetilde{V}_-$ is form bounded with respect to P^2. Consequently, there exist constants $a, b > 0$ such that

$$\langle \varphi_0, V_-\varphi_0 \rangle = \langle \widetilde{\varphi}_0, \widetilde{V}_-\widetilde{\varphi}_0 \rangle \leq a\|P\widetilde{\varphi}_0\|^2 + b\|\widetilde{\varphi}_0\|^2.$$

By Lemma D.1.3 we have $\widetilde{\varphi}_0 \in L^2(\mathbb{R}^d)$ and also $\|P\widetilde{\varphi}_0\|^2 < \infty$. This completes the proof of statement (a).

We proceed by proving *statement (b)*. Let $R > 0$ be given, and choose $\{\chi_1, \chi_2\}$ to be a quadratic partition of unity such that $\operatorname{supp}(\chi_1) \subset \{x \in \mathbb{R}^d : |x| \leq 2R\}$ and $\operatorname{supp}(\chi_2) \subset \{x \in \mathbb{R}^d : |x| \geq R\}$. Then, since $\chi_1^2 + \chi_2^2 = 1$ we can write

$$\langle \varphi_0, V_-\varphi_0 \rangle = \langle \varphi_0\chi_1, V_-\varphi_0\chi_1 \rangle + \langle \varphi_0\chi_2, V_-\varphi_0\chi_2 \rangle, \tag{D.1.8}$$

which splits the expression into two terms.
Next, we estimate each term on the right-hand side of (D.1.8) separately. We begin with the term involving χ_1. For all $n \in \mathbb{N}$, we have the following decomposition:

$$\begin{aligned}\langle \varphi_0\chi_1, V_-\varphi_0\chi_1 \rangle = {} & \langle \varphi_0\chi_1, V_-(\varphi_0 - \psi_n)\chi_1 \rangle \\ & + \langle (\varphi_0 - \psi_n)\chi_1, V_-\psi_n\chi_1 \rangle + \langle \psi_n\chi_1, V_-\psi_n\chi_1 \rangle.\end{aligned}$$

Let $I_1 \coloneqq \langle \varphi_0\chi_1, V_-(\varphi_0 - \psi_n)\chi_1 \rangle$ and $I_2 \coloneqq \langle (\varphi_0 - \psi_n)\chi_1, V_-\psi_n\chi_1 \rangle$. We now aim to show

$$\lim_{n\to\infty} \langle \psi_n\chi_1, V_-\psi_n\chi_1 \rangle = \langle \varphi_0\chi_1, V_-\varphi_0\chi_1 \rangle, \tag{D.1.9}$$

by proving that both I_1 and I_2 tend to zero as $n \to \infty$. We begin by estimating I_1. Using Hölder's inequality we find

$$|I_1|^2 \le \|V_-^{1/2}\chi_1\varphi_0\|^2\|V_-^{1/2}\chi_1(\varphi_0 - \psi_n)\|^2. \tag{D.1.10}$$

By assumption, V_- is infinitesimally form bounded. Therefore, for any $\varepsilon > 0$, there exists $C_\varepsilon > 0$ such that

$$\|V_-^{1/2}\chi_1\varphi_0\|^2 \le \varepsilon\|P(\chi_1\varphi_0)\|^2 + C_\varepsilon\|\chi_1\varphi_0\|^2. \tag{D.1.11}$$

Since $\varphi_0 \in \dot{H}^1(\mathbb{R}^d)$, it follows that $\varphi_0 \in L^2_{\text{loc}}$, and consequently, $\|\chi_1\varphi_0\|^2 < \infty$. To estimate the first term on the right-hand side of (D.1.11), we note that

$$\|P(\chi_1\varphi_0)\|^2 \le 2\|P\varphi_0\|^2 + 2\|(\nabla\chi_1)\varphi_0\|$$

which is finite because $\varphi_0 \in \dot{H}^1(\mathbb{R}^d)$. Therefore, we have shown

$$\|V_-^{1/2}\chi_1\varphi_0\|^2 < \infty. \tag{D.1.12}$$

Next, to conclude that $I_1 \to 0$ as $n \to \infty$, we show that for any $\varepsilon > 0$, there exists $C > 0$ independent of ε such that

$$\lim_{n\to\infty} \|V_-^{1/2}\chi_1(\varphi_0 - \psi_n)\|^2 < C\varepsilon. \tag{D.1.13}$$

Since V_- is infinitesimally form bounded with respect to P^2, for any $\varepsilon > 0$, there exists $C_\varepsilon > 0$ such that

$$\|V_-^{1/2}\chi_1(\varphi_0 - \psi_n)\|^2 \le \varepsilon\|P(\varphi_0 - \psi_n)\|^2 + C_\varepsilon\|(\chi_1)(\varphi_0 - \psi_n)\|^2.$$

A short calculation shows that

$$\|P(\varphi_0 - \psi_n)\|^2 \le 4\|P\varphi_0\|^2 + 4\|P\psi_n\|^2 \le 8,$$

and since $\text{supp}(\chi_1) \subset \{x \in \mathbb{R}^d : |x| \le 2R\}$, we can apply Lemma D.1.1 to find

$$\lim_{n\to\infty} \|\chi_1(\varphi_0 - \psi_n)\|^2 = 0.$$

Thus, we have shown that (D.1.13) holds. Summarizing, we obtain $|I_1| \le C\varepsilon$ as $n \to \infty$ for some $C > 0$ independent of n and ε. Taking the limit $\varepsilon \to 0$, we conclude that $|I_1| \to 0$ as $n \to \infty$. Similar estimates show that $|I_2| \to 0$ as $n \to \infty$, and consequently, (D.1.9) holds. Next, we show that

$$\lim_{n\to\infty} \langle\psi_n\chi_2, V_-\psi_n\chi_2\rangle = \langle\varphi_0\chi_2, V_-\varphi_0\chi_2\rangle. \tag{D.1.14}$$

Note that

$$\begin{aligned}\langle\varphi_0\chi_2, V_-\varphi_0\chi_2\rangle =& \langle\varphi_0\chi_2, V_-\left(\varphi_0 - \psi_n\right)\chi_2\rangle + \langle\left(\varphi_0 - \psi_n\right)\chi_2, V_-\psi_n\chi_2\rangle \\ &+ \langle\psi_n\chi_2, V_-\psi_n\chi_2\rangle.\end{aligned}$$

Let $J_1 \coloneqq \langle \varphi_0 \chi_2, V_- (\varphi_0 - \psi_n) \chi_2 \rangle$ and $J_2 \coloneqq \langle (\varphi_0 - \psi_n) \chi_2, V_- \psi_n \chi_2 \rangle$. Recall that $\mathrm{supp}(\chi_2) \subset \{x \in \mathbb{R}^d : |x| \geq R\}$. We will show that both J_1 and J_2 vanish uniformly in n as $R \to \infty$. Recall $\tilde{f} = (1 + |\cdot|)^{-1-\theta} f$ for any mapping f, and $\widetilde{V}_- \coloneqq (1 + |\cdot|)^{2+2\theta} V_-$. Then

$$|J_2|^2 = |\langle (\widetilde{\varphi}_0 - \widetilde{\psi}_n)\chi_2, \widetilde{V}_- \widetilde{\psi}_n \chi_2 \rangle|^2 \leq \|\widetilde{V}_-^{1/2} \widetilde{\psi}_n \chi_2\|^2 \|\widetilde{V}_-^{1/2} (\widetilde{\varphi}_0 - \widetilde{\psi}_n)\chi_2\|^2. \tag{D.1.15}$$

