Point Interactions in Systems of Fermions

by

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List of Publications

This thesis contains the following publications:

Chapter 2: T. Moser, R. Seiringer, *Stability of a fermionic* $N + 1$ *particle system with point interactions*, Commun. Math. Phys. **356**, pp. 329–355 (2017).

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About the Author

Thomas Moser started his studies in Physics at University of Vienna in 2008. In the second semester, he decided to take several mathematic courses and eventually he studied both fields simultaneously. He finished both Bachelors in the academic year 2011/2012 and continued with a Master in Physics and Mathematics at University of Vienna. In 2012, he went to New York University for one exchange semester.

Thomas started his master thesis in the area of mathematical many-body physics in 2013. He focused his research interests exploring the connection between Bose Einstein condensation and superfluidity in one dimensional point interacting systems in a random potential. He finished his Master in Physics in 2014.

In 2014, Thomas started his PhD at IST Austria and continued his research in many-body quantum-mechanics. During the years of his PhD he specialized in point interactions and more specifically in point-interacting systems of fermions.

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Abstract

In this thesis we will discuss systems of point interacting fermions, their stability and other spectral properties. Whereas for bosons a point interacting system is always unstable this question is more subtle for a gas of two species of fermions. In particular the answer depends on the mass ratio between these two species.

Most of this work will be focused on the $N + M$ model which consists of two species of fermions with N, M particles respectively which interact via point interactions. We will introduce this model using a formal limit and discuss the $N + 1$ system in more detail. In particular, we will show that for mass ratios above a critical one, which does not depend on the particle number, the $N + 1$ system is stable. In the context of this model we will prove rigorous versions of Tan relations which relate various quantities of the point-interacting model.

By restricting the $N + 1$ system to a box we define a finite density model with point interactions. In the context of this system we will discuss the energy change when introducing a point-interacting impurity into a system of non-interacting fermions. We will see that this change in energy is bounded independently of the particle number and in particular the bound only depends on the density and the scattering length.

As another special case of the $N + M$ model we will show stability of the $2 + 2$ model for mass ratios in an interval around one.

Further we will investigate a different model of point interactions which was discussed before in the literature and which is, contrary to the $N + M$ model, not given by a limiting procedure but is based on a Dirichlet form. We will show that this system behaves trivially in the thermodynamic limit, i.e. the free energy per particle is the same as the one of the non-interacting system.

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CHAPTER 1

Introduction

1.1 Motivation

Point interactions are a common choice to model systems where one or many length scales vanish or diverge. An example are short range forces where the underlying physics is largely independent of the detailed structure of the potential. The history of point interactions reaches back to the 1930ties and sometimes they are also called zero-range or on-site interactions. Originally they were introduced to model nuclear interactions [5, 6, 19, 68, 72], but they are also used for polarons (see [40] and references there) or cold atomic gases [74].

In recent years the application for cold atomic gases is of particular interest as it is now possible to explore strongly point-interacting fermionic systems in laboratories. For this reason we will briefly discuss why a point interacting model is a good choice for certain experimental setups in section 1.1.1. We note though that the results proven in later chapters are independent on any specific setup.

In this work we will only consider three-dimensional systems but there are also interesting results for the two-dimensional case [15, 16, 28, 35]. These two-dimensional systems behave very differently and in section 1.2.2 we will discuss the fundamental reasons for this. There we will also see why there are no point interactions in higher dimensions.

A popular model of point interactions, which we will denote in the following by the $N + M$ model and which we introduce in detail in section 1.2.3, consists of N fermions of one kind with mass one, M fermions of another species with mass m and point interactions between the species. We emphasize that setting the mass of one of the species to one is no restriction as an overall factor in the Hamiltonian is unimportant for our analysis. In particular, we are interested in specific values for N, M, i.e. the $1 + 1$, the $N + 1$ and the $2 + 2$ model. We note that because of antisymmetry there are no point interactions between fermions of the same species. As the species are allowed to have different masses, the $N + M$ and $M + N$ model describe in general different systems, but they can be connected as the $N + M$ model with mass m is equivalent to the $M + N$ problem with mass m^{-1} up to an overall factor in the Hamiltonian.

The first of these systems which was rigorously understood was the $1 + 1$ model which consists of two point interacting particles. For a good overview about this system see [1] and references therein. We will use the $1 + 1$ model in section 1.2.1 as a toy model to introduce the relevant notations and concepts.

A priori it is not clear what is even meant by point interactions as a $\delta(x-y)$ interaction potential is ill-defined in dimensions larger than one. A common way to define point interactions is by realizing that any point-interacting Hamiltonian would act on a state in which interacting particles are separated in the same way as the corresponding non-interacting Hamiltonian. We define the hyperplanes of interaction as the set in configuration space where two interacting particles are on top of each other. Using above fact we define a point-interacting Hamiltonian to be a self adjoint extension of a non-interacting Hamiltonian restricted to functions with support away from these hyperplanes. We note that this definition is very general as it also allows for non-local point interactions. These are non-local in the sense that the strength of the point interaction between two particles depends on the position of all the other particles and these interactions are therefore unphysical. In case of the $1+1$ system it is possible to classify all self-adjoint extensions which we will do in section 1.2.1.

Beyond the $1+1$ model it is highly non-trivial to explicitly define a physically realistic point interacting model. A common way to introduce it is to regularize in momentum space and then renormalize the interaction strength while taking a formal limit [20]. We will follow this approach in section 1.2.3 to introduce the general $N+M$ model. In two dimensions this formal limit was made rigorous in [15, 16, 35].

From a physical point of view it would be desirable to show that the $N+M$ model is a limit of Hamiltonians interacting with potentials with shrinking support and which are close to a two-body zero-energy resonance. This is true for the two particle case [1] and for three particles in one dimension [3] but has not been established for any other case. In section 1.2.1, we will discuss this limit in more detail. We also note that for sufficiently enough interaction potential this convergence is true in the norm resolvent sense. Contrary to this the rigorous constructions using momentum cutoffs carried out in [16, 28, 35] only show strong resolvent convergence.

The study of the three-body point interacting system is relatively old and dates back to Thomas [68] who investigated point interacting bosons. Later there was more work done by G.V. Skorniakov and K. A. Ter-Martirosian [65] who gave their name to the STM-Extension (sometimes also TMS-Extension). These are the point-interacting self-adjoint extensions of the non-interacting Hamiltonian restricted away from the hyperplanes of interactions which behave physically, avoiding non-local point interactions. We will discuss this issue in more detail in section 1.2.1. A first rigorous analysis of the three particle problem was given by Minlos and Faddeev [49].

It turns out that a model of three point interacting bosons is unstable, i.e. the spectrum of the associated Hamiltonian is not bounded from below. This is even true if one considers a system of two different species of bosons with point-interactions only between the species [11, 13]. Because of this unbounded spectrum it is not clear whether an associated self adjoint operator exists at all.

Contrary to this, the three-body problem of two species of fermions with point interactions between different species is well posed under suitable conditions [11–13, 44–48, 59]. An important parameter is the mass ratio between the mass of the single particle and the mass of the other two, which is critical to the question of stability. By setting the mass of one of the species to one, the mass of the second species is equivalent to the mass ratio. In the following we will therefore denote the mass ratio simply by the mass.

It was shown in [11] that there exists a critical mass $m^* = 0.0735$ such that for all masses

$m \geq m^*$ the energy is bounded from below. This bound is sharp and for $m < m^*$ it was shown in [59] that the system is indeed unstable. The reason that one can calculate such sharp analytic bounds is that the question of stability can be reduced to a one body problem as point interactions effectively only happen when two particles sit on top of each other.

Being effectively a one body problem the $2 + 1$ model allows studying more detailed questions about the spectrum going beyond a lower bound [4]. Another question one can ask is if it possible to define physically interesting point-interacting systems beside the one we will introduce in section 1.2.3. It was shown in [12] that there is a critical mass $m^{**} = 0.116$ such that for the unitary system, i.e. for infinite scattering length, with masses $m^* \leq m \leq m^{**}$ there are additional self adjoint extensions possible which correspond to three body interactions. Also in [47,48] it was shown that there are other extensions possible but their interpretation is not as clear.

In [11] it was also shown that there is a critical mass $m^*(N)$ for the $N + 1$ problem, i.e. N non-interacting fermions and a point interacting impurity, such that the system is stable if $m > m^*(N)$. This critical mass behaves by far not optimal and in particular $m^*(N) \sim N$. We emphasize that one would expect that $m^*(N) \leq 1$ uniformly in N. Only then there exists a mass range independent on N such that the $N + 1$ and the $1 + N$ problem is stable. We recall that the $1 + N$ system is, up to an overall factor, equivalent to the $N + 1$ system with inverted mass. The reason that we expect this is that we suspect that the $N + M$ model, i.e. two species of fermions with interactions between them, is stable for certain masses, which is suggested by experiments (see [75] and references therein). By separating particles it is clear that this can only be the case if the $N + 1$ and the $1 + M$ system is stable for a given mass and arbitrary N and M.

We were able to show stability for the $N + 1$ system for masses above an N independent critical mass $\tilde{m}_1 = 0.36$ [50] which we will present in Chapter 2. This result tells us that there are no $N+1$ particle states with negative energy for the unitary gas. The existence of states with negative energy for the unitary gas is, due to scale invariance, which we will define properly in section 1.1.2, directly linked to instability.

Besides studying the $N + 1$ model one can also investigate few body problems in more detail. In particular the $2 + 2$ model is of interest as it is not clear whether a four body collapse can happen for masses where the $2 + 1$ and the $1 + 2$ system is stable. Numerically this problem was discussed in [42] where the authors concluded that the system is indeed stable for a mass equal to one. Further, in [18] it was claimed that the critical mass of stability should be equal to the one of the $2 + 1$ system. In [53] we were able to prove that there is a critical mass $\tilde{m}_2 = 0.58$ such that the system is stable for $m \in [\tilde{m}_2, \tilde{m}_2^{-1}]$. In Chapter 4, we present this proof.

The results for the $N + 1$ and the $2 + 2$ model suggest that the $N + M$ model might be stable for certain mass regions. Still, it could be that a energy collapse happens for states with higher number of particle in both species and causes the spectrum to be unbounded. We will introduce in 1.2.3 the general $N + M$ problem and point out the difficulties in showing stability.

Another question we investigated in [52] and which we will discuss in Chapter 3 is to investigate the energy contribution of introducing an impurity into the system. For this it is not suitable to work with a zero-density model, i.e. a fixed number of particles on $\mathbb{R}^3$, as we will see that the particles will separate in an approximate ground state even though the interaction is attractive. Instead, we will restrict to wavefunctions which have support in a fixed box and obtain a system with a fixed mean density. Because of this restriction, the energy will be to leading order the non-interacting kinetic energy. We will prove that the corrections for introducing an impurity can be bounded uniformly in N in terms of the mean density and the scattering length. As this bound depends only on local quantities, we view the impurity as a local perturbation.

In 2008 Tan discussed in a series of papers [62–64] a collection of relations, named Tan relations, connecting basic quantities of a point-interacting model. These Tan relations are of high interest also for the experimental implementation as they allow getting crucial information about the point-interacting part of the wavefunction out of its abnormally large momentum tail. In Chapter 2, we will put these relations for the $N + 1$ system on a solid mathematical basis.

The $N + M$ model is a specific system of point interactions and in general one can raise the question if there are other interesting models describing a point-interacting gas. In [25] a model based on a Dirichlet form was investigated and a Lieb-Thirring type inequality was proved. This system models point interactions and is well-defined for any number of particles but it contains many-body point interactions, i.e. the strength of the point interactions between two particles depends on the position of all the others. In [51] we showed that the model becomes trivial in the thermodynamic limit for fixed temperature, in the sense that the free energy per particle is the one of non-interacting particles in the thermodynamic limit. We will present this proof in Chapter 5.

1.1.1 Cold atomic gases

As mentioned above an experimentally accessible way of investigating point interactions is by using cold gases. We consider a gas of atoms in a three-dimensional box with mean density ρ. In the following we will discuss the appearing length scales and argue why a point interacting model can be a suitable description and what the advantages of this system are. For a more thorough introduction see [8, 75].

We start by defining relevant length scales appearing in this trapped gas. The first one is the mean particle distance which is comparable to $\rho^{-1/3}$ as long as there are no bound states. Further the thermal wavelength λ_T measures how much each particle wavefunction is spread out. The interaction range of the atomic potentials we denote by r_0 and the S-wave scattering length by a. See [33] for a rigorous definition of the scattering length and [8] for a different approach. At low energies the interaction range r_0 is, in most setups, basically the van der Waals length [75].