We begin by estimating the first factor on the right-hand side of (D.1.15). Since $\widetilde{V}_-$ is form-bounded with respect to P^2, there exist constants $a, b > 0$ such that

$$\|\widetilde{V}_-^{1/2} \widetilde{\psi}_n \chi_2\|^2 \leq a \|P(\widetilde{\psi}_n \chi_2)\|^2 + b \|\widetilde{\psi}_n \chi_2\|^2. \tag{D.1.16}$$

Using the fact that $\|P\psi_n\| = 1$ for all $n \in \mathbb{N}$, and that $\mathrm{supp}(\chi_2) \subset \{x \in \mathbb{R}^d : |x| \geq R\}$, we obtain from Lemma D.1.3

$$\|\widetilde{\psi}_n \chi_2\| \leq (1 + R)^{-\theta} \|P\psi_n\| \leq (1 + R)^{-\theta}. \tag{D.1.17}$$

Similarly, the first term in (D.1.16) can be bounded with the help of Lemma D.1.3 by

$$\|P(\widetilde{\psi}_n \chi_2)\| \lesssim (1 + R)^{-\theta} \|P(\psi_n \chi_2)\| \leq (1 + R)^{-\theta} (\|\chi_2 P\psi_n\| + \|\nabla \chi_2 \psi_n\|) .$$

Since the support of $\nabla \chi_2$ is compact and $\nabla \chi_2$ is bounded, Lemma D.1.1 shows $\|\nabla \chi_2 \psi_n\| \lesssim \|P\psi_n\| \leq 1$ for all $n \in \mathbb{N}$. Thus

$$\|P(\widetilde{\psi}_n \chi_2)\| \lesssim (1 + R)^{-\theta} \tag{D.1.18}$$

for all $n \in \mathbb{N}$, where the implicit constant is independent of n. Combining (D.1.16), (D.1.17) and (D.1.18) we arrive at

$$\|\widetilde{V}_-^{1/2} \widetilde{\psi}_n \chi_2\| \lesssim (1 + R)^{-\theta} . \tag{D.1.19}$$

Next, we estimate the second factor in the right–hand side of (D.1.15). Since $\widetilde{V}_-$ is form–bounded with respect to P^2, there exist constants $a, b > 0$ such that

$$\|\widetilde{V}_-^{1/2} (\widetilde{\varphi}_0 - \widetilde{\psi}_n)\chi_2\|^2 \leq a \|P(\widetilde{\varphi}_0 - \widetilde{\psi}_n)\chi_2\|^2 + b \|(\widetilde{\varphi}_0 - \widetilde{\psi}_n)\chi_2\|^2. \tag{D.1.20}$$

Using a similar argument as before, we find

$$\|(\widetilde{\varphi}_0 - \widetilde{\psi}_n)\chi_2\|^2 \leq 2(1 + R)^{-2\theta} \left(\|P\varphi_0\|^2 + \|P\psi_n\|^2 \right) \leq 2(1 + R)^{-2\theta}. \tag{D.1.21}$$

Moreover, similarly as before, we see that

$$\|P(\widetilde{\varphi}_0 - \widetilde{\psi}_n)\chi_2\|^2 \lesssim (1 + R)^{-2\theta} (\|P\varphi_0\| + \|P\psi_n\|) \lesssim (1 + R)^{-2\theta}. \tag{D.1.22}$$

Combining (D.1.20), (D.1.21) and (D.1.22) we find

$$\|\widetilde{V}_-^{1/2} (\widetilde{\varphi}_0 - \widetilde{\psi}_n)\chi_2\|^2 \lesssim (1 + R)^{-2\theta}. \tag{D.1.23}$$

Inserting (D.1.23) and (D.1.19) into (D.1.15) yields

$$|J_2|^2 \lesssim (1+R)^{-2\theta}.$$

Similarly, we find that

$$|J_1|^2 \lesssim (1+R)^{-2\theta}.$$

This proves (D.1.14) as $R \to \infty$. Combining this with (D.1.9), we conclude

$$\lim_{n\to\infty} \langle \psi_n, V_-\psi_n\rangle = \langle \varphi_0, V_-\varphi_0\rangle,$$

which completes the proof of statement (b).
It remains to prove *statement (d)*, which says

$$\langle \varphi_0, V_+\varphi_0\rangle \le \liminf_{n\to\infty} \langle \psi_n, V_+\psi_n\rangle.$$

Let χ_T be the characteristic function of the set $\{x \in \mathbb{R}^d : |x| \le T\}$. By Lemma D.1.1, for any $T > 0$, we have $\chi_T\psi_n \to \chi_T\varphi_0$ in $L^2(\mathbb{R}^d)$. Hence, there exists a subsequence of $(\chi_R\psi_n)_{n\in\mathbb{N}}$ that converges pointwise almost everywhere to $\chi_T\varphi_0$. For this subsequence, we can apply Fatou's Lemma to get

$$\langle \chi_T\varphi_0, V_+\chi_T\varphi_0\rangle \le \liminf_{n\to\infty} \langle \psi_n, V_+\psi_n\rangle.$$

Thus, statement (d) follows from the monotone convergence theorem as $T \to \infty$. ∎

D.2 Uniqueness of Resonances and the Energy Gap

In this section, we show that the resonance solution φ is unique under a small additional assumption on the potential. Moreover, this uniqueness implies that on the space $\dot{H}^1(\mathbb{R}^d) \cap \dot{Q}(V_+)$ the operator $H = \frac{1}{2}P^2 + V$ has an energy gap for functions orthogonal to the resonance φ_0 with respect to the scalar product in the homogenous Sobolev space $\dot{H}^1$.

Theorem D.2.1 (Uniqueness of Resonances and the Energy Gap)**.** *We consider dimension $d \ge 3$. In addition to the short–range condition from Theorem D.1.2) (=Theorem 1.4.11) we assume that the potential $V \in L^{d/2}_{\mathrm{loc}}$ as well as $V_+ \in K_{d,\mathrm{loc}}$ and $V_- \in K_d$.*
Then the resonance solution φ_0 from Theorem D.1.2 is unique and can be chosen to be strictly positive. Moreover, there exists a constant $\mu > 0$ such that, as quadratic forms,

$$\langle \psi, H\psi\rangle \ge \mu \|P\psi\|^2 \tag{D.2.1}$$

for all $\psi \in \dot{H}^1(\mathbb{R}^d) \cap \dot{Q}(V_+)$ orthogonal to the resonance φ_0 in $\dot{H}^1(\mathbb{R}^d)$, i.e., $\langle P\psi, P\varphi_0\rangle = 0$.

Remark D.2.2. *The conditions of Theorem D.2.1 are satisfied if the potential V is a short–range potential of the form*

$$V = (1+|\cdot|)^{-2-\theta}\, W$$

for some $\theta > 0$ and $W \in L^{d/2}_{\text{loc}} \cap K_d$.

Proof. Let φ_0 be the resonance solution from Theorem D.1.2. The complex conjugate $\overline{\varphi_0}$ is also a solution of (D.1.1) since H commutes with complex conjugation. By linearity, $\mathrm{Re}(\varphi_0)$ and $\mathrm{Im}(\varphi_0)$ are solutions of (D.1.1). Hence, we can assume that the resonance φ_0 is real–valued. Moreover, since V_+ is in the local Kato–class $K_{d,\text{loc}}$ and $V_- \in K_d$, and φ_0 is a local solution of $H\varphi_0 = 0$ (see Remark 1.4.7), the results of [3] show that φ_0 is continuous. With an argument slightly different from the one given in [3] we also explain in the proof of Theorem D.5.2 why resonances are continuous when the potential satisfies the short range condition of Remark D.2.2 above.

If the bound (D.2.1) is false, then for any $\delta > 0$ there exists $\psi \in \dot{H}^1(\mathbb{R}^d) \cap \dot{Q}(V_+)$ with $\langle P\psi, P\varphi_0\rangle = 0$ such that

$$\langle \psi, H\psi\rangle < \delta/2\|P\psi\|^2 .$$

Taking a sequence $(\delta_n)_N \in (0,1)$ with $\delta_n \downarrow 0$ yields a sequence $\psi_n \in \dot{H}^1(\mathbb{R}^d) \cap \dot{Q}(V_+)$ with $\langle P\psi_n, P\varphi_0\rangle = 0$ and

$$\langle \psi_n, H\psi_n\rangle < \delta_n/2\|P\psi_n\|^2 . \tag{D.2.2}$$

Again, since $\psi_n \neq 0$ we can assume that $\|P\psi_n\| = 1$ by normalizing the sequence ψ_n, so (D.2.2) gives

$$\langle \psi_n, H\psi_n\rangle < \delta_n/2 \tag{D.2.3}$$

with $\psi_n \in \dot{H}^1(\mathbb{R}^d) \cap \dot{Q}(V_+)$, $\|P\psi_n\| = 1$, and $\langle P\psi_n, P\varphi_0\rangle = 0$ for all $n \in \mathbb{N}$. In particular, since $\|P\psi_n\| = 1$ we have

$$\frac{1-\delta_n}{2} + \langle \psi_n, V\psi_n\rangle = \langle \psi_n, H\psi_n\rangle - \delta_n/2 < 0 \tag{D.2.4}$$

which is the same bound as (D.1.3), but now for a sequence with $\langle P\psi_n, P\varphi_0\rangle = 0$.

Taking a subsequence, again denoted by $(\psi_n)_{n\in\mathbb{N}}$ which converges weakly in $\dot{H}^1$ and almost everywhere to some $\psi_0 \in H^1$. By weak convergence, we have $\langle P\psi_0, P\varphi_0\rangle = 0$.

Using (D.2.4), the same arguments as in the proof of Theorem D.1.2 can be used to show that $\|P\psi_0\| = 1$, $\langle \psi_0, V_+\psi_0\rangle \leq \langle \psi_0, V_-\psi_0\rangle - 1 < \infty$, and $\langle \psi_0, H\psi_0\rangle = q_H(\psi_0, \psi_0) = 0$, i.e., ψ_0 is also an energy minimizer on $\dot{H}^1 \cap \dot{Q}(V_+)$. In particular, (D.1.1) and (D.1.2) hold with φ_0 replaced by ψ_0. Again, since $V_+ \in K_{d,\text{loc}}$ and $V_- \in K_d$, the results of [3] show that ψ_0 is continuous.

Since φ_0 is real–valued and ψ_0 is orthogonal to φ_0 in $\dot{H}^1$, also the real and imaginary parts of ψ_0 are orthogonal to φ_0 in $\dot{H}^1$. Moreover, they are both minimizers of the energy (on $\dot{H}^1 \cap \dot{Q}(V_+)$). Hence we can assume that both φ_0 and ψ_0 are real–valued and continuous.

The space

$$L = \mathrm{span}\{\psi_0, \varphi_0\} = \{\alpha\psi_0 + \beta\varphi_0 : \alpha, \beta \in \mathbb{R}\}$$

is a two–dimensional subspace of $\dot{H}^1 \cap \dot{Q}(V_+)$) and by bi–linearity and (D.1.1) we have for all $\psi = \alpha\psi_0 + \beta\varphi_0 \in L$

$$\begin{aligned}\langle\psi, H\psi\rangle &= \langle\alpha\psi_0 + \beta\varphi_0, H\alpha\psi_0 + \beta\varphi_0\rangle \\ &= \alpha^2\langle\psi_0, H\psi_0\rangle + \alpha\beta\langle\psi_0, H\varphi_0\rangle + \alpha\beta\langle\varphi_0, H\psi_0\rangle + \beta^2\langle\varphi_0, H\varphi_0\rangle \\ &= \alpha^2\langle\psi_0, H\psi_0\rangle + \beta^2\langle\varphi_0, H\varphi_0\rangle = 0\end{aligned}$$

where in the last step we also used (D.1.2). Note that L is a real two dimensional subspace of $\dot{H}^1$ with scalar product $\langle\nabla\varphi, \nabla\psi\rangle_1$ for $\varphi, \psi \in L$. Since L is finite–dimensional, any other scalar product on L will will be equivalent to $\langle\nabla\varphi, \nabla\psi\rangle_1$. We choose

$$\langle\varphi, \psi\rangle_2 = \langle\varphi, (1 + |\cdot|)^{-2}\psi\rangle = \int \frac{\varphi(x)\psi(x)}{(1 + |x|^2)^2}\, dx\,.$$

Recall that any $\psi \in L$ is real–valued. Since L is a two–dimensional real vector space, there must exist a function $f \in L$ which changes sign or is zero on a non–empty open subset of $\mathbb{R}^d$. Otherwise, any function in L is either non-negative or non-positive and zero only on a set of Lebesgue measure zero, Hence $\langle\varphi, \psi\rangle_2 \neq 0$ for all $\varphi, \psi \in L$, which is not possible since the dimension of L is two.

Taking a real–valued continuous function $f \in L$ which changes sign, consider its positive and negative parts f_+ and f_-, which are elements of $L \subset \dot{H}^1 \cap \dot{Q}(V_+)$ due to the well–known inequality $|\nabla|f|| \leq |\nabla f|$. The sets $\{f_+ > 0\}$ and $\{f_- > 0\}$ are open and disjoint. Hence, since H or, more precisely, its quadratic form q_H, is local, we have

$$\begin{aligned}0 = \langle f, Hf\rangle = q_H(f, f) &= q_H(f_+ - f_-, f_+ - f_-) \\ &= q_H(f_+, f_+) - q_H(f_+, f_-) - q_H(f_-, f_+) + q_H(f_-, f_-) \\ &= q_H(f_+, f_+) + q_H(f_-, f_-)\end{aligned}$$

and since $q_H(f_\pm, f_\pm) \geq 0$, we get $q_H(f_\pm, f_\pm) = 0$. If both f_+ and f_- are non–trivial, then f_+ and f_- are both zero on non–empty open sets. Since $V \in L^{d/2}_{\mathrm{loc}}$, the unique continuation theorem from [62], see Theorem D.3.2, shows that both f_+ and f_- are identically zero, which is a contradiction. Thus, either f_+ or f_- are identically zero. This contradicts the fact that L is two–dimensional. Thus, (D.2.1) holds for some $\mu > 0$.

If the resonance solution φ_0 is not unique, there exists a nontrivial $\psi_0 \notin \mathrm{span}(\varphi_0)$ with $q_H(\psi_0, \psi_0) = 0$. Write $\psi_0 = c\varphi_0 + g$ with a non–trivial $g \in \dot{H}^1 \cap \dot{Q}(V_+)$ which is orthogonal to φ_0 in $\dot{H}^1$. Then (D.1.1), (D.1.2), and (D.2.1) imply

$$\begin{aligned}\langle\psi_0, H\psi_0\rangle = q_H(\psi_0, \psi_0) &= |c|^2 q_H(\varphi_0, \varphi_0) + 2\,\mathrm{Re}(c q_H(g, \varphi_0)) + q_H(g, g) \\ &= q_H(g, g) \geq \delta\|Pg\|^2 > 0\end{aligned}$$

which is a contradiction. So φ_0 is unique.