The interaction for a two-body system is determined by the scattering length for low energies, i.e. low temperatures and therefore large λ_T in comparison with r_0. In a many particle system this also holds under the condition that $\rho^{-1/3} \gg r_0$ which ensures that scattering is dominated by two particle collisions. In this case the particles are effectively separated such that only two-body collisions can occur. Hence, we want to ensure the relation [75]

$$r_0 \ll \rho^{-1/3} \lesssim \lambda_T. \tag{1.1.1}$$

We cannot expect to choose these scales freely within a real life experiment, and we discuss next which ones are accessible in an experiment. The density can be chosen freely within certain limits and particularly it is easy to create low densities. By adjusting the temperature we can control λ_T. Here it becomes clear why we need cold atomic gases as λ_T grows with decreasing temperature. The range of the interaction r_0 is hard to change, and we have to consider it to be fixed. Crucial to fulfill (1.1.1) is to choose ρ and the temperature small.

One of the reasons why cold gases are an ideal way of investigating point interactions experimentally is that it is also possible to tune the scattering length to arbitrary values, even infinity, using Feshbach resonances [8]. These resonances happen if the energy of bound states in a closed scattering channel is close to the energy of an open channel. Usually the energy of the bound state is tuned magnetically but in cases where this is not possible there exists also an optical version.

The ability of tuning the scattering length allows one to investigate the gas with infinite scattering length which is called the unitary limit (sometimes we say unitary system for a system in the unitary limit). This is a special case and in particular interesting as it develops additional symmetries.

A crucial ingredient for the above arguments was that the mean particle distance is of order $\rho^{-1/3}$. For an unstable model, like for bosons, bound states will exist and particles would be much closer to each other. We cannot assume that a point-interacting model will accurately describe thermal states of these systems.

1.1.2 Efimov effect, Thomas effect and Stability

Already in 1935 Thomas [68] realized that a system of three bosons interacting with point interactions is inherently unstable. With unstable we mean that the Hamiltonian is not bounded from below which is, in this setting, also called the Thomas effect.

The Thomas effect is inherently linked to the existence of states with negative energy for the unitary gas. Let in the following F denote the quadratic form associated to the unitary gas on $\mathbb{R}^3$ which we will introduce properly in Section 1.2.3. As this system has no associated length scales it is easy to see that the quadratic form F is scale invariant, i.e.

$$F(\psi^\eta) = \eta^2 F(\psi) \tag{1.1.2}$$

for $\psi^\eta(x) = \eta^{3N/2}\psi(\eta x)$ where N is the total particle number and $x \in \mathbb{R}^{3N}$ the set of coordinates. This scale invariance immediately shows that as soon as we find a state with negative energy we can rescale it to smaller length scales to find a state with arbitrary negative energy. Hence, the unitary gas can only be stable if the ground state energy is positive.

The above argumentation also works for finite scattering length. In this case, when rescaling lengths as in (1.1.2) by η, we have to additionally rescale the scattering length by $a \to \eta a$. As we want to take the limit $\eta \to \infty$ we see that also $\eta a \to \infty$ and the problem reduces to the unitary case. In other words, the reason the argument works is that even a finite scattering length is large in comparison with the length scale associated with a small collapsed state.

Another widely discussed concept is the Efimov effect first described by Efimov in 1970 [17]. For a review see [8]. It applies to a system of particles with two-body interactions where only two-body resonances exist. Contrary to point interactions the microscopic structure of the potential is not neglected and in particular the effective range r_0 is finite. The Efimov effect says that there is an infinite sequence of three-body bound states with energies $(E_n)_n$ accumulating at zero. For large n, i.e. E_n close to zero, the states are spatially extended in comparison with

r_0 and because of that the microscopic structure of the interaction is unimportant. In particular one finds the universal behavior

$$\frac{E_{n+1}}{E_n} \to \frac{1}{515.03}. \tag{1.1.3}$$

In contrast to the spatially extended wavefunctions associated with E_n for n large, the wavefunctions for small n have a spatial size of the same order as r_0. On this scale the behavior is dominated by the microscopic structure of the potential and one cannot expect any universal behavior.

The two effects described above are linked as we obtain the Thomas effect by taking a scaling limit of a system where the Efimov effect applies. The scaling effectively decreases r_0 and in the limit there will be states for arbitrary negative energies.

The above argumentation shows that investigating the ground state in a model of point interactions for bosons is a bad idea as its physical ground state will depend strongly on r_0 which is neglected in a point interacting model.

In an experimental setup it can still be useful to describe the unitary Bose gas by a point interacting model (see [22, 23] and references therein). Such a system has no thermal states as the spectrum is unbounded from below. Hence, such a model cannot predict the energy of a cold gas of bosons in an experiment at thermal equilibrium. Nevertheless, it is possible that such a point interacting model gives a good approximation for the energies of states where particles have a mean particle distance larger than the effective range of the interaction. It is not clear if the physical system can be accurately described by a self-adjoint Hamiltonian.

Due to the rapid formation of three-body bound states the lifetime of a bosonic point-interacting gas is much shorter than the, at least for certain masses, stable fermionic counterpart. In fact, the experimental setup is ill described by a particle number conserving model as the three-body bound states usually escape the trap and are effectively removed from the system. Still, it is possible to measure the energy and the particle decay of artificially prepared states during the short lifetime of the gas. Such experiments were for example done in [22,23], and they give interesting insight into how three-body losses affect the system.

1.2 Models

A priori it is not clear what is even meant with a model of point interactions. Roughly speaking we want to give a meaning to the formal Hamiltonian

$$\text{“}H = -\frac{1}{2}\sum_{i=1}^{N} \Delta_{x_i} - \frac{1}{2m}\sum_{j=1}^{M} \Delta_{y_j} + \gamma \sum_{i=1}^{N}\sum_{j=1}^{M} \delta(x_i - y_j)\text{”} \tag{1.2.1}$$

for $N, M \geq 1$ and $y_i, x_j \in \mathbb{R}^3$ for $1 \leq i \leq N, 1 \leq j \leq M$. The Hamiltonian H is ill-defined as functions in $H^1(\mathbb{R}^3)$, which is the form domain of the Laplacian, are non-continuous and therefore the δ interaction term has no a priori meaning.

In section 1.2.1, we will show how to solve this problem for the two particle case. In this toy model case everything can be solved explicitly as it is effectively a one body problem. We discussed that a good notion for defining point interactions is looking for extensions of the non-interacting operator defined on functions supported away from the hyperplanes of interactions. Constructing all self-adjoint extensions will be easy in this toy model case, and we follow this approach in section 1.2.1.

In the main part of this section we will derive a model for $N+M$ particles interacting with point interactions following [20]. The model is obtained by a formal limit using a cutoff in momentum space. We will not make this limit rigorous but it should be viewed as a motivation to define the corresponding quadratic form.

In the last section 1.2.4 we will discuss how the $N+M$ model simplifies for $M = 1$. In particular it is then convenient to separate the center of mass motion and work in relative coordinates.

We note that this limit was carried out rigorously in two dimensions [15, 16, 35].

1.2.1 The two particle problem

In this section we will discuss the $1+1$ model and how it can be defined. We will use it to introduce an electrostatic point of view and associated surface charges. We will see that this two particle model will agree with the $N+1$ system in relative coordinates, which we will introduce in section 1.2.4, if $N = 1$.

We denote the non-interacting two-particle Hamiltonian for one particle with mass 1 and one with mass m in three dimensions by

$$H_0 = -\frac{1}{2}\Delta_{x_1} - \frac{1}{2m}\Delta_{x_2} \tag{1.2.2}$$

where $x_1, x_2 \in \mathbb{R}^3$. We define the hyperplane of interactions as

$$\mathcal{S} = \{(x_1, x_2) \mid x_1, x_2 \in \mathbb{R}^3, x_1 = x_2\}. \tag{1.2.3}$$

The idea is that H_0 is identical to the operator of point interactions if we restrict to functions in $C_0^\infty(\mathbb{R}^6 \setminus \mathcal{S})$. The full Hamiltonian can be recovered using self adjoint extensions.

For further analysis it is convenient to work in the relative frame using the variable transformation

$$y = x_2 - x_1, \qquad Y = \frac{1}{m+1}x_1 + \frac{m}{m+1}x_2. \tag{1.2.4}$$

Applying this transformation to H_0 we get

$$H_0 = -\frac{1}{2(m+1)}\Delta_Y - \frac{m+1}{2m}\Delta_y \tag{1.2.5}$$

and the hyperplane of interactions can be written in the new variables as $\mathcal{S} = \{(Y, y) \mid y = 0\} = \mathbb{R}^3 \times \{0\}$. To find self adjoint extensions of H_0 it suffices to find them for Δ_Y and Δ_y separately. As $\mathcal{S}$ does not restrict Y and because Δ_Y is essentially self adjoint on $\mathbb{C}_0^\infty(\mathbb{R}^3)$, the problem reduces to finding extensions of

$$\tilde{H}_0 = -\left.\Delta_y\right|_{C_0^\infty(\mathbb{R}^3 \setminus \{0\})}. \tag{1.2.6}$$

To apply von Neumann extensions theory (see [56] as a reference) to $\tilde{H}_0$ we need to find in particular non-trivial L^2 solutions to the equation

$$\tilde{H}_0^* \psi = E\psi \tag{1.2.7}$$

for $E = \pm i$. More generally the function

$$\psi_E = \sqrt{\frac{\pi}{2}} \frac{e^{i\sqrt{E}|x|}}{|x|} \quad \text{with } \operatorname{Im}(\sqrt{E}) > 0 \tag{1.2.8}$$

solves the equation for $E \in \mathbb{C}$ fixed and it is the only non-trivial solution in $L^2(\mathbb{R}^3)$. In the sense of distributions we get $(-\Delta - E)\psi_E = (2\pi)^{3/2}\delta$ and we will call ψ_E therefore the fundamental solution of $(-\Delta - E)$. For short, we will denote $\psi_+ = \psi_i$ and $\psi_- = \psi_{-i}$. Using von Neumann extension theory we find a one parameter family of self adjoint extensions H_κ for $\kappa \in (-\pi, \pi]$:

$$\begin{aligned} D(H_\kappa) &= \{\phi + \eta(\psi_+ + e^{i\kappa}\psi_-) \mid \phi \in H^2(\mathbb{R}^3), \phi(0) = 0, \eta \in \mathbb{C}\} \\ H_\kappa(\phi + \eta(\psi_+ + e^{i\kappa}\psi_-)) &= H_0\phi + i\eta(\psi_+ - e^{i\kappa}\psi_-) \end{aligned} \tag{1.2.9}$$

The conditions on ϕ are the ones needed such that ϕ is in the domain of the closure of $\tilde{H}_0$. The case $\kappa = \pi$ corresponds to the non-interacting system as $\psi_+ - \psi_- \in H^2(\mathbb{R}^3)$.

It will be convenient to reformulate this definition. We note that

$$\psi_+ + e^{i\kappa}\psi_- - (1 + e^{i\kappa})\psi_{-\mu} \in H^2(\mathbb{R}^3) \tag{1.2.10}$$

where $\mu > 0$ is an arbitrary smoothing parameter. We define $\eta = \xi/(1 + e^{i\kappa})$,

$$\alpha = 2\pi^2 \frac{i\sqrt{i} + i\sqrt{-i}e^{i\kappa}}{(1 + e^{i\kappa})} = \sqrt{2}\pi^2 (\tan(\kappa/2) - 1) \in \mathbb{R} \cup \{\infty\} \tag{1.2.11}$$

and

$$\phi_\mu = \phi + \xi \frac{(\psi_+ + e^{i\kappa}\psi_-)}{(1 + e^{i\kappa})} - \xi\psi_{-\mu}. \tag{1.2.12}$$

With these notations we can reformulate the operator as $\tilde{H}_\alpha = H_{\kappa(\alpha)}$ and get

$$\begin{aligned} D(\tilde{H}_\alpha) &= \{\phi_\mu + \xi\psi_{-\mu} \mid \phi_\mu(0) = (2\pi)^{-3/2}\xi(\alpha + 2\pi^2\sqrt{\mu})\} \\ (\tilde{H}_\alpha + \mu)(\phi_\mu + \xi\psi_{-\mu}) &= (H_0 + \mu)\phi_\mu. \end{aligned} \tag{1.2.13}$$

It is easy to check that α can take indeed all values in $\mathbb{R} \cup \{\infty\}$. We emphasize that even though μ appears explicitly in above formula the Hamiltonian and its domain are independent of it. The choice of α might seem arbitrary but it is directly linked to the scattering length. For ψ with $\psi \in H_\alpha$ we get for small $|x|$ that

$$\psi(x) \propto \frac{2\pi^2}{\alpha|x|} + 1 + o(1). \tag{1.2.14}$$

Hence, α is connected to the scattering length a by $\alpha = -2\pi^2 a^{-1}$.