As before, the real part $\varphi_r = \mathrm{Re}(\varphi_0)$ and imaginary part $\varphi_i = \mathrm{Im}(\varphi_0)$ of φ_0 are also resonance solutions. If both are nontrivial and linearly independent, then $\varphi_r = c\varphi_i + g$ with g non–trivial and orthogonal to φ_r in $\dot{H}^1$. As before, this leads to the contradiction

$$0 = \langle \psi_r, H\psi_r \rangle = q_H(\psi_r, \psi_r) = |c|^2 q_H(\varphi_i, \varphi_i) + 2\,\mathrm{Re}(q_H(g, c\varphi_i)) + q_H(g, g)$$
$$= q_H(g, g) \geq \delta \|Pg\|^2 > 0\,.$$

So $\mathrm{Re}(\varphi_0)$ and $\mathrm{Im}(\varphi_0)$ are linearly dependent, hence φ_0 can be chosen to be real–valued and continuous. If the positive and negative parts of φ_0 are non-trivial, then as before, we get a contradiction using the unique continuation theorem. This proves that φ_0 can be chosen to be strictly positive and finishes the proof of Theorem D.2.1. ∎

D.3 Unique Continuation à la Jerison and Kenig

In this section, we give a proof of the following unique continuation type result. First, some notation. Let $\Omega \subset \mathbb{R}^d$ be an open set. We say that a function $f \in L^2_{\mathrm{loc}}(\Omega)$ vanishes to infinite order at a point $x_0 \in \Omega$ if for any $n \in \mathbb{N}$ there exists positive constants C_n and t_n such that for any $0 < t \leq t_n$

$$\int_{|x-x_0|\leq t} |f(x)|^2\,dx \leq C_n t^n\,. \tag{D.3.1}$$

Remark D.3.1. *Note that if f vanishes to infinite order at a point x_0, then Hölder's inequality implies that for any $1 \leq q < 2$ we have*

$$\int_{|x-x_0|\leq t} |f|^q\,dx \leq \left(\int_{|x-x_0|\leq t} 1\,dx\right)^{(2-q)/2} \left(\int_{|x-x_0|\leq t} |f|^2\,dx\right)^{2/q} \lesssim t^{(2d+(n-d)q)/2}$$

for all $n \in \mathbb{N}$, so f vanishes to infinite order also with respect to any L^q-norm as long as $1 \leq q \leq 2$.

The main unique continuation result we need is

Theorem D.3.2 (= Theorem 6.3 in [62])**.** *Let $\Omega \subset \mathbb{R}^d$ be open and connected and $d \geq 3$. Assume that $V \in L^{d/2}_{\mathrm{loc}}(\Omega)$, $f \in H^1_{\mathrm{loc}}(\Omega)$ with distributional Lapalacian $\Delta f \in L^1_{\mathrm{loc}}(\Omega)$, and*

$$|\Delta f| \leq |Vf| \quad \text{in } \Omega\,.$$

If f vanished at a point $x_0 \in \Omega$ to infinite order, then f is identically zero on Ω.

Remark D.3.3. *In their landmark paper, Jerison and Kenig proved this theorem under the additional assumption that f is in the second oder Sobolev space $W^{2,q}_{\mathrm{loc}}(\Omega)$ with $q = \frac{2d}{d+2}$ and $d \geq 3$. Of course, in the application to solutions of the Schrödinger equation, we have $f \in H^1_{\mathrm{loc}}$, hence, by Sobolev's embedding theorem, also $f \in L^{2d/(d-2)}_{\mathrm{loc}}$. The inequality $|\Delta f| \leq |Vf|$, with $V \in L^{d/2}_{\mathrm{loc}}(\Omega)$ and $f \in H^1_{\mathrm{loc}}(\Omega)$, together with Hölder's inequality then implies*

$$\Delta f \in L^{2d/(d+2)}_{\mathrm{loc}}(\Omega)\,.$$

Calderón–Zygmund theory, see [80], shows that all mixed weak second order derivatives of f are in $L^{2d/(d+2)}_{\text{loc}}(\Omega)$. *Indeed, it is shown in Exercise 7.4 in [80] that for all* $j,k=1,\dots,d$ *the operators* $R_{j,k}=\partial_j\partial_k\Delta^{-1}$ *are operators given by singular integrals. By Calderón–Zygmund theory they are bounded from* L^p *to* L^p *as long as* $1<p<\infty$. *So, see for example Corollary 7.7 in [80], one has*

$$\sup_{j,k=1,\dots,d}\left\|\partial_j\partial_k u\right\|_{L^p}\le C_{p,d}\|\Delta u\|_{L^p}\,.$$

Using cut–off functions and bounding the commutators, shows that $\partial_j\partial_k f\in L^p_{\text{loc}}(\Omega)$ *for all* $j,k=1\dots,d$ *as soon as* $\Delta f\in L^p_{\text{loc}}(\Omega)$.
Together with the fact that $L^2_{\text{loc}}(\Omega)\subset L^{2d/(d+2)}_{\text{loc}}(\Omega)$, *this shows that any function* f *satisfying the assumptions of Theorem D.3.2 is indeed in* $W^{2,q}_{\text{loc}}(\Omega)$ *with* $q=\frac{2d}{d+2}$, *as assumed in [62].*

D.4 Uniformly Integrable Potentials and the Kato–class

Recall that $L^P_{\text{loc,unif}}(\mathbb{R}^d)$, the space of *uniformly locally* p-times integrable functions is given by all (Borel measurable) functions f such that

$$\|f\|_{L^p_{\text{loc,unif}}}\coloneqq\sup_{x\in\mathbb{R}^d}\left(\int_{|x-y|\le 1}|f(y)|^p\,dy\right)^{1/p}<\infty\,. \tag{D.4.1}$$

It is easy to see that for all $r>0$ the norms

$$\|f\|_{L^p_{\text{loc,unif}},r}\coloneqq\sup_{x\in\mathbb{R}^d}\left(\int_{|x-y|\le r}|f(y)|^p\,dy\right)^{1/p} \tag{D.4.2}$$

are equivalent to (D.4.1). Recall also that for $d\ge 2$ the Kato–class K_d defined in Definition 1.2.8, is given by all potentials V such that with

$$g_d(x)=\begin{cases}|\ln(|x|)| & d=2\\ |x-y|^{2-d} & d\ge 2\end{cases}, \tag{D.4.3}$$

one has

$$\lim_{\delta\to 0}\sup_{x\in\mathbb{R}^d}\int_{|x-y|\le\delta}g_d(x-y)|V(y)|\,dy=0\,.$$

Also, $K_1\coloneqq L^1_{\text{loc,unif}}(\mathbb{R})$, but we will not use this. Furthermore, for $d\ge 2$ we define $K_{d,1}$ as the set of all potentials V such that

$$\lim_{\delta\to 0}\sup_{x\in\mathbb{R}^d}\int_{|x-y|\le\delta}|x-y|^{1-d}|V(y)|\,dy=0\,.$$

Since $g_d(x) \geq 1$ for $|x| \leq 1$ and $d \geq 3$, respectively $g_2(x) \geq \ln(2)$ for $|x| \leq 1/2$, one easily sees from (D.4.1), respectively (D.4.2), that $K_d \subset L^1_{\text{loc,unif}}(\mathbb{R}^d)$. Similarly, $K_{d,1} \subset L^1_{\text{loc,unif}}(\mathbb{R}^d)$. Furthermore, Hölder's inequality shows that $L^p_{\text{loc,unif}}(\mathbb{R}^d) \subset K_d$ for all $p > d/2$ and $L^p_{\text{loc,unif}}(\mathbb{R}^d) \subset K_{d,1}$ for all $p > d$.
The following Lemma is a key observation for our proof of the precise asymptotics of virtual levels.

Lemma D.4.1. a) *For all $W \in L^1_{\text{loc,unif}}(\mathbb{R}^d)$ and all $L \geq 0$*

$$\sup_{x \in \mathbb{R}^d} \int_{|x-y| \leq L} |W(y)| \, dy \leq \|W\|_{L^1_{\text{loc,unif}}} (1+L)^d \,. \tag{D.4.4}$$

Moreover, for any $\theta > 0$ we have

$$\sup_{x \in \mathbb{R}^d} \int (1 + |x-y|)^{-d-\theta} |W(y)| \, dy < \infty \,. \tag{D.4.5}$$

b) *Assume that $d \geq 2$ and for some $\theta > 0$ the potential V is given by*

$$V(y) = (1+|y|)^{-2-\theta} W(y) \quad \text{for a.e. } y \in \mathbb{R}^d$$

where $W \in K_d$. Then

$$\sup_{x \in \mathbb{R}^d} \int g_d(x-y) |V(y)| \, dy < \infty \,. \tag{D.4.6}$$

Proof. Clearly, with $|B_1^d|$ the volume of a ball of radius one in $\mathbb{R}^d$ we have

$$\int \mathbb{1}_{\{|y-z| \leq 1\}} \, dz = |B_1^d| \quad \text{for all } y \in \mathbb{R}^d \,.$$

Thus

$$\int_{|x-y| \leq L} |W(y)| \, dy = \frac{1}{|B_1^d|} \iint \mathbb{1}_{\{|x-y| \leq L\}} \mathbb{1}_{\{|y-z| \leq 1\}} |W(y)| \, dy dz$$

and since $|x-z| \leq |x-y| + |y-z| \leq L+1$, we see that

$$\begin{aligned}
\int_{|x-y| \leq L} |W(y)| \, dy &\leq \frac{1}{|B_1^d|} \int_{|x-z| \leq 1+L} \int_{|y-z| \leq 1} |W(y)| \, dy \, dz \\
&\leq \frac{1}{|B_1^d|} \|W\|_{L^1_{\text{loc,unif}}} \int_{|x-z| \leq 1+L} dz = \|W\|_{L^1_{\text{loc,unif}}} (1+L)^d
\end{aligned}$$

for all $x \in \mathbb{R}^d$. This proves (D.4.4).

Using the identity

$$(1+|z|)^{-\alpha} = \alpha \int_0^\infty (1+r)^{-(\alpha+1)} \mathbb{1}_{\{r\geq |z|\}} dr, \quad \forall z \in \mathbb{R}^d \text{ and } \alpha > 0,$$

together with (D.4.4) we have

$$\begin{aligned}\int_{\mathbb{R}^d} (1+|x-y|)^{-d-\theta} |W(y)| dy &= (d+\theta) \int_0^\infty (1+r)^{-(d+\theta+1)} \int_{|x-y|<r} |W(y)| dy dr \\ &\leq C(d+\theta) \int_0^\infty (1+r)^{-(\theta+1)} dr < \infty \,,\end{aligned}$$

which proves (D.4.5).
We only give the proof of (D.4.6) for $d \geq 3$. The proof for $d = 2$ is similar. By the definition of the Kato–class we have

$$\sup_{x\in\mathbb{R}^d} \int_{|x-y|\leq\delta_0} |x-y|^{2-d} |V(y)| \, dy < \infty$$

for some $\delta_0 > 0$. Thus it remains to check that

$$\sup_{x\in\mathbb{R}^d} \int_{|x-y|>\delta_0} |x-y|^{2-d} |V(y)| \, dy < \infty \,. \tag{D.4.7}$$

For $|x - y| \geq \delta_0$ we have $|x-y|^{2-d} \lesssim (1 + |x-y|)^{2-d}$, so

$$\int_{|x-y|>\delta_0} |x-y|^{2-d} |V(y)| \, dy \lesssim \int (1+|x-y|)^{2-d} (1+|y|)^{-2-\theta} |W(y)| \, dy \,.$$

Since $W \in K_d \subset L^1_{\text{loc,unif}}(\mathbb{R}^d)$ the claim (D.4.7) follows from Lemma D.6.1. ∎

D.5 Integral Representation of Zero–Energy Solutions

To prove Theorem 3.2.5, we need the following result on solutions of Poisson's equation

Theorem D.5.1 (= Theorem 6.21 in [74])**.** *Let $f \in L^1_{\text{loc}}(\mathbb{R}^d)$, $d \geq 1$. Assume that for almost every $x \in \mathbb{R}^d$ the function*

$$y \mapsto G(x-y) f(y) \in L^1(\mathbb{R}^d)$$

where

$$G(x-y) = \begin{cases} c_d \ln(|x-y|) & d = 2 \\ c_d |x-y|^{2-d} & d \neq 2 \end{cases},$$

with $c_d = (d-2)^{-1}\left|\mathbb{S}^{d-1}\right|^{-1}$ *for* $d \geq 3$ *and* $c_2 = -\left|\mathbb{S}^1\right|^{-1}$. *Define the function* $u : \mathbb{R}^d \to \mathbb{C}$ *by*

$$u(x) = \int_{\mathbb{R}^d} G(x-y) f(y)\, dy.$$

Then $u \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ *and* $-\Delta u = f$ *in the sense of distributions. Moreover, the function* u *has a distributional derivative that is a function; it is given, for almost every* $x \in \mathbb{R}^d$, *by*

$$\nabla u(x) = \int_{\mathbb{R}^d} \nabla G(x-y) f(y)\, dy. \tag{D.5.1}$$

We prove the following, which is in large parts an application of Theorem D.5.1.

Theorem D.5.2. *Let* $d \geq 3$ *and* $V : \mathbb{R}^d \to \mathbb{R}$ *such that there exists* $W \in K_d$ *and* $\theta > 0$ *such that*

$$V(x) = W(x)(1+|x|)^{-2-\theta} \quad \forall x \in \mathbb{R}^d. \tag{D.5.2}$$

Assume that $H = \frac{1}{2}P^2 + V$ *has a virtual level and* φ_0 *is the corresponding weak local zero energy eigenfunction with finite kinetic energy (i.e.,* $\varphi_0 \in \dot{H}^1$*). Then* φ_0 *has a continuous version, it is bounded with* $V\varphi \in L^1(\mathbb{R}^d)$*, and satisfies the integral equation*

$$\varphi_0(x) = -2c_d \int_{\mathbb{R}^d} |x-y|^{-(d-2)} V(y)\varphi_0(y) dy, \quad \forall x \in \mathbb{R}^d, \tag{D.5.3}$$

with $c_d = (d-2)^{-1}\left|\mathbb{S}^{d-1}\right|^{-1}$, *where* $\left|\mathbb{S}^{d-1}\right| = d\left|B_1^d\right|$ *is the surface area of the unit sphere in* $\mathbb{R}^d$ *and* $\left|B_1^d\right|$ *the volume of the unit ball in* $\mathbb{R}^d$. *If additionally* $W \in K_{d,1}$ *then* $\nabla\varphi_0$ *has a continuous version and satisfies the integral equation*

$$\nabla\varphi_0(x) = 2(d-2)c_d \int_{\mathbb{R}^d} \frac{x-y}{|x-y|^d} V(y)\varphi_0(y) dy, \quad \forall x \in \mathbb{R}^d. \tag{D.5.4}$$

Remark D.5.3. *Equation* (D.5.1) *shows that for almost every* $x \in \mathbb{R}^d$ *the integral equation* (D.5.4) *holds. If* $W \in K_{d,1}$, *the the right hand side of* (D.5.1) *is continuous in* x *and yields the continuous version of* $\nabla\varphi_0$.

Proof of Theorem D.5.2. The proof proceeds in two steps. In the first step we assume that the zero-energy solution φ_0 is bounded and use this, together with a–priori bound from Proposition 3.2.7, to see that Theorem D.5.1 applies. Thus the integral representations in (D.5.3) and (D.5.4) are valid for almost every $x \in \mathbb{R}^d$. Then we use this to show that φ_0 is continuous, more precisely, has a continuous version when $W \in K_d$ and that $\nabla\varphi_0$ is continuous when $W \in K_{d,1}$. In the second step, we show that φ_0 is indeed bounded.