We can derive the quadratic form in a straight-forward way from the Hamiltonian. Denoting $\varphi = \phi_\mu + \xi\psi_{-\mu}$ we get

$$\begin{aligned}\langle\varphi|(\tilde{H}_\alpha + \mu)\varphi\rangle &= \langle\varphi|(H_0 + \mu)\phi_\mu\rangle \\ &= \langle\phi_\mu|(H_0 + \mu)\phi_\mu\rangle + \xi^*\langle\psi_{-\mu}|(H_0 + \mu)\phi_\mu\rangle \\ &= \langle\phi_\mu|(H_0 + \mu)\phi_\mu\rangle + (2\pi)^{3/2}\xi^*\phi_\mu(0) \\ &= \langle\phi_\mu|(H_0 + \mu)\phi_\mu\rangle + |\xi|^2(\alpha + 2\pi^2\sqrt{\mu})\end{aligned}$$

This allows us to define the quadratic form F_α by

$$\begin{aligned}D(F_\alpha) &= \{\phi = \phi + \xi\psi_{-\mu} \mid \phi \in H^1(\mathbb{R}^3), \xi \in \mathbb{C}\} \\ F_\alpha(\psi) &= \langle\phi|(H_0 + \mu)\phi\rangle - \mu\,||\psi||^2 + |\xi|^2(\alpha + 2\pi^2\sqrt{\mu})\end{aligned} \tag{1.2.15}$$

The term $\langle\phi|(H_0+\mu)\phi\rangle$ should be interpreted as the quadratic form associated with $H_0+\mu$ which has the form domain $H^1(\mathbb{R}^3)$.

The quantities ξ and $\psi_{-\mu}$ can be interpreted in an electrostatic picture. Here ξ is a charge sitting at the origin and $(H_0 + \mu)^{-1}\xi\delta = \xi\psi_{-\mu}$ is the field it creates. The overall wavefunction consists of a regular part ϕ_μ which does not see the interaction at all and a singular part $\xi\psi_{-\mu}$ which originates from the interaction. We call ξ the surface charge because it lives on the hyperplanes of interactions which consist only of the origin in this toy model. In the following we will call the ξ dependent terms of the quadratic form its singular part and $\langle\phi_\mu|(H_0 + \mu)\phi_\mu\rangle$ the regular part.

At first glance it seems that the quadratic form is more involved than the operator given by (1.2.13) but the complexity is hidden in the condition for $\phi_\mu(0)$. For more particles the connection between ϕ_μ and ξ on the operator level will be given by a complicated integral equation. For the quadratic form on the other hand ϕ_μ and ξ can be chosen completely independent of each other but its action is more involved than for the Hamiltonian.

For this $1 + 1$ model there is no problem with stability as we see from the definition of $F(\psi)$ that

$$\frac{F(\psi)}{||\psi||^2} \geq -\mu + |\xi|^2(\alpha + 2\pi^2\sqrt{\mu}) \geq -\frac{\alpha_-^2}{4\pi^4} \tag{1.2.16}$$

choosing $\mu = (4\pi^4)^{-1}\alpha_-^2$ with α_- being the negative part of α, i.e. $\alpha_- = \frac{1}{2}(|\alpha| - \alpha)$. In particular the whole family of extensions is stable independent of the masses of both particles.

Because every function in $\psi \in H^1(\mathbb{R}^3)$ is a valid trial function for $F(\psi)$ we see that

$$\inf_{\psi\in D(\tilde{H}_\alpha)}\langle\psi|\tilde{H}_\alpha\psi\rangle \leq \inf_{\psi\in D(H_0)}\langle\psi|H_0\psi\rangle. \tag{1.2.17}$$

In this sense all the interactions are attractive which will also be true in the general case.

In this simple model we can also see the large momentum tail of the wavefunction which was first discovered by Tan [62–64]. Consider $\varphi = \phi_\mu + \xi\psi_{-\mu} \in D(\tilde{H}_\alpha)$. Even though φ is not in $H^1(\mathbb{R}^3)$ we get that

$$\hat{\varphi}(p) - \frac{\xi}{p^2 + \mu} \in L^2(\mathbb{R}^3, (1 + p^2)) \tag{1.2.18}$$

and in this sense the wavefunction falls off slowly in momentum space. We emphasize that if we would choose any other constant than ξ in (1.2.18), the resulting function would fail to be in $L^2(\mathbb{R}^3, (1+p^2))$. This connection allows one to determine ξ from investigating the large momentum tail which is commonly done in experiments. We emphasize that (1.2.18) is a simple version applying only to the $1+1$ model. We will discuss a more general case in Chapter 2 where we will formulate rigorous versions of the Tan relations for the $N+1$ model.

There are various ways of how to construct $\tilde{H}_\alpha$. One physically intuitive approach is to take a Hamiltonian of two particles interacting with a potential V having a zero-energy resonance and take a scaling limit. Hence, we ask if there is a limiting object for

$$-\frac{1}{2}\Delta_1 - \frac{1}{2m}\Delta_2 + \varepsilon^{-2} V\left(\frac{x-y}{\varepsilon}\right). \tag{1.2.19}$$

For nice potentials this limit exists in the norm resolvent sense and equals the unitary two-body point interacting Hamiltonian $\tilde{H}_0$ [1]. This result can be extended to arbitrary scattering lengths if one considers an additional $\varepsilon^{-1} V\left(\frac{x-y}{\varepsilon}\right)$ term with a suitable prefactor [1].

We consider this approach to be most realistic as this scaling limit is approximately implemented in experiments. Nevertheless, this limit in the norm resolvent sense, is rigorously only established in the case of two particles [1] and for three particles in one dimension [3]. As mentioned before, we note that the rigorous constructions using momentum cutoffs in two dimensions are only valid in the weaker strong resolvent sense.

The simplicity of this $1+1$ system hides one major complication in constructing an extension. Because the hyperplane of interactions is, after removing the center off mass motion, just zero dimensional we get a one parameter family of extensions. As soon as the hyperplane has a higher dimension, there are a lot more extensions possible, and they need to be parameterized using functions [44]. Most of these are physically uninteresting because they violate locality in the sense that the strength of the point-interaction between two particles can depend on the coordinates of all the others.

To avoid these issues one usually considers a subset of all possible extensions called the STM-Extensions. For our construction of the $N+M$ model in section 1.2.3 we will use a different approach where we regularize using a cutoff in momentum space. With this approach the interactions between two particles are naturally independent of all other particles and if the limiting form gives rise to an operator it should be an STM-Extension.

We note that the results we present in Chapter 5 will not consider an STM-Extension as the model discussed contains non-local point interactions.

1.2.2 Dimensionality

In the context of this three-dimensional $1+1$ model we will discuss the differences in other dimensions. The dimension entered in solving (1.2.7). In momentum space we can write the equation $\tilde{H}_0^* \psi = \pm i\psi + (2\pi)^{3/2}\delta$ as

$$p^2 \hat{\psi} = \pm i \hat{\psi} + 1 \tag{1.2.20}$$

with the solutions

$$\hat{\psi}_\pm(p) = \frac{1}{p^2 \pm i}. \tag{1.2.21}$$

Its derivative is given by $\widehat{\nabla\psi_\pm} = i(2\pi)^{-3/2} p(p^2 \pm i)^{-1}$ and falls off like p^{-1}.

$d = 1$**:** In one dimension both $(p^2 \pm i)^{-1}$ and $p(p^2 \pm i)^{-1}$ are functions in $L^2(\mathbb{R})$ which allows us to implement the point interactions as a potential. This is equivalent to noticing that $H^1(\mathbb{R})$ functions are continuous which makes a delta interaction well-defined. For two particles, the Hamiltonian can be constructed as a norm resolvent limit of

$$-\frac{1}{2}\partial_1^2 - \frac{1}{2m}\partial_2^2 + \varepsilon^{-1}V\left(\frac{x-y}{\varepsilon}\right) \tag{1.2.22}$$

for $\varepsilon \to 0$ and a sufficiently regular potential V [1].

$d = 2, 3$**:** In these cases the function $(p^2 + \mu)^{-1}$ is in $L^2(\mathbb{R}^2)$ and $L^2(\mathbb{R}^3)$ respectively but the derivative $p(p^2 + \mu)^{-1}$ is not. Still, the behavior in these cases is very different.

In three dimensions we have argued that there is a unitary limit which is scale invariant. This scale invariance is responsible for the unboundedness of the spectrum if a state with negative energy exists. The invariance naturally shows when writing the unitary two-body system as a limit of the operators with regular potentials V as above:

$$-\frac{1}{2}\Delta_1 - \frac{1}{2m}\Delta_2 + \varepsilon^{-2}V\left(\frac{x-y}{\varepsilon}\right) \tag{1.2.23}$$

This limit was establish in the norm resolvent sense for $\varepsilon \to 0$ in [1].

In two dimensions there is no unitary case and in particular the singular part of the functional scales differently than the regular part. As a consequence, the functional is always bounded from below. In [1] it was shown that the Hamiltonian can be obtained by a norm resolvent limit of the operators

$$-\frac{1}{2}\Delta_1 - \frac{1}{2m}\Delta_2 + \lambda\left((\log(\varepsilon))^{-1}\right)\varepsilon^{-2}V\left(\frac{x-y}{\varepsilon}\right) \tag{1.2.24}$$

with $\lambda(\eta) = \lambda_1\eta + \lambda_2\eta^2 + o(\eta^2)$ for certain values of λ_1, λ_2 and $\varepsilon \to 0$ with V sufficiently regular.

$d \geq 4$**:** In high dimensions with $d \geq 4$ the fundamental solutions $(p^2 + \mu)^{-1}$ are not in $L^2(\mathbb{R}^d)$ and therefore there are no non-trivial solutions to (1.2.7) which makes point interactions impossible.

1.2.3 The $N + M$ model

In this section we will introduce a model for N particles of one kind and M particles of another kind interacting with point interactions in three dimensions. The model will be presented for general particles but in section 1.2.3.1 we will simplify it in the case of fermions which will be our primary focus. We will give a rigorous meaning to (1.2.1) which is ill-defined in three dimensions. There are various ways how to achieve this, but we will restrict to a regularization in momentum space similar to [20]. We will not prove any rigorous statement about the convergence, but we see this as a motivation for defining the quadratic form. For a rigorous version in two dimensions see [15, 16, 35].

In momentum space the Hamiltonian is formally given by

$$\widehat{H\psi}(p,q) = h_0(p,q)\hat{\psi}(p,q) - \gamma\sum_{(i,j)}\langle \mathrm{id}_{i,j}|\hat{\psi}\rangle \tag{1.2.25}$$

with $p=(p_1,\dots,p_N), q=(q_1,\dots,q_M), \sum_{(i,j)}=\sum_{i=1}^N\sum_{j=1}^M$,

$$h_0(p,q)=\sum_{i=1}^N \frac{p_i^2}{2}+\sum_{j=1}^M \frac{q_j^2}{2m} \tag{1.2.26}$$

and

$$\begin{aligned}&\langle \mathrm{id}_{i,j}|\hat\psi\rangle(p_i+q_j,\hat p_i,\hat q_j)\\ &\quad=\int \hat\psi(p_1,\dots,\underset{\substack{\uparrow\\ i\text{-th}}}{p_i+z},\dots,p_N,q_1,\dots,\underset{\substack{\uparrow\\ j\text{-th}}}{q_j-z},\dots,q_M)\,\mathrm{d}z\\ &\quad=\int \hat\psi(p_1,\dots,\frac{1}{m+1}(p_i+q_j)+z,\dots,\\ &\qquad\qquad p_N,q_1,\dots,\frac{m}{m+1}(p_i+q_j)-z,\dots,q_N)\,\mathrm{d}z.\end{aligned} \tag{1.2.27}$$

The last equality we obtain using the substitution $z\to z-(\frac{m}{m+1}p_i-\frac{1}{m+1}q_j)$ and $\hat p_i=(p_1,\dots,p_{i-1},p_{i+1},\dots,p_N)$, $\hat q_j=(q_1,\dots,q_{j-1},q_{j+1},\dots,q_M)$. The non-interacting Hamiltonian, which we obtain by a Fourier transform of h_0, we denote by H_0.