Step 1:

Assume that φ_0 is bounded then

$$\int_{\mathbb{R}^d} |G(x-y)V(y)\varphi_0(y)|dy \lesssim \int_{\mathbb{R}^d} |x-y|^{-(d-2)}(1+|y|)^{-2-\theta}|W(y)|dy \tag{D.5.5}$$

where $\lesssim$ means that the inequality holds up to a positive constant. Thanks to (D.4.6), we have that for every $x \in \mathbb{R}^d$ the map $y \mapsto G(x-y)V(y)$ is integrable. Therefore we may apply Theorem D.5.1 to conclude that

$$u(x) = 2c_d \int_{\mathbb{R}^d} G(x-y)V(y)\varphi_0(y) \in L^1_{\text{loc}}(\mathbb{R}^d)\,.$$

for almost every $x \in \mathbb{R}^d$. Note that the right–hand side of the above equation is finite uniformly in $x \in \mathbb{R}^d$.
Next we show that u has a continuous version by showing that the right–hand–side of the above equation is continuous in x. Let $\chi \in C_0^\infty(\mathbb{R}^d)$ $\delta > 0$ with $0 \leq \chi \leq 1$, $\chi(x) = 1$ for $|x| \leq 1$ and $\chi(x) = 0$ for $|x| \geq 2$. For $\delta > 0$ define $\chi_\delta(x) = \chi(x/\delta)$ and

$$u_\delta(x) = 2c_d \int (1-\chi_\delta(x-y))G(x-y)V(y)\varphi_0(y)dy\,.$$

Since $\chi_\delta(x-y) = 1$ for $|x-y| \leq \delta$ the map $x \mapsto (1-\chi_\delta(x-y))G(x-y)V(y)\varphi_0(y)$ is continuous for for fixed $y \in \mathbb{R}^d$. Because of (D.4.6), we can use Lebesgue's dominated convergence theorem to see that $\lim_{n\to\infty} u_\delta(x_n) = u_\delta(x)$ for any sequence $(x_n)_n$ which converges to x. Thus, u_δ is continuous. Since $V(y) = (1+|y|)^{-(2+\theta)}W(y)$ with W in the Kato–class K_d, we have

$$\sup_{x\in\mathbb{R}^d} |u(x) - u_\delta(x)| \lesssim \sup_{x\in\mathbb{R}^d} \int_{|x-y|\leq 2\delta} |x-y|^{2-d}|W(y)|\,dy \to 0 \quad \text{for } \delta \to 0$$

and consequently, u is the uniform limit of continuous functions, hence continuous. This shows that the zero–energy solution φ_0 indeed has a continuous version. If, in addition, the function $W \in K_{d,1}$, this also implies that $\nabla\varphi_0$ can be chosen to be continuous. Define

$$f_\delta(x) = 2(d-2)c_d \int_{|x-y|>\delta} (1-\chi_\delta(x-y))\frac{x-y}{|x-y|^d}V(y)\psi(y)\,dy$$

which is again continuous, and $f(x)$ by the right hand side of (D.5.1) and note that

$$\sup_{x\in\mathbb{R}^d} |f(x) - f_\delta(x)| \lesssim \sup_{x\in\mathbb{R}^d} \int_{|x-y|\leq\delta} |x-y|^{1-d}|W(y)|\,dy \to 0 \quad \text{as } \delta \to 0\,.$$

So $\nabla\varphi_0$ has a continuous version if $W \in K_{d,1}$.

Step 2:

We show that φ_0 is indeed bounded. Following [3, Lemma Theorem 6.1], for any $\delta > 0$ small enough there exists $C_\delta > 0$ with

$$|\varphi_0(x)| \leq C_\delta \int_{|x-y|\leq\delta} |\varphi_0(y)|dy\,.$$

The constant C_δ depends on local norms Kato–norms of V_- and can be chosen independently of x. However, C_δ will blow up as $\delta \to 0$. Using Cauchy–Schwarz, we get

$$|\varphi_0(x)| \leq C_\delta |B_\delta^d|^{1/2} \|\varphi_0\|_{L^2(B_\delta^d(x))}$$

and

$$\|\varphi_0\|^2_{L^1(B_\delta^d)} \leq |B_\delta| \int\limits_{|x-y|<\delta} \delta^2 \frac{|\varphi_0(y)|^2}{|x-y|^2} dy \leq \left|B_\delta^d\right| \delta^2 \int\limits_{|x-y|<\delta} \frac{|\varphi_0(y)|^2}{|x-y|^2} dy\,. \tag{D.5.6}$$

Since $\varphi_0 \in \dot{H}^1$, we can use translation invariance and Hardy's inequality to see that

$$\sup_{x\in\mathbb{R}^d} \int\limits_{|x-y|<\delta} \frac{|\varphi_0(y)|^2}{|x-y|^2} dy \lesssim \|\nabla\varphi_0\|^2 < \infty\,.$$

This proves that $\sup_{x\in\mathbb{R}^d} |\varphi_0(x)| \lesssim \|\nabla\varphi_0\| < \infty$, i.e., φ_0 is bounded. ∎

D.6 Useful Integral Estimates

Lemma D.6.1. *Let $0 \leq U \in L^1_{\text{loc,unif}}(\mathbb{R}^d)$. Given parameters $\alpha, \beta > 0$ with $\alpha + \beta > d$ define for any $x \in \mathbb{R}^d$*

$$h_{\alpha,\beta}(x) \coloneqq \int_{\mathbb{R}^d} (1+|x-y|)^{-\beta}(1+|y|)^{-\alpha} U(y)dy. \tag{D.6.1}$$

Then there exists a constant $c > 0$ depending on $\alpha, \beta > 0$ such that

$$\left|h_{\alpha,\beta}(x)\right| \leq \begin{cases} c(1+|x|)^{d-(\alpha+\beta)} & \text{if } \alpha,\beta < d \text{ and } d < \alpha+\beta \\ c(1+|x|)^{-\alpha}\ln(2+|x|) & \text{if } \beta = d, \text{ and } \alpha < d \\ c(1+|x|)^{-\beta}\ln(2+|x|) & \text{if } \alpha = d \text{ and } \beta < d \\ c(1+|x|)^{-\beta} & \text{if } \beta < d < \alpha \\ c(1+|x|)^{-\alpha} & \text{if } \alpha < d < \beta \end{cases} \tag{D.6.2}$$

for all $x \in \mathbb{R}^d$.

Remark D.6.2. *The estimate* (D.6.2) *is symmetric under the exchange of α and β, even though the expression $h_{\alpha,\beta}$ itself is not symmetric under this exchange. Substituting $x-y=z$ in* (D.6.1) *and noting that for any $z \in \mathbb{R}^d$ the potential $U(\cdot - z) \in L^1_{\text{loc,unif}}$ uniformly in z if $U \in L^1_{\text{loc,unif}}$ helps clarify this behavior.*

Proof. Inserting the identity

$$(1+|z|)^{-\alpha} = \alpha \int_0^\infty (1+r)^{-(\alpha+1)} \mathbb{1}_{\{r \geq |z|\}} dr, \quad \forall z \in \mathbb{R}^d$$

into the right–hand side of (D.6.1) we arrive at

$$h_{\alpha,\beta}(x) = \alpha\beta \int_0^\infty \int_0^\infty (1+s)^{-(\beta+1)}(1+t)^{-(\alpha+1)} \int_{\mathbb{R}^d} \mathbb{1}_{\{s \geq |x-y|\}} \mathbb{1}_{\{t \geq |y|\}} U(y) dy ds dt\,. \tag{D.6.3}$$

Applying Lemma D.4.1 we have with $C = \|U\|_{L^1_{\text{loc,unif}}}$ and all $s, t > 0$ and $x \in \mathbb{R}^d$

$$\int_{\mathbb{R}^d} \mathbb{1}_{\{s \geq |x-y|\}} \mathbb{1}_{\{t \geq |y|\}} U(y) dy \leq \int_{s \geq |x-y|} |U(y)| dy \leq C(1+s)^d, \tag{D.6.4}$$

and similar

$$\int_{\mathbb{R}^d} \mathbb{1}_{\{s \geq |x-y|\}} \mathbb{1}_{\{t \geq |y|\}} U(y) dy \leq C(1+t)^d\,. \tag{D.6.5}$$

So

$$\int_{\mathbb{R}^d} \mathbb{1}_{\{s \geq |x-y|\}} \mathbb{1}_{\{t \geq |y|\}} U(y) dy \leq C \min((1+s)^d, (1+t)^d), \tag{D.6.6}$$

Furthermore, for $|x-y| \leq s$ and $|y| \leq t$ also have $|x| \leq |x-y| + |y| \leq s+t$. Thus, using (D.6.6) in (D.6.3) we find

$$\left|h_{\alpha,\beta}(x)\right| \leq C\alpha\beta \iint\limits_{s,t \geq 0, |x| \leq s+t} (1+s)^{-(\beta+1)}(1+t)^{-(\alpha+1)} \min\{(1+t)^d, (1+s)^d\} ds dt\,.$$

We split the integral in the regions where $s < t$ and $t < s$ to find

$$\begin{aligned} \left|h_{\alpha,\beta}(x)\right| \leq & C\alpha\beta \iint\limits_{0 \leq s < t, |x| \leq 2t} (1+s)^{d-(\beta+1)}(1+t)^{-(\alpha+1)} ds dt \\ & + C\alpha\beta \iint\limits_{0 \leq t < s, |x| \leq 2s} (1+s)^{-(\beta+1)}(1+t)^{d-(\alpha+1)} ds dt\,. \end{aligned}$$

We define

$$\begin{aligned} I_1 &:= \iint\limits_{0 \leq s < t, |x| \leq 2t} (1+s)^{d-(\beta+1)}(1+t)^{-(\alpha+1)} ds dt, \\ I_2 &:= \iint\limits_{0 \leq t < s, |x| \leq 2s} (1+s)^{-(\beta+1)}(1+t)^{d-(\alpha+1)} ds dt\,. \end{aligned}$$

It suffices to estimate I_1 since both integrals are the same after renaming $s > 0$ and $t > 0$. Note that

$$I_1 = \int_{|x|/2}^{\infty} \int_0^t (1+s)^{d-(\beta+1)} ds (1+t)^{-(\alpha+1)} dt$$

and by direct calculations

$$\int_0^t (1+s)^{d-(\beta+1)} ds \leq \begin{cases} (d-\beta)^{-1}(1+t)^{d-\beta}, & \beta \neq d \\ \ln(1+t), & \beta = d \end{cases}$$

In the case $\beta = d$, $\alpha > 0$ after substitution and partial integration

$$I_1 \leq \int_{|x|/2}^{\infty} \ln(1+t)(1+t)^{-(\alpha+1)} dt = \alpha^{-1}(1+|x|/2)^{-\alpha} \left(\ln(1+|x|/2) + \alpha^{-1} \right)$$

and consequently for $\beta = d$ there exists some $c_1 > 0$ depending on $\alpha > 0$ such that

$$I_1 \leq c_1 (1+|x|)^{-\alpha} \ln(2+|x|) \quad \forall x \in \mathbb{R}^d .$$

In the case $\beta \neq d$ and using $\alpha + \beta > d$ we have

$$I_1 \leq (d-\beta)^{-1} \int_{|x|/2}^{\infty} (1+t)^{d-(\beta+\alpha)-1} dt = (d-\beta)^{-1}(\alpha+\beta-d)^{-1}(1+|x|/2)^{d-(\alpha+\beta)} .$$

Hence for some $c_2 > 0$ depending on $\alpha, \beta > 0$ it follows

$$|I_1| \leq c_2 (1+|x|)^{d-(\alpha+\beta)}$$

Choosing $c = \max\{c_1, c_2\}$ proves the assertion of Lemma D.6.1. ∎

Lemma D.6.3. *Let $d \geq 3$, $\theta > 0$ and $W \in K_d$. For any $x \in \mathbb{R}^d$ let $L(x) > 0$ such that $L(x) < |x|/2$ for $|x| > 1$ large enough. For $p < d$ we define*

$$\begin{aligned}
\sigma_1(x) &:= \int_{|y|>L(x)} (1+|y|)^{-(d+\theta)} |W(y)| dy, \\
\sigma_{2,p}(x) &:= \int_{|y|<L(x)} \left(|x-y|^{-(d-p)} - |x|^{-(d-p)} \right) (1+|y|)^{-(d+\theta)} |W(y)| dy, \\
\sigma_{3,p}(x) &:= \int_{|y|>L(x)} |x-y|^{-(d-p)} (1+|y|)^{-(d+\theta)} |W(y)|) dy \\
\sigma_4(x) &:= \int_{|y|<L(x)} \left| \frac{x-y}{|x-y|^d} - \frac{x}{|x|^d} \right| (1+|y|)^{-(d+\theta)} |W(y)| dy .
\end{aligned}$$

Then for $|x| > 1$ *large enough*

$$\begin{aligned}|\sigma_1(x)| &\lesssim (1+L(x))^{-\theta}\,,\\ \left|\sigma_{2,p}(x)\right| &\lesssim (1+L(x))^{-\theta}\,(|x|-L(x))^{p-d-1}\,,\\ |\sigma_4(x)| &\lesssim (1+L(x))^{-\theta}\,|x|\,(|x|-L(x))^{-d-1}\,,\end{aligned}$$

and if $p=1$ *and* $W \in K_d$*, or* $p=2$ *and* $W \in K_{d,1}$*, then for* $|x| > 1$ *large enough*

$$\left|\sigma_{3,p}(x)\right| \lesssim (1+L(x))^{-\theta}\,(1+|x|)^{p-d}\ .$$

Proof. We begin with the estimate for σ_1. The estimate follows similar to the proof of Lemma D.4.1. Using the identity

$$(1+|y|)^{-\gamma} = \gamma \int_0^\infty (1+r)^{-(\gamma+1)} \mathbb{1}_{\{r\geq |y|\}} dr, \quad \forall y \in \mathbb{R}^d, \gamma > 0 \tag{D.6.7}$$

one finds for $\gamma = d+\theta$ by application of Lemma D.4.1

$$\begin{aligned}\sigma_1(x) &= (d+\theta)\int_{L(x)}^\infty (1+r)^{-(d+\theta+1)} \int_{\mathbb{R}^d} \mathbb{1}_{\{r\geq|y|\geq L(x)\}} |W(y)| dy dr\\ &\leq (d+\theta)\int_{L(x)}^\infty (1+r)^{-(d+\theta+1)} \int_{|y|\leq r} |W(y)| dy dr\\ &\lesssim \int_{L(x)}^\infty (1+r)^{-(\theta+1)} dr \lesssim (1+L(x))^{-\theta}\,.\end{aligned}$$

We continue by estimating $\sigma_{3,p}$. We split the domain of integration into the sets where $|x-y| < 1$ and $|x-y| > 1$ to find

$$\sigma_{3,p}(x) = I_1(x) + I_2(x),$$

where

$$\begin{aligned}I_1(x) &\coloneqq \int_{\substack{|x-y|\leq 1\\ |y|\geq L(x)}} |x-y|^{-(d-p)} (1+|y|)^{-(d+\theta)} |W(y)| dy,\\ I_2(x) &\coloneqq \int_{\substack{|x-y|\geq 1\\ |y|\geq L(x)}} |x-y|^{-(d-p)} (1+|y|)^{-(d+\theta)} |W(y)| dy\,.\end{aligned}$$