For some $R>0$ we introduce the cutoff function $\chi_R^{i,j}$ which is given by

$$\chi_R^{i,j}(p,q)=\chi_{B_R}\left(\frac{m}{m+1}p_i-\frac{1}{m+1}q_j\right) \tag{1.2.28}$$

where B_R denotes the ball with radius R and χ_{B_R} its indicator function. For a fixed R we define the operator:

$$\widehat{H_R\psi}=h_0(p,q)\hat\psi(p,q)-\gamma_R\sum_{(i,j)}\langle\chi_R^{i,j}|\hat\psi\rangle(p_i+q_j,\hat p_i,\hat q_j)\chi_{B_R}\left(\frac{m}{m+1}p_i-\frac{1}{m+1}q_j\right) \tag{1.2.29}$$

with

$$\langle\chi_R^{i,j}|\hat\psi\rangle=\int\chi_{B_R}(z)\hat\psi\left(p_1,\dots,\frac{m}{m+1}(p_i+q_j)+z,\dots,p_N,q_1,\dots,\frac{m}{m+1}(p_i+q_j)-z,\dots,q_N\right) \tag{1.2.30}$$

The operator $H_R\psi$ is, differently than (1.2.25), well-defined and in the following we will establish a limiting quadratic form for $R\to\infty$ by choosing γ_R in the right way.

For short, we define the following quantities

$$\begin{aligned}\hat\xi_{i,j}^R(p_i+q_j,\hat p_i,\hat q_j)&:=\gamma_R\langle\chi_R^{i,j}|\hat\psi\rangle(p_i+q_j,\hat p_i,\hat q_j)\\ \hat\rho_{i,j}^R(p,q)&:=\hat\xi_{i,j}^R(p_i+q_j,\hat p_i,\hat q_j)\chi_{B_R}\left(\frac{m}{m+1}p_i-\frac{1}{m+1}q_j\right)\\ \hat\rho^R(p,q)&:=\sum_{(i,j)}\hat\rho_{i,j}^R(p,q)\end{aligned}$$

and we fix ϕ_μ^R by

$$\hat\psi=\hat\phi_\mu^R+\widehat{G_\mu\rho^R},\qquad \widehat{G_\mu\rho^R}:=\frac{\hat\rho^R}{h_0+\mu} \tag{1.2.31}$$

where $\mu > 0$ is a smoothing parameter. We will also use $G_\mu(p,q) = (h_0(p,q)+\mu)^{-1}$. For the quadratic form we get

$$\begin{aligned}\langle\psi|H_R\psi\rangle &= \langle\psi|H_0\psi\rangle - \langle\hat{\psi}|\hat{\rho}^R\rangle \\ &= \langle\hat{\phi}^R_\mu + \widehat{G_\mu\rho^R}|(h_0+\mu)(\hat{\phi}^R_\mu + \widehat{G_\mu\rho^R})\rangle - \mu\,\|\psi\|^2 - \langle\hat{\psi}|\hat{\rho}^R\rangle \\ &= \langle\hat{\phi}^R_\mu|(h_0+\mu)\hat{\phi}^R_\mu\rangle + \langle\hat{\rho}^R|\hat{\phi}^R_\mu\rangle + \langle\hat{\phi}^R_\mu|\hat{\rho}^R\rangle + \langle\widehat{G_\mu\rho^R}|\hat{\rho}^R\rangle - \mu\,\|\psi\|^2 - \langle\hat{\psi}|\hat{\rho}^R\rangle \\ &= \langle\hat{\phi}^R_\mu|(h_0+\mu)\hat{\phi}^R_\mu\rangle - \mu\,\|\psi\|^2 - \langle\widehat{G_\mu\rho^R}|\hat{\rho}^R\rangle + \langle\hat{\psi}|\hat{\rho}^R\rangle \end{aligned} \tag{1.2.32}$$

With the aid of $\xi^R_{i,j}$ we can rewrite $\langle\hat{\psi}|\hat{\rho}^R\rangle$ in a more convenient form:

$$\langle\hat{\psi}|\hat{\rho}^R\rangle = \sum_{(i,j)}\langle\hat{\psi}|\langle\chi^{i,j}_R|\hat{\psi}\rangle\otimes|\chi^{i,j}_R\rangle\rangle = \gamma_R^{-1}\sum_{(i,j)}\left\|\gamma\langle\chi^{i,j}_R|\hat{\psi}\rangle\right\|^2 = \gamma_R^{-1}\sum_{(i,j)}\left\|\xi^R_{i,j}\right\|^2. \tag{1.2.33}$$

The second to last term in (1.2.32) contains a double sum which we use to split (1.2.32) into four different parts and get

$$\begin{aligned}\langle\widehat{G_\mu\rho^R}|\hat{\rho}^R\rangle &=: -\sum_{i=0}^{3}\tilde{\Phi}^R_i(\vec{\rho}^R) \\ &= \sum_{(i,j)}\int|\xi^R_{i,j}(p_i+q_j,\hat{p}_i,\hat{q}_j)|^2\langle\chi^{i,j}_R|G_\mu|\chi^{i,j}_R\rangle\,\mathrm{d}p\,\mathrm{d}q \\ &+ \sum_{(i,j)}\sum_{\substack{n=1\\n\neq j}}^{N}\int\langle\chi^{i,j}_R|\overline{\hat{\xi}^R_{i,j}}(p_i+q_j,\hat{p}_i,\hat{q}_j)\hat{\xi}^R_{n,j}(p_n+q_j,\hat{p}_n,\hat{q}_j)G_\mu(p,q)|\chi^{n,j}_R\rangle\,\mathrm{d}p\,\mathrm{d}q \\ &+ \sum_{(i,j)}\sum_{\substack{m=1\\n\neq j}}^{M}\int\langle\chi^{i,j}_R|\overline{\hat{\xi}^R_{i,j}}(p_i+q_j,\hat{p}_i,\hat{q}_j)\hat{\xi}^R_{i,m}(p_i+q_m,\hat{p}_i,\hat{q}_m)G_\mu(p,q)|\chi^{i,m}_R\rangle\,\mathrm{d}p\,\mathrm{d}q \\ &+ \sum_{(i,j)}\sum_{\substack{(m,n)\\m\neq i\\n\neq j}}\int\langle\chi^{i,j}_R|\overline{\hat{\xi}^R_{i,j}}(p_i+q_j,\hat{p}_i,\hat{q}_j)\hat{\xi}^R_{n,m}(p_n+q_m,\hat{p}_n,\hat{q}_m)G_\mu(p,q)|\chi^{n,m}_R\rangle\,\mathrm{d}p\,\mathrm{d}q\end{aligned} \tag{1.2.34}$$

using $\vec{\rho}^R = (\rho^R_{i,j})_{(i,j)}$. We note that $\tilde{\Phi}^R_2, \tilde{\Phi}^R_3$ vanish if we fix $M = 1$ and similarly $\tilde{\Phi}^R_1, \tilde{\Phi}^R_3$ vanish if we set $N = 1$. In this sense we view $\tilde{\Phi}_1$ as the $N+1$, $\tilde{\Phi}^R_2$ as the $1+M$ and $\tilde{\Phi}_3$ as the full $N+M$ particle contribution.

The expressions $\tilde{\Phi}^R_1, \tilde{\Phi}^R_2$ and $\tilde{\Phi}^R_3$ are all well-defined if we take the formal limit $R \to \infty$. This is not true for $\tilde{\Phi}_0$ which contains the divergent part. Because $|\xi(p_i+q_j,\hat{p}_i,\hat{q}_j)|^2$ is not dependent of $\frac{m}{m+1}p_i - \frac{1}{m+1}q_j$ we can perform the integration explicitly and obtain

$$\begin{aligned}\tilde{\Phi}^R_0 &= \sum_{(i,j)}\int|\xi^R_{i,j}(p_i+q_j,\hat{p}_i,\hat{q}_j)|^2\langle\chi^{i,j}_R|G_\mu|\chi^{i,j}_R\rangle\,\mathrm{d}p\,\mathrm{d}q \\ &= \sum_{(i,j)}\int\chi_{B_R}(z)\frac{|\hat{\xi}^R_{i,j}(w,\hat{p}_i,\hat{q}_j)|^2}{\frac{1}{2(m+1)}w^2+\frac{m+1}{2m}z^2+\frac{1}{2}\hat{p}_i^2+\frac{1}{2m}\hat{q}_j^2+\mu}\,\mathrm{d}\hat{p}_i\,\mathrm{d}\hat{q}_j\,\mathrm{d}w\,\mathrm{d}z.\end{aligned} \tag{1.2.35}$$

We used the transformation $q_j = \frac{m}{m+1}w - z$, $p_i = \frac{1}{m+1}w + z$ which allows us to write $h_0(\vec{p},\vec{q})$ as

$$h_0(\vec{p},\vec{q}) = \frac{1}{2(m+1)}w^2 + \frac{m+1}{2m}z^2 + \frac{1}{2}\hat{p}_i^2 + \frac{1}{2m}\hat{q}_j^2. \tag{1.2.36}$$

We can evaluate the integral over z explicitly

$$\int_{B_R} \frac{1}{\frac{1}{2(m+1)}w^2 + \frac{m+1}{2m}z^2 + \frac{1}{2}\hat{p}_i^2 + \frac{1}{2m}\hat{q}_j^2 + \mu}\,\mathrm{d}z \\ = \frac{8\pi m}{m+1}R - 4\pi^2\left(\frac{m}{m+1}\right)^{3/2}\sqrt{\frac{1}{m+1}w^2 + \hat{p}_i^2 + \frac{1}{m}\hat{q}_j^2 + 2\mu} + o(1) \tag{1.2.37}$$

where the $o(1)$ part vanishes if $R \to \infty$. Choosing

$$\gamma_R = \left(\frac{8\pi m}{m+1}R + \alpha\frac{2m}{m+1}\right)^{-1} \tag{1.2.38}$$

such that the linear term in R in (1.2.37) cancels with (1.2.33) which allows us to take a formal limit.

Combining the above statements we define the following limit functional $\tilde{F}_\alpha$

$$D(\tilde{F}_\alpha) = \{\psi \mid \psi = \phi + G_\mu\vec{\xi},\ \phi \in H^1(\mathbb{R}^{3(N+M)}), \xi_{i,j} \in H^{1/2}(\mathbb{R}^{3(N+M-1)}) \text{ for } 1 \le i \le N\}$$

$$\tilde{F}_\alpha(\psi) = \langle\phi|H_0\phi\rangle + \mu\,\|\phi\|^2 - \mu\,\|\psi\|^2 + \frac{2m}{m+1}\alpha\sum_{(i,j)}\left\|\xi_{i,j}\right\|^2 + \sum_{k=0}^{3}\tilde{\Phi}_k(\vec{\xi}) \tag{1.2.39}$$

with $\vec{\xi} = (\xi_{i,j})_{(i,j)}$ and

$$G_\mu\vec{\xi}(p,q) = \sum_{(i,j)}\frac{\xi_{(i,j)}(p_i + q_j, \hat{p}_i, \hat{q}_j)}{h_0(p,q) + \mu}$$

$$\tilde{\Phi}_0(\vec{\xi}) = 2\pi^2\left(\frac{2m}{m+1}\right)^{3/2}\sum_{(i,j)}\int_{\mathbb{R}^{3(N+M-1)}}\sqrt{\frac{1}{2(m+1)}w^2 + \frac{1}{2}\hat{p}_i^2 + \frac{1}{2m}\hat{q}_j^2 + \mu}|\xi_{i,j}(w,\hat{p}_i,\hat{q}_j)|^2\,\mathrm{d}w\,\mathrm{d}\hat{p}_i\,\mathrm{d}\hat{q}_j$$

$$\tilde{\Phi}_1(\vec{\xi}) = -\sum_{(i,j)}\sum_{\substack{n=1\\n\neq j}}^{N}\int\overline{\hat{\xi}_{i,j}}(p_i + q_j, \hat{p}_i, \hat{q}_j)\hat{\xi}_{n,j}(p_n + q_j, \hat{p}_n, \hat{q}_j)G_\mu(p,q)\,\mathrm{d}p\,\mathrm{d}q$$

$$\tilde{\Phi}_2(\vec{\xi}) = -\sum_{(i,j)}\sum_{\substack{m=1\\n\neq j}}^{M}\int\overline{\hat{\xi}_{i,j}}(p_i + q_j, \hat{p}_i, \hat{q}_j)\hat{\xi}_{i,m}(p_i + q_m, \hat{p}_i, \hat{q}_m)G_\mu(p,q)\,\mathrm{d}p\,\mathrm{d}q$$

$$\tilde{\Phi}_3(\vec{\xi}) = -\sum_{(i,j)}\sum_{\substack{(m,n)\\m\neq i\\n\neq j}}\int\overline{\hat{\xi}_{i,j}}(p_i + q_j, \hat{p}_i, \hat{q}_j)\hat{\xi}_{n,m}(p_n + q_m, \hat{p}_n, \hat{q}_m)G_\mu(p,q)\,\mathrm{d}p\,\mathrm{d}q \tag{1.2.40}$$

The requirement that $\xi_i \in H^{1/2}(\mathbb{R}^{3(N+M-1)})$ originates from $\tilde{\Phi}_0$ which is equivalent to the $H^{1/2}(\mathbb{R}^{3(N+M-1)})$ norm. On the other hand this is also sufficient to make the terms $\tilde{\Phi}_1, \tilde{\Phi}_2$ and $\tilde{\Phi}_3$ well-defined which can be seen by a Schur test [20]. We emphasize that even though μ explicitly appears in the terms of $\tilde{F}_\alpha$ the quadratic form itself is independent of the choice of μ. As we can choose ϕ_μ and ξ in the $D(\tilde{F}_\alpha)$ independently, we will frequently drop the subscript μ.

1.2.3.1 Antisymmetry

So far we did not assume any antisymmetry constraints on the particles. From now on we demand antisymmetry in the coordinates p and separately in q. From the definition of $\xi_{i,j}$ in (1.2.31) we see using $\xi := \xi_{1,1} \in H^{1/2}(\mathbb{R}^3) \otimes H^{1/2}_{\mathrm{as}}(\mathbb{R}^{3(N-1)}) \otimes H^{1/2}_{\mathrm{as}}(\mathbb{R}^{3(M-1)})$ that

$$\xi_{i,j}(p_i + q_j, \hat{p}_i, \hat{q}_j) = (-1)^{j+i}\xi(p_i + q_j, \hat{p}_i, \hat{q}_j) \tag{1.2.41}$$

With $H^{1/2}_{\mathrm{as}}$ we denote the functions in $H^{1/2}$ which are antisymmetric in all coordinates. Because $\tilde{\Phi}_0$ only depends on the absolute value of ξ we get

$$\tilde{\Phi}_0(\vec{\xi}) = 2\pi^2 NM\left(\frac{2m}{m+1}\right)^{3/2} \int_{\mathbb{R}^{3(N+M-1)}} \sqrt{\frac{1}{2(m+1)}w^2 + \frac{1}{2}\hat{p}_i^2 + \frac{1}{2m}\hat{q}_j^2 + \mu}|\xi(w, \hat{p}_i)|^2 \, \mathrm{d}w \, \mathrm{d}\hat{p}_i \, \mathrm{d}\hat{q}_j. \tag{1.2.42}$$

For $\tilde{\Phi}_1$ we get

$$\begin{aligned}\tilde{\Phi}_1(\vec{\xi}) &= -\sum_{(i,j)} \sum_{\substack{n=1\\n\neq j}}^{N} (-1)^{i+2j+n} \int \overline{\hat{\xi}}(p_i + q_j, \hat{p}_i, \hat{q}_j)\hat{\xi}(p_n + q_j, \hat{p}_n, \hat{q}_j) G_\mu(p,q) \, \mathrm{d}p \, \mathrm{d}q \\ &= \sum_{(i,j)} \sum_{\substack{n=1\\n\neq j}}^{N} \int \overline{\hat{\xi}}(p_1 + q_1, \hat{p}_1, \hat{q}_1)\hat{\xi}(p_2 + q_1, \hat{p}_2, \hat{q}_1) G_\mu(p,q) \, \mathrm{d}p \, \mathrm{d}q \\ &= NM(N-1) \int \overline{\hat{\xi}}(p_1 + q_1, \hat{p}_1, \hat{q}_1)\hat{\xi}(p_2 + q_1, \hat{p}_2, \hat{q}_1) G_\mu(p,q) \, \mathrm{d}p \, \mathrm{d}q \end{aligned} \tag{1.2.43}$$

using

$$\begin{aligned}&\int \overline{\hat{\xi}}(p_i + q_j, \hat{p}_i, \hat{q}_j)\hat{\xi}(p_n + q_j, \hat{p}_n, \hat{q}_j) G_\mu(p,q) \, \mathrm{d}p \, \mathrm{d}q \\ &\quad = \int \overline{\hat{\xi}}(p_1 + q_1, p_i, p_n, p_3, \ldots, p_{i-1}, p_{i+1}, \ldots, p_2, \ldots p_N, q_j, \ldots, q_{j-1}, q_{j+1}, \ldots, q_N) \\ &\qquad \times \overline{\hat{\xi}}(p_2 + q_1, p_i, p_n, p_3, \ldots, p_1, \ldots, p_{n-1}, p_{n+1}, \ldots p_N, q_j, \ldots, q_{j-1}, q_{j+1}, \ldots, q_N) G_\mu(p,q) \, \mathrm{d}p \, \mathrm{d}q \\ &\quad = (-1)^{1+i+n} \int \overline{\hat{\xi}}(p_1 + q_1, \hat{p}_1, \hat{q}_1)\hat{\xi}(p_2 + q_1, \hat{p}_2, \hat{q}_1) G_\mu(p,q) \, \mathrm{d}p \, \mathrm{d}q\end{aligned}$$

for $i < n$ and an analogous calculation otherwise. In the same way we obtain

$$\begin{aligned}\tilde{\Phi}_2(\vec{\xi}) &= NM(M-1) \int \overline{\hat{\xi}}(p_1 + q_1, \hat{p}_1, \hat{q}_1)\hat{\xi}(p_1 + q_2, \hat{p}_1, \hat{q}_2) G_\mu(p,q) \, \mathrm{d}p \, \mathrm{d}q \\ \tilde{\Phi}_3(\vec{\xi}) &= -NM(N-1)(M-1) \int \overline{\hat{\xi}}(p_1 + q_1, \hat{p}_1, \hat{q}_1)\hat{\xi}(p_2 + q_2, \hat{p}_2, \hat{q}_2) G_\mu(p,q) \, \mathrm{d}p \, \mathrm{d}q \end{aligned} \tag{1.2.44}$$

We note that if we would consider bosons the sign in front of $\tilde{\Phi}_1$ and $\tilde{\Phi}_2$ would be inverted. We define in the following F_α which is the restriction of $\tilde{F}_\alpha$ to fermionic wavefunctions. The quadratic form F_α is given by

$$\begin{aligned}D(F_\alpha) &= \{\psi \mid \psi = \phi + G_\mu\xi, \ \phi \in H^1_{\mathrm{as}}(\mathbb{R}^{3N}) \otimes H^1_{\mathrm{as}}(\mathbb{R}^{3M}), \\ &\qquad \xi \in H^{1/2}(\mathbb{R}^3) \otimes H^{1/2}_{\mathrm{as}}(\mathbb{R}^{3(N-1)}) \otimes H^{1/2}_{\mathrm{as}}(\mathbb{R}^{3(M-1)})\} \\ F_\alpha(\psi) &= \langle\phi|H_0\phi\rangle + \mu\,\|\phi\|^2 - \mu\,\|\psi\|^2 + NM\left(\frac{2m}{m+1}\alpha\,\|\xi\|^2 + \sum_{k=0}^{3}\Phi_k(\xi)\right)\end{aligned} \tag{1.2.45}$$

with $G_\mu\xi(p,q) = \sum_{(i,j)} G_\mu(p,q)\xi(p_i+q_j,\hat{p}_i,\hat{q}_j)$ and

$$\Phi_0(\xi) = 2\pi^2\left(\frac{2m}{m+1}\right)^{3/2}\int_{\mathbb{R}^{3(N+M-1)}}\sqrt{\frac{1}{2(m+1)}w^2+\frac{1}{2}\hat{p}_i^2+\frac{1}{2m}\hat{q}_j^2+\mu}|\xi_{i,j}(w,\hat{p}_i,\hat{q}_j)|^2\,\mathrm{d}w\,\mathrm{d}\hat{p}_i\,\mathrm{d}\hat{q}_j$$

$$\Phi_1(\xi) = (N-1)\int\bar{\hat{\xi}}(p_1+q_1,\hat{p}_1,\hat{q}_1)\hat{\xi}(p_2+q_1,\hat{p}_2,\hat{q}_1)G_\mu(p,q)\,\mathrm{d}p\,\mathrm{d}q$$

$$\Phi_2(\xi) = (M-1)\int\bar{\hat{\xi}}(p_1+q_1,\hat{p}_1,\hat{q}_1)\hat{\xi}(p_1+q_2,\hat{p}_1,\hat{q}_2)G_\mu(p,q)\,\mathrm{d}p\,\mathrm{d}q$$

$$\Phi_3(\xi) = -(N-1)(M-1)\int\bar{\hat{\xi}}(p_1+q_1,\hat{p}_1,\hat{q}_1)\hat{\xi}(p_2+q_2,\hat{p}_2,\hat{q}_2)G_\mu(p,q)\,\mathrm{d}p\,\mathrm{d}q. \tag{1.2.46}$$

The latter three terms Φ_1,Φ_2 and Φ_3 are neither positive nor negative and, as they come with different signs, we expect cancellations between them when investigating the ground state energy.

Clearly if we are able to show that the singular part is positive for a fixed $\mu > 0$ then we showed stability as $-\mu\,\|\psi\|^2$ is bounded from below and the regular part is also positive.

Conversely, let for fixed $\mu > 0$, ξ_- be such that $\sum_{j=1}^4 \Phi_j(\xi_-) = -\gamma < 0$. We define a trial function such that $\phi = 0$ and further $\psi^\eta = \eta^{3(N+M)/2}G_\mu\xi_-(\eta\vec{x},\eta\vec{y}) = G_{\eta^2\mu}\xi_-^\eta(\vec{x},\vec{y})$ with $\hat{\xi_-^\eta}(p_0+p_i,\hat{p}_i) = \eta^{(-3(N+M))/2+2}\hat{\xi}_-((p_i+q_j)/\eta,\hat{p}_i/\eta,\hat{q}_j/\eta)$ and ξ_- chosen such that $\|\psi^\eta\| = 1$. Using the scaling properties of Φ_j we get

$$\begin{aligned}F_\alpha(\psi^\eta) &= \eta^2\left(\frac{2m}{m+1}\frac{\alpha}{\eta}\sum_{i=1}^N\|\xi_-\|^2+\sum_{j=1}^4\Phi_j(\xi_-)-\mu\right)\\ &= \eta^2\left(\frac{2m}{m+1}\frac{\alpha}{\eta}N\,\|\xi_-\|^2-\gamma-\mu\right).\end{aligned} \tag{1.2.47}$$

As $F_\alpha(\psi^\eta)\to-\infty$ for $\eta\to\infty$ the quadratic form is not bounded from below.

The term Φ_0 is positive and to show stability we need to show that it is larger than $-\Phi_1 - \Phi_2 - \Phi_3$. In the general case, where $N, M \geq 2$, a major difficulty are the strong cancellations between Φ_1,Φ_2,Φ_3. This is the reason why we will restrict in the next section to the $N+1$ model where $\Phi_2 = \Phi_3 = 0$ which significantly simplifies the model.

If we are able to show that the quadratic form is closed, the abstract theory tells us that there exists a self adjoint Hamiltonian associated to it. To show that the form is closed we need to prove that the quadratic form is equivalent to the norms appearing in the domain of F_α. Obviously the regular part is equivalent to $\|\phi\|^2_{H^1(\mathbb{R}^{3(N+M)})}$. If we show that $\Phi_0 \gtrsim \sum_{j=0}^3\Phi_j \gtrsim \Phi_0$, the singular part of the quadratic form is equivalent to the $\|\xi\|^2_{H^{1/2}(\mathbb{R}^{3(N+M-1)})}$ norm. The lower bound proves stability and is rather difficult whereas the upper bound, i.e. the first inequality, is easy, and we already needed it to ensure that all terms Φ_j are well-defined.

Assuming the stability results we prove in Chapter 2, we will discuss in the end of the following section the Hamiltonian associated to the quadratic form for the $N+1$ model.

1.2.4 The $N+1$ model

In the case that we set $M = 1$ the model reduces significantly as $\Phi_2 = \Phi_3 = 0$. In particular, we are able to single out the center of mass motion and switch to relative coordinates in a way which preserves the antisymmetry. For sake of generality we will work with $\tilde{F}_\alpha$ but similar analysis can be done for F_α.

For working with the $N+1$ model it is convenient to simplify the notation a bit. We will drop the index j from $\xi_{i,j}$ and label $p_0 = q_1$. Further we denote with $(x_1, \dots, x_N)$ the coordinates of the N particles and with x_0 the coordinate of the distinct particle.

The coordinate transformation we look at transforms $x = (x_0, x_1, \dots, x_N) \to (X, y_1, \dots, y_N) = y$ with

$$\begin{aligned} X &= \frac{mx_0 + \sum_{i=1}^N x_i}{m+N} \\ y_i &= x_i - x_0. \end{aligned} \tag{1.2.48}$$

We denote with $(P, k_1, \dots, k_N)$ the corresponding momentum variables. The transformation matrix between these two parameterizations is

$$\begin{pmatrix} X \\ y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} = \begin{pmatrix} \frac{m}{m+N} & \frac{1}{m+N} & \frac{1}{m+N} & \dots & \frac{1}{m+N} \\ -1 & 1 & 0 & \dots & 0 \\ -1 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & 0 & 0 & \dots & 1 \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_N \end{pmatrix} \tag{1.2.49}$$

and we denote it by K_N (or simply by K).

Lemma 1.2.1.

$$\det(K_N) = 1 \tag{1.2.50}$$

Proof. We will prove the result inductively. For $N = 0$ the statement is trivial. Let us assume that it is shown for N. Using the Laplace expansion of the determinant we get

$$\det(K_{N+1}) = \frac{m+N}{m+N+1} \underbrace{\det(K_N)}_{=1} + (-1)^{2N} \frac{1}{m+N+1} = 1 \tag{1.2.51}$$

□

where let $p = (p_0, p_1, \dots, p_N)$ be the coordinates in momentum space. For any function $f(x)$ we get

$$\begin{aligned} \hat{f}(p) &= \frac{1}{(2\pi)^{3(N+1)/2}} \int e^{ip\cdot x} f(x)\, \mathrm{d}x = \frac{1}{(2\pi)^{3(N+1)/2}} \int e^{ip\cdot K^{-1}y} f(K^{-1}y)\, \mathrm{d}y \\ &= \frac{1}{(2\pi)^{3(N+1)/2}} \int e^{i(K^{-1^t}p)\cdot y} f(K^{-1}y)\, \mathrm{d}y \;\Rightarrow\; (\mathcal{F}f)\circ K^t = \mathcal{F}(f\circ K^{-1}) \end{aligned} \tag{1.2.52}$$

using $x = K^{-1}y$ and $\mathcal{F}$ being the Fourier transformation. In particular, we see that

$$\begin{pmatrix} p_0 \\ p_1 \\ p_2 \\ \vdots \\ p_N \end{pmatrix} = \begin{pmatrix} \frac{m}{m+N} & -1 & -1 & \dots & -1 \\ \frac{1}{m+N} & 1 & 0 & \dots & 0 \\ \frac{1}{m+N} & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{1}{m+N} & 0 & 0 & \dots & 1 \end{pmatrix} \begin{pmatrix} P \\ k_1 \\ k_2 \\ \vdots \\ k_N \end{pmatrix} \tag{1.2.53}$$

and therefore

$$p_0 = \frac{m}{m+N}P - \sum_{i=1}^{N} k_i \qquad p_i = \frac{1}{m+N}P + k_i \tag{1.2.54}$$

We define $\psi^{\mathrm{rel}}(P,\vec{k}) = \psi(p_0,\vec{p})$ and $\phi^{\mathrm{rel}}(P,\vec{k}) = \phi(p_0,\vec{p})$ and in particular for the case that the N particles are fermions, ψ^{rel} and ϕ^{rel} are anti-symmetric functions in the last N coordinates. Using the coordinate transformation we can rewrite h_0 as

$$\begin{aligned} h_0(p,p_0) &= \frac{1}{2m}\left(\frac{m}{m+N}P - \sum_{i=1}^{N} k_i\right)^2 + \frac{1}{2}\sum_{i=1}^{N}\left(\frac{1}{m+N}P + k_i\right)^2 \\ &= \frac{m+1}{2m}\Bigg(\frac{m}{(m+1)(m+N)}P^2 + \underbrace{\frac{1}{m+1}\sum_{i\neq j} k_i\cdot k_j + \sum_{i=1}^{N} k_i^2}_{=:h_0^{\mathrm{rel}}(\vec{k})}\Bigg) \end{aligned} \tag{1.2.55}$$

and

$$\begin{aligned} \hat{\xi}_i(p_i+p_0,\hat{p}_i) &= \hat{\xi}_i\left(\frac{m+1}{m+N}P - \sum_{j\neq i}^{N} k_j, \frac{1}{m+N}P + k_1,\ldots,\frac{1}{m+N}P + k_N\right) \\ &=: \frac{m+1}{2m}\hat{\xi}_i^{\mathrm{rel}}(P,\hat{k}_i). \end{aligned} \tag{1.2.56}$$

The choice of the prefactor $(m+1)/2m$ is arbitrary but will be convenient in further calculations. The Fourier transform of h_0^{rel} we denote by H_0^{rel}. In a similar way we introduced $\widehat{G_\mu\xi_i}$ we define

$$\widehat{G_\mu^{\mathrm{rel}}\xi_i^{\mathrm{rel}}}(P,\vec{k}) := \frac{1}{h_0^{\mathrm{rel}}(\vec{k})+\mu}\hat{\xi}_i^{\mathrm{rel}}(P,\hat{k}_i). \tag{1.2.57}$$

We can express $\widehat{G_\mu\xi}$ in relative coordinates

$$\begin{aligned} G_\mu(p,p_0)\hat{\xi}_i(p_0+p_i,\hat{p}_i) &= \frac{1}{h_0(\vec{p},p_0)+\mu}\hat{\xi}(p_0+p_i,\hat{p}_i) \\ &= \frac{1}{h_0^{\mathrm{rel}}(P,\vec{k}) + \frac{m}{(m+1)(m+N)}P^2 + \frac{2m}{m+1}\mu}\hat{\xi}_i^{\mathrm{rel}}(P,\hat{k}_i) \\ &=: G^{\mathrm{rel}}_{\frac{m}{(m+1)(m+N)}P^2+\frac{2m}{m+1}\mu}\hat{\xi}_i^{\mathrm{rel}}(P,\hat{k}_i) \end{aligned} \tag{1.2.58}$$

which shows in particular the splitting $\psi^{\mathrm{rel}} = \phi^{\mathrm{rel}} + G_{\tilde{\mu}}^{\mathrm{rel}}\xi^{\mathrm{rel}}$. We define $\tilde{\mu} := \frac{m}{(m+1)(m+N)}P^2 + \frac{2m}{m+1}\mu$ and use

$$\begin{aligned} \frac{1}{m+1}w^2 + \hat{p}_i^2 + 2\mu &= \frac{1}{m+1}\left(\frac{m+1}{m+N}P - \sum_{j\neq i}^{N} k_j\right)^2 + \sum_{j\neq i}^{N}\left(\frac{1}{m+N}P + k_j\right)^2 + 2\mu \\ &= \frac{m+1}{m}\Bigg[\frac{m}{(m+1)^2}\sum_{\substack{j\neq\ell \\ j,\ell\neq i}} k_j\cdot k_\ell + \frac{m(m+2)}{(m+1)^2}\sum_{j\neq i} k_j^2 + \tilde{\mu}\Bigg] \end{aligned} \tag{1.2.59}$$

on $\tilde{\Phi}_0$ to obtain

$$\begin{aligned}
\tilde{\Phi}_0(\vec{\xi}) &= \int \sum_{i=1}^{N} \int \sqrt{2}\pi^2 \left(\frac{2m}{m+1}\right)^{-1/2} \left(\frac{m+1}{m}\right)^{1/2} \\
&\qquad \times \left[\frac{m}{(m+1)^2} \sum_{\substack{j\neq\ell \\ j,\ell\neq i}} k_j \cdot k_\ell + \frac{m(m+2)}{(m+1)^2} \sum_{j\neq i} k_j^2 + \tilde{\mu}\right]^{1/2} |\hat{\xi}_i^{\mathrm{rel}}(P,\vec{k})|^2 \,\mathrm{d}\hat{k}_i \,\mathrm{d}P \\
&= \frac{m+1}{2m} \int \sum_{i=1}^{N} \int 2\pi^2 \left[\frac{m}{(m+1)^2} \sum_{\substack{j\neq\ell \\ j,\ell\neq i}} k_j \cdot k_\ell + \frac{m(m+2)}{(m+1)^2} \sum_{j\neq i} k_j^2 + \tilde{\mu}\right]^{1/2} \\
&\qquad \times |\hat{\xi}_i^{\mathrm{rel}}(P,\vec{k})|^2 \,\mathrm{d}\hat{k}_i \,\mathrm{d}P \\
&=: \frac{m+1}{2m} \int \tilde{\Phi}_0^{\mathrm{rel}}(\xi^{\mathrm{rel}}(P,\cdot)) \,\mathrm{d}P. \qquad (1.2.60)
\end{aligned}$$

A similar computation for $\tilde{\Phi}_1$ gives

$$\begin{aligned}
\sum_{i\neq j} \langle \hat{\xi}_i(p_0+p_i,\hat{p}_i) | G_\mu \hat{\xi}_j(p_0+p_j,\hat{p}_j)\rangle &= \frac{m+1}{2m} \sum_{i\neq j} \langle \hat{\xi}_i^{\mathrm{rel}}(P,\hat{k}_i) | G_{\tilde{\mu}}^{\mathrm{rel}} \hat{\xi}_j^{\mathrm{rel}}(P,\hat{k}_j)\rangle \\
&= \frac{m+1}{2m} \int \int \frac{\overline{\hat{\xi}_i(P,\hat{k}_i)}\hat{\xi}_j(P,\hat{k}_j)}{h_0^{\mathrm{rel}}(\vec{k})+\tilde{\mu}} \,\mathrm{d}\vec{k}\,\mathrm{d}P \\
&=: \frac{m+1}{2m} \int \tilde{\Phi}_1^{\mathrm{rel}}(\xi^{\mathrm{rel}}(P,\cdot)) \,\mathrm{d}P. \qquad (1.2.61)
\end{aligned}$$

The last term of the singular part of $\tilde{F}_\alpha$ can be expressed by

$$\frac{2m}{m+1}\alpha \sum_{i=1}^{N} \|\xi_i\|^2 = \frac{m+1}{2m} \int \mathrm{d}P \int |\xi_i^{\mathrm{rel}}(P,\vec{k})|^2 \,\mathrm{d}\vec{k}\,\mathrm{d}P. \qquad (1.2.62)$$

The regular part can be written as

$$\langle \phi | (h_0+\mu)\phi\rangle = \frac{m+1}{2m} \int \langle \phi^{\mathrm{rel}}(P,\cdot) | (h_0^{\mathrm{rel}}+\tilde{\mu})\phi^{\mathrm{rel}}(P,\cdot)\rangle \,\mathrm{d}P \qquad (1.2.63)$$

and we can write $-\mu\,\|\psi\|^2$ as

$$-\mu\,\|\psi\| = \int \left(-\frac{m+1}{2m}\tilde{\mu} + \frac{1}{2(m+N)}P^2\right) \int |\psi^{\mathrm{rel}}(P,\vec{k})|^2 \,\mathrm{d}\vec{k}\,\mathrm{d}P \qquad (1.2.64)$$

Combining (1.2.60), (1.2.61) and (1.2.64) with (1.2.39) we get

$$\begin{aligned}
\tilde{F}_\alpha(\psi) = \frac{m+1}{2m} \int \Big(&\langle \phi^{\mathrm{rel}}(P,\cdot) | (h_0^{\mathrm{rel}}(\vec{k})+\tilde{\mu})\phi^{\mathrm{rel}}(P,\cdot)\rangle - \tilde{\mu} \int |\psi^{\mathrm{rel}}(P,\vec{k})|^2 \,\mathrm{d}\vec{k} \\
&+ \tilde{\Phi}_0^{\mathrm{rel}}(\xi^{\mathrm{rel}}(P,\cdot)) + \tilde{\Phi}_1^{\mathrm{rel}}(\xi^{\mathrm{rel}}(P,\cdot))\Big) \,\mathrm{d}P \\
+ \int \frac{1}{2(m+N)} &P^2 |\psi^{\mathrm{rel}}(P,\vec{k})|^2 \,\mathrm{d}\vec{k}\,\mathrm{d}P. \qquad (1.2.65)
\end{aligned}$$

For a fixed P the expression inside the integrals does not depend on the choice of $\tilde{\mu}$ and hence we can view $\tilde{\mu}$ as a P independent constant. This motivates the definition of the relative energy functional, where we drop the center of mass energy, i.e. last term in (1.2.65), as

$$\begin{aligned} D(\tilde{F}_\alpha^{\mathrm{rel}}) &= \{\psi^{\mathrm{rel}} \mid \psi^{\mathrm{rel}} = \phi^{\mathrm{rel}} + G_{\tilde{\mu}}^{\mathrm{rel}}\xi^{\mathrm{rel}},\ \phi \in H^1_{\mathrm{as}}(\mathbb{R}^{3N}), \xi^{\mathrm{rel}} \in H^{1/2}_{\mathrm{as}}(\mathbb{R}^{3(N-1)})\} \\ \tilde{F}_\alpha^{\mathrm{rel}}(\psi^{\mathrm{rel}}) &= \langle \phi^{\mathrm{rel}} | (H_0^{\mathrm{rel}} + \tilde{\mu})\phi^{\mathrm{rel}}\rangle - \tilde{\mu}\left\|\psi^{\mathrm{rel}}\right\|^2 \\ &\quad + N\left[\alpha\left\|\xi^{\mathrm{rel}}\right\|^2 + T^{\mathrm{rel}}_{\mathrm{diag}}(\xi^{\mathrm{rel}}) + T^{\mathrm{rel}}_{\mathrm{off}}(\xi^{\mathrm{rel}})\right] \end{aligned} \tag{1.2.66}$$

with

$$\begin{aligned} T^{\mathrm{rel}}_{\mathrm{diag}}(\xi^{\mathrm{rel}}) &= 2\pi^2 \sum_{i=1}^N \int_{\mathbb{R}^{3(N-1)}} |\xi_i^{\mathrm{rel}}(\hat{k}_i)|^2 \sqrt{\frac{m}{(m+1)^2}\sum_{t,j\neq i, t\neq j} k_i\cdot k_t + \frac{m(m+2)}{(m+1)^2}\hat{k}_i^2 + \tilde{\mu}}\, \mathrm{d}\vec{k} \\ T^{\mathrm{rel}}_{\mathrm{off}}(\xi^{\mathrm{rel}}) &= -\sum_{i\neq j}\int_{\mathbb{R}^{3(N+1)}} \frac{\overline{\xi}_i^{\mathrm{rel}}(\hat{k}_i)\xi_j^{\mathrm{rel}}(\hat{k}_j)}{h_0^{\mathrm{rel}}(\vec{k}) + \tilde{\mu}}\, \mathrm{d}\vec{k} \end{aligned} \tag{1.2.67}$$

In the case where $N = 1$ we see that $\tilde{F}_\alpha^{\mathrm{rel}}$ is equivalent to the $1 + 1$ model which was rigorously introduced in (1.2.15).

For analyzing stability it suffices to discuss this quadratic form $\tilde{F}_\alpha^{\mathrm{rel}}$, or better its antisymmetric restriction F_α^{rel}, as the kinetic energy of the center of mass motion is always positive.

At this point it is not clear that the quadratic form is bounded from below and gives rise to a self-adjoint operator. We refer to Chapter 2 for rigorous details and will continue in this section rather formally. Assuming stability we can define Γ as a positive selfadjoint operator given by

$$T^{\mathrm{rel}}_{\mathrm{diag}}(\xi^{\mathrm{rel}}) + T^{\mathrm{rel}}_{\mathrm{off}}(\xi^{\mathrm{rel}}) = \langle \xi^{\mathrm{rel}} | \Gamma \xi^{\mathrm{rel}}\rangle \tag{1.2.68}$$

on $L^2_{\mathrm{as}}(\mathbb{R}^{3(N-1)})$.

Using this operator we define the Hamiltonian associated to F_α^{rel} by

$$\begin{aligned} D(H_\alpha^{\mathrm{rel}}) = \Big\{&\psi^{\mathrm{rel}} \in L^2_{\mathrm{as}}(\mathbb{R}^{3N}) \mid \psi^{\mathrm{rel}} = \phi_\mu^{\mathrm{rel}} + G_\mu^{\mathrm{rel}}\xi, \\ &\phi_\mu^{\mathrm{rel}} \in H^2_{\mathrm{as}}(\mathbb{R}^{3N}), \xi^{\mathrm{rel}} \in D(\Gamma), \phi_\mu^{\mathrm{rel}}\restriction_{y_N=0} = (2\pi)^{-3/2}(-1)^{N+1}(\alpha+\Gamma)\xi^{\mathrm{rel}}\Big\} \end{aligned} \tag{1.2.69}$$

with H_α^{rel} acting on $\psi^{\mathrm{rel}} \in D(H_\alpha)$ as

$$\left(H_\alpha^{\mathrm{rel}} + \mu\right)\psi^{\mathrm{rel}} = (H_0^{\mathrm{rel}} + \mu)\phi_\mu^{\mathrm{rel}}. \tag{1.2.70}$$

The following computation connects H_α^{rel} to F_α^{rel}. Given $\psi \in D(H_\alpha^{\mathrm{rel}})$ we get

$$\begin{aligned} \langle \psi^{\mathrm{rel}} | (H_\alpha^{\mathrm{rel}} + \mu)\psi^{\mathrm{rel}}\rangle &= \langle \psi^{\mathrm{rel}} | (H_\alpha^{\mathrm{rel}} + \mu)\phi_\mu^{\mathrm{rel}}\rangle \\ &= \langle \phi_\mu^{\mathrm{rel}} | (H_\alpha^{\mathrm{rel}} + \mu)\phi_\mu^{\mathrm{rel}}\rangle + \langle G_\mu^{\mathrm{rel}}\xi^{\mathrm{rel}} | (H_0^{\mathrm{rel}} + \mu)\phi_\mu^{\mathrm{rel}}\rangle \\ &= \langle \phi_\mu^{\mathrm{rel}} | (H_\alpha^{\mathrm{rel}} + \mu)\phi_\mu^{\mathrm{rel}}\rangle + \langle \xi^{\mathrm{rel}} | \phi_\mu^{\mathrm{rel}}\restriction_{y_N=0}\rangle \\ &= F_\alpha^{\mathrm{rel}}(\psi^{\mathrm{rel}}) + \mu\left\|\psi^{\mathrm{rel}}\right\|^2 \end{aligned} \tag{1.2.71}$$

using the boundary condition of the Hamiltonian. We emphasize that ϕ_μ^{rel} and ξ^{rel} for a function $\psi^{\mathrm{rel}} \in D(H_\alpha^{\mathrm{rel}})$ cannot be chosen independently of each other. Hence, even though the action of H_α^{rel} is rather simple, the real difficulty lies in the boundary condition involving the many-particle operator Γ.

1.3 Main Results

1.3.1 The $N + 1$ model

The results from [11,13] are not completely limited to the three particles case but also show that there exists a critical mass $m^*(N)$ such that the $N+1$ system is stable if $m > m^*(N)$. This critical mass diverges linearly in N which makes it only applicable to systems with small particle numbers. We recall that a critical mass smaller than one is necessary to show simultaneous stability of the $N + 1$ and the $1 + N$ system.

Our results for the $N + 1$ system on $\mathbb{R}^3$ are covered in Chapter 2. The main theorem will show that there is a critical mass $\tilde{m}_1 = 0.36$ such that the $N + 1$ model is stable if $m \geq \tilde{m}_1$. Differently to previous work we manage to take the antisymmetry into account which allows us to find a critical mass independent of the particle number N.

We will define this critical mass using the quantity $\Lambda(m)$ which is given by

$$\begin{aligned}\Lambda(m) &= \sup_{s,K\in\mathbb{R}^3,Q>0} \frac{s^2+Q^2}{\pi^2(m+1)} \ell_m(s,K,Q)^{-1/2} \int_{\mathbb{R}^3} \frac{1}{t^2} \ell_m(t,K,Q)^{-1/2} \\ &\times \frac{|(s+AK)\cdot(t+AK)|}{\left[(s+AK)^2+(t+AK)^2+\frac{m}{m+1}(Q^2+AK^2)\right]^2 - \left[\frac{2}{(m+1)}(s+AK)\cdot(t+AK)\right]^2}\,\mathrm{d}t \end{aligned} \tag{1.3.1}$$

with $A = 1/(m + 2)$ and

$$\ell_m(s,K,Q) := \left(\frac{m}{(m+1)^2}(s+K)^2 + \frac{m}{m+1}(s^2+Q^2)\right)^{1/2}. \tag{1.3.2}$$

We note that it is possible to bound (1.3.1) using the Cauchy-Schwarz inequality (see section 2.6) by

$$\Lambda(m) \leq \frac{4(m+1)^2(2+4m+m^2)^{3/2}}{\sqrt{2}\pi\,[m(m+2)]^3} \tag{1.3.3}$$

and in particular $\Lambda(m) \to 0$ as $m \to \infty$.

The following theorem proves stability for the $N + 1$ system in the case that $\Lambda(m) < 1$.

Theorem 2.2.1. *For any $\xi \in H^{1/2}_{\mathrm{as}}(\mathbb{R}^{3(N-1)})$, $\mu > 0$ and $N \geq 2$,*

$$T_{\mathrm{off}}(\xi) \geq -\Lambda(m) T_{\mathrm{diag}}(\xi) \tag{1.3.4}$$

In particular, if m is such that $\Lambda(m) < 1$, then F_α is closed and bounded from below by

$$F_\alpha(u) \geq \begin{cases} 0 & \text{for } \alpha \geq 0 \\ -\left(\frac{\alpha}{2\pi^2(1-\Lambda(m))}\right)^2 \|u\|^2_{L^2(\mathbb{R}^{3N})} & \text{for } \alpha < 0 \end{cases} \tag{1.3.5}$$

for all $u \in D(F_\alpha)$.

Proof. See section 2.4. ◻

The bound obtained in (1.3.3) is not very good as it does not show that $\Lambda(1) < 1$ for $m = 1$. Using numerical methods we will show in section 2.7 that for $m \geq \tilde{m}_1 = 0.36$ we get that $\Lambda(m) \leq 1$. This shows together with Theorem 2.2.1 stability for these masses.

The numerics needed to prove the statement above is limited to a numeric integration and an optimization on a compact set. The possibility of bounding $\Lambda(m)$ by an analytic expression is limited as such bounds quickly increase $\Lambda(m)$ to the point where the bound is larger than one for all masses smaller than one.

1.3.2 The finite density problem

Even though Theorem 2.2.1 does show stability for $m \geq \tilde{m}_1$ we do not learn anything about the effect a point interacting impurity has on the energy. In particular, we see from (1.3.5) that the ground state energy is independent of the interaction strength if $\alpha \geq 0$. The reason for this is that we work with a zero density model and particles in low energy states tend to spatially separate.

In [52], see Chapter 3, we avoid these problems by confining the wavefunction to be supported in a box $B = (0, L)^3$ in all coordinates, giving rise to a finite mean density $\rho = N/L^3$. This system has a well-defined ground state which allows us to investigate the change in energy when introducing an impurity.

In the following theorem we show that the change in energy can be bounded uniformly in N and in particular the bound only depends on ρ and α. With E_N^D we denote the ground state energy of the non-interacting system of N fermions with Dirichlet boundary conditions on B. As long as the density is fixed we get that $E_N^D \sim N\rho^{2/3}$.

Theorem 3.2.1. *Let $\psi \in D(F_\alpha)$, supported in $(0, L)^{3(N+1)}$, with $\|\psi\| = 1$. Let $\rho = NL^{-3}$, and assume that $\Lambda(m) < 1$. Then*

$$F_\alpha(\psi) \geq E_N^D - const\left(\frac{\rho^{2/3}}{(1 - \Lambda(m))^{9/2}} + \frac{\alpha_-^2}{(1 - \Lambda(m))^2}\right) \tag{1.3.6}$$

where the constant is independent of ψ, m, N, L and α, and α_- denotes the negative part of α, i.e., $\alpha_- = \frac{1}{2}(|\alpha| - \alpha)$.

Proof. See Chapter 3. □

As the interactions are always attractive the upper bound for $F_\alpha(\psi)$ is trivially E_N^D. Hence the change of energy when introducing a point interacting impurity is of order one in N and therefore small in comparison to the kinetic energy E_N^D.

1.3.3 The 2+2 case

Models for $N, M \geq 2$ are inherently more difficult to deal with because of the additional terms Φ_2, Φ_3. The easiest model of this kind is the $2 + 2$ model where one does not have to take into account the anti-symmetry of ξ. In [42] a numerical analysis on the $2 + 2$ system was done and in particular for the ground state strong cancellations between Φ_1, Φ_2 and Φ_3 were found. It was suggested in [18] that the critical mass for a four body collapse should be the same as for the one with three bodies.

In Chapter 4, we will confirm that there is a stable mass region for the 2 + 2 problem. The critical mass we determine is not sharp as we need to use several non optimal bounds. In particular, we are not able to fully take into account cancellations between Φ_1, Φ_2 and Φ_3. The question whether there is a mass region where the system is unstable due to four-body bound states is still open.

For $a \in \mathbb{R}^3$, $b \geq 0$ and $m > 0$, let $O^m_{a,b}$ be the bounded operator on $L^2(\mathbb{R}^3)$ with integral kernel

$$O^m_{a,b}(p_1, p_2) = \tag{1.3.7}$$
$$\left[(p_1 + a)^2 + b^2\right]^{-1/4} \frac{1}{p_1^2 + p_2^2 + \frac{2}{m+1} p_1 \cdot p_2 + \frac{2(2+m)}{(m+1)^2} a^2 + \frac{2m}{(m+1)^2} b^2} \left[(p_2 + a)^2 + b^2\right]^{-1/4}$$

Let further

$$\Lambda_2(m) = -\frac{1}{2\pi^2} \frac{m+1}{\sqrt{m}} \inf_{a \in \mathbb{R}^3, b \geq 0} \inf \operatorname{spec} O^m_{a,b} \tag{1.3.8}$$

Theorem 4.3.1. *For m such that $\Lambda_2(m) + \Lambda_2(1/m) < 1$, we have*

$$F_\alpha(\psi) \geq \begin{cases} 0 & \alpha \geq 0 \\ -\alpha^2 \left(\frac{m+1}{m}\right)^3 \frac{1}{2\pi^4 (1 - \Lambda_2(m) - \Lambda_2(1/m))^2} \|\psi\|_2^2 & \alpha < 0 \end{cases} \tag{1.3.9}$$

for any $\psi \in D(F_\alpha)$.

Proof. See the proof of Theorem 4.3.1 in Chapter 4. □

In particular, we will show that if m such that $0.58 \lesssim m \lesssim 1.73$ then $\Lambda_2(m) + \Lambda_2(1/m) < 1$ which shows stability for these masses.

As discussed before, the cancellations in the singular part of F_α are very difficult to deal with. In the case of 2 + 2 particles it is possible to bound $\Phi_0 + \Phi_3$ from below by a positive quantity. We show that this quantity is large enough to bound the negative part of Φ_1 and Φ_2.

1.3.4 A Dirichlet form model

In Chapter 5, we will discuss a point interacting model based on a Dirichlet form which was formerly investigated in [25]. This model is stable in all cases but contains many particle point interactions which make it physically less realistic. We show that in the thermodynamic limit the free energy per particle is equal to the non-interacting one. In this sense the model behaves trivially.

Deriving the two particle point interacting system can be done using multiple approaches. In section 1.2.1, we have seen that it can be constructed using self adjoint extensions. In [1, Appendix F] it was shown that one can also formulate the system as a Dirichlet form

$$\mathcal{E}_2(\phi) = \frac{\int |\nabla\phi(x)|^2 \left(\frac{1}{a} - \frac{1}{|x|}\right) \mathrm{d}x}{\int |\phi(x)|^2 \left(\frac{1}{a} - \frac{1}{|x|}\right) \mathrm{d}x} \tag{1.3.10}$$

as long as the scattering length a is negative. Of particular interest is the unitary case, i.e. $a = \infty$ which we will generalize below. We note that as a Dirichlet form this system is well-defined [2] and in particular positive.

An integration by parts gives for $\varepsilon > 0$

$$\int_{|x|\geq\epsilon}\left(\frac{1}{|x|}-\frac{1}{a}\right)^2|\nabla\phi(x)|^2\,\mathrm{d}x = \int_{|x|\geq\epsilon}\left|\nabla\left(\frac{1}{|x|}-\frac{1}{a}\right)\phi(x)\right|^2\,\mathrm{d}x - \int_{|x|=\epsilon}\left(\frac{1}{|x|}-\frac{1}{a}\right)\frac{1}{|x|^2}|\phi(x)|^2\mathrm{d}\omega. \tag{1.3.11}$$

The last term corresponds to point interactions and is only non-trivial in the limit $\varepsilon \to 0$ if ϕ vanishes slower than $|x|^{1/2}$ at the origin. This shows that $\mathcal{E}_2$ is indeed a model of point interactions.

Along the same lines we can extend this model to a many particle system and for simplicity we restrict to the unitary case. We define

$$\mathcal{E}_g(\psi) = \frac{\sum_{i=1}^N \int |\nabla_i\psi(x)|^2 g(x)\,\mathrm{d}x}{\int |\psi(x)|^2 g(x)\,\mathrm{d}x} \tag{1.3.12}$$

with $x = (x_1, \ldots, x_N)$, $x_i \in \mathbb{R}^3$ and

$$g(x) = \sum_{1\leq i<j\leq N}\frac{1}{|x_i - x_j|}. \tag{1.3.13}$$

We will restrict ψ to an antisymmetric subspace of some kind. Because this model is always well-defined, it is possible to allow arbitrary many species of fermions and the number of species we denote by q. This is very different to the systems we introduced in section 1.2.3 where every system with more than two species is unstable.

With the same argument as in (1.3.11) we get that $\mathcal{E}_g$ models a system of N point interacting particles. It turns out though that the system contains non-local multi-particle point interactions which are physically undesirable.

In the following we will consider the system described by $\mathcal{E}_g$ restricted to wavefunctions in the box $[0, L]^3$ and we define the density $\rho = N/L^3$. The free energy of the system with an inverse temperature $\beta > 0$ is then given by

$$F_g(\beta, N, L) = -T\ln \sup_{\substack{\{\psi_k\}\\ \langle\psi_i|\psi_j\rangle_g=\delta_{ij}}} \sum_k e^{-\beta\mathcal{E}_g(\psi_k)} \tag{1.3.14}$$

and the free energy density in the thermodynamic limit with fixed density $\rho > 0$ as

$$f_g(\beta,\rho) = \lim_{N\to\infty}\frac{\rho}{N}F_g(\beta, N, (N/\rho)^{1/3}). \tag{1.3.15}$$

The non-interacting free energy density is given by

$$f(\beta,\rho) = \sup_{\mu\in\mathbb{R}}\left[\mu\rho - \frac{qT}{(2\pi)^3}\int_{\mathbb{R}^3}\ln\left(1 + e^{-\beta(p^2-\mu)}\right)dp\right] \tag{1.3.16}$$

In Chapter 5, we will show that both energies per particle are equal and in this sense the model behaves trivially in the thermodynamic limit.

Theorem 5.2.1. *For any $\beta > 0$ and $\rho > 0$, and any $q \geq 1$,*

$$f_g(\beta, \rho) = f(\beta, \rho) \tag{1.3.17}$$

Proof. See the proof of Theorem 5.2.1 in Chapter 5. □

We have seen for the two particle case for a finite scattering length that it can be defined by a Dirichlet form with a weight function of $x \mapsto |x|^{-1} - a^{-1}$. When we look at the point interactions between particles with coordinates x_1 and x_2, the weight function g can be written as

$$g(x) = \frac{1}{|x_1 - x_2|} + \sum_{\substack{1 \leq i < j \leq N \\ (i,j) \neq (1,2)}} \frac{1}{|x_i - x_j|}. \tag{1.3.18}$$

The first part is similar to the $|x|^{-1}$ of the two particle case and the second part takes the role of $-a^{-1}$ and therefore defines an effective scattering length. Assuming there are two interacting particles beside the pair $(1, 2)$ we see that the second term in (1.3.18) is very large if these particles are close together. In particular this effect is independent of the distance between these two pairs. These are the non-local point interactions we discussed above as the strength of the point interactions can be influenced by particles far away.

Because we consider a thermodynamic limit with density ρ, we expect a mean particle distance of $\rho^{-1/3}$. A heuristic calculation gives an effective scattering length of $N^{-5/3}\rho^{-1/3}$ using (1.3.18). In particular this means that the interactions should be very weak in the thermodynamic limit as the effective scattering length formally vanishes. This is what we show rigorously in Theorem 5.2.1.

CHAPTER 2

Stability of a fermionic $N + 1$ particle system with point interactions

Thomas Moser, Robert Seiringer

Abstract

We prove that a system of N fermions interacting with an additional particle via point interactions is stable if the ratio of the mass of the additional particle to the one of the fermions is larger than some critical m^*. The value of m^* is independent of N and turns out to be less than 1. This fact has important implications for the stability of the unitary Fermi gas. We also characterize the domain of the Hamiltonian of this model, and establish the validity of the Tan relations for all wave functions in the domain.

2.1 Introduction

Models of particles with point interactions are ubiquitously used in physics, as an idealized description whenever the range of the interparticle interactions is much shorter than other relevant length scales. They were introduced in the early days of quantum mechanics as models of nuclear interactions [6, 19, 68, 72], but have proved useful in other branches of physics, like polarons (see [40] and references there) and cold atomic gases [74]. While the two-particle problem is mathematically completely understood [1], for more than two particles the existence of a self-adjoint Hamiltonian that is bounded from below and models pairwise point interactions is a challenging open problem. It is known that such a Hamiltonian can only exist for fermions with at most two components (or two different species of fermions), due do the Thomas effect [8, 61, 68, 73].

For $N \geq 2$, we consider here a system of N (spinless) fermions of mass 1, interacting with another particle of mass m via point interactions. The latter are characterized by a parameter $\alpha \in \mathbb{R}$, where $-1/\alpha$ is proportional to the scattering length of the pair interaction [1]. Purely formally, the Hamiltonian of the system can be thought of as

$$H = -\frac{1}{2m}\Delta_{x_0} - \frac{1}{2}\sum_{i=1}^{N}\Delta_{x_i} + \gamma\sum_{i=1}^{N}\delta(x_0 - x_i) \tag{2.1.1}$$

where $x_i \in \mathbb{R}^3$, and γ represents an infinitesimal coupling constant. Models of this kind have been studied extensively in the literature (see, e.g., [10–13, 15, 16, 21, 41–43, 45–47, 49, 65, 71]) and can be defined via a suitable regularization procedure. More precisely, the formal expression (2.1.1) can be given a meaning in terms of a suitable quadratic form [11, 15, 21], which will be introduced in the next section. However, only in case the quadratic form is stable, i.e., bounded from below, does it give rise to a unique self-adjoint operator and hence gives a precise meaning to (2.1.1). We are interested in this question of stability. We shall show that there exists a critical mass m^*, independent of N, such that stability holds for $m > m^*$. The value of m^* is determined by a two-dimensional optimization problem of a certain analytic function. A numerical evaluation of the expression yields $m^* \approx 0.36$.

In particular, the system under consideration is stable for $m = 1$. This latter case is of particular importance, in view of constructing a model of a gas of spin 1/2 fermions close to the unitary limit, where the scattering length becomes much larger than the range of the interactions. For $N + 1$ such fermions, our result can be interpreted as proving the existence of such a model in the sector of total spin $(N-1)/2$, i.e., 1 less than the maximal value. Of course stability holds trivially in the sector of total spin $(N+1)/2$, since the particles do not interact in this case due to the total antisymmetry of the spatial part of the wave functions. We note that stability in other spin sectors is still an open problem, whose solution would be of great interest because of the relevance of the model for cold atomic gases (see [74] and references there). For its solution, it is necessary to understand the problem of stability for general systems of $N+M$ particles mutually interacting via point interactions. In the case $N = M = 2$, a numerical analysis suggests stability, see [42] for the case $m = 1$ and [18] for the full range of mass ratios where stability for the 2 + 1 problem holds, i.e., for $0.0735 < m < (0.0735)^{-1} \approx 13.6$ [8].

2.2 Model and Main Results

Because of translation