For the integral I_1 we have by using Lemma D.4.1 for the cases $p=1$ and $p=2$

$$I_1(x) \lesssim (1+|x|)^{-(d+\theta)} \sup_{x\in\mathbb{R}^d} \int_{|x-y|\leq 1} |x-y|^{-(d-p)} |W(y)| dy \lesssim (1+|x|)^{-(d+\theta)}\ . \tag{D.6.8}$$

To estimate I_2 note that

$$I_2(x) \lesssim \int_{|y|\geq L(x)} (1+|x-y|)^{-(d-p)} \, (1+|y|)^{-(d+\theta)} |W(y)| dy \,. \tag{D.6.9}$$

Inserting the identity (D.6.7) for $\gamma = p-d$ and $\gamma = d+\theta$ we arrive at

$$\begin{aligned} &I_2(x) \\ &\lesssim \iint_{s,t\geq 0} (1+s)^{-(d-p+1)} (1+t)^{-(d+\theta+1)} \int_{|y|\geq L(x)} \mathbb{1}_{\{s\geq|x-y|\}} \mathbb{1}_{\{t\geq|y|\}} |W(y)| dy ds dt \,. \end{aligned} \tag{D.6.10}$$

Not that on that the constraints $s \geq |x-y|$ and $t \geq |y| \geq L(x)$ directly imply

$$|x| \leq |x-y| + |y| \leq s+t$$

and $t \geq L(x)$. Applying Lemma D.4.1 we find

$$\int_{|y|\geq L(x)} \mathbb{1}_{\{s\geq|x-y|\}} \mathbb{1}_{\{t\geq|y|\}} |W(y)| dy \lesssim \min\{(1+s)^d, (1+t)^d\} \mathbb{1}_{\{t\geq L(x)\}} \mathbb{1}_{\{s+t\geq|x|\}} \,. \tag{D.6.11}$$

Inserting (D.6.11) into (D.6.10) and splitting the domain of integration into the sets for which $s > t$ and $t < s$ we arrive at

$$\begin{aligned} &I_2(x) \\ &\lesssim \iint_{\substack{s,t\geq 0 \\ s+t\geq|x|}} (1+s)^{-(d-p+1)} (1+t)^{-(d+\theta+1)} \min\{(1+s)^d, (1+t)^d\} \mathbb{1}_{\{t\geq L(x)\}} ds dt \\ &\lesssim \iint_{\substack{0\leq s\leq t \\ |x|\leq 2t}} (1+s)^{d-(d-p+1)} (1+t)^{-(d+\theta+1)} \mathbb{1}_{\{t\geq L(x)\}} ds dt \\ &+ \iint_{\substack{0\leq t\leq s \\ |x|\leq 2s}} (1+s)^{-(d-p+1)} (1+t)^{d-(d+\theta+1)} \mathbb{1}_{\{t\geq L(x)\}} ds dt \,. \end{aligned} \tag{D.6.12}$$

We estimate the remaining two integrals independently. We begin with the integral in the second line of (D.6.12) and find

$$\begin{aligned} &\iint\limits_{\substack{0\leq s\leq t \\ |x|\leq 2t}} (1+s)^{d-(d-p+1)} (1+t)^{-(d+\theta+1)} \mathbb{1}_{\{t\geq L(x)\}} ds dt \\ &\qquad \lesssim \int\limits_{\max\left\{L(x), \frac{|x|}{2}\right\}}^{\infty} (1+t)^{p-d-\theta-1} dt \lesssim \left(1 + \max\left\{L(x), \frac{|x|}{2}\right\}\right)^{p-d-\theta} \,. \end{aligned} \tag{D.6.13}$$

For the integral in the third line of (D.6.12) we have

$$\begin{aligned}
&\iint_{\substack{0\le t\le s\\ |x|\le 2s}} (1+s)^{-(d-p+1)}(1+t)^{d-(d+\theta+1)}\mathbb{1}_{\{t\ge L(x)\}} \\
&\quad\lesssim \int_{|x|/2}^{\infty}(1+s)^{-(d-p+1)}ds\int_{L(x)}(1+t)^{-(\theta+1)}dt \\
&\quad\lesssim (1+|x|)^{-(d-p)}\,(1+L(x))^{-\theta}\ .
\end{aligned} \tag{D.6.14}$$

For $|x|>1$ large enough $L(x)<|x|/2$ by assumption. Comparing the estimates in (D.6.8), (D.6.13) and (D.6.14) proves

$$\sigma_{3,p}(x)\lesssim (1+|x|)^{-(d-p)}\,(1+L(x))^{-\theta}$$

for $|x|>1$ large enough.
We continue by estimating $\sigma_{2,p}$. Note that for $|y|<|x|$ we have $|x-y|\ge|x|-|y|>0$ and consequently

$$\begin{aligned}
\big||x-y|^{p-d}-|x|^{p-d}\big| \le (|x|-|y|)^{p-d}-|x|^{p-d} &= (d+1-p)\int_0^{|y|}(|x|-s)^{p-d-1}\,ds \\
&\le (d+1-p)|y|(|x|-|y|)^{p-d-1}\ .
\end{aligned}$$

By assumption $L(x)<|x|/2$ for $|x|>1$ large enough and therefore this implies

$$\begin{aligned}
\sigma_{2,p}(x) &= \int_{|y|<L(x)}\left(|x-y|^{-(d-p)}-|x|^{-(d-p)}\right)(1+|y|)^{-(d+\theta)}|W(y)|dy \\
&\lesssim (|x|-L(x))^{p-d-1}\int_{|y|<L(x)}|y|(1+|y|)^{-(d+\theta)}|W(y)|dy\,.
\end{aligned}$$

Using $|y|<1+|y|$ the remaining integral can be estimated similar to the estimate of σ_1 to find

$$\int_{|y|<L(x)}|y|(1+|y|)^{-(d+\theta)}|W(y)|dy\lesssim (1+L(x))^{1-\theta}\ . \tag{D.6.15}$$

This directly proves the estimate on $\sigma_{3,p}$ and finishes the proof of Lemma D.6.3.
It remains to estimate σ_4. Note that

$$\begin{aligned}
\left|\frac{x-y}{|x-y|^d}-\frac{x}{|x|^d}\right| &= \left|x\left(|x-y|^{-d}-|x|^{-d}\right)-y|x|^{-d}\right| \\
&\le |x|\big||x-y|^{-d}-|x|^{-d}\big|+|y||x|^{-d}
\end{aligned}$$

and consequently

$$|\sigma_4(x)| \leq |x| \int_{|y|<L(x)} \big||x-y|^{-d} - |x|^{-d}\big|(1+|y|)^{-(d+\theta)}|W(y)|dy$$
$$+ |x|^{-d} \int_{|y|<L(x)} |y|(1+|y|)^{-(d+\theta)}|W(y)|dy\,.$$

Comparing this with $\sigma_{2,0}$ shows

$$|\sigma_4(x)| \leq |x|\,(1+L(x))^{-\theta}\,(|x|-L(x))^{-d-1}$$
$$+ |x|^{-d} \int_{|y|<L(x)} |y|(1+|y|)^{-(d+\theta)}|W(y)|dy\,.$$

The last remaining integral is the same as in (D.6.15), and consequently we arrive at

$$|\sigma_4(x)| \leq |x|\,(1+L(x))^{-\theta}\,(|x|-L(x))^{-d-1} + |x|^{-d}(1+L(x))^{1-\theta}$$
$$\lesssim |x|\,(1+L(x))^{-\theta}\,(|x|-L(x))^{-d-1}\;\;.$$

which completes the proof of Lemma D.6.3. ■

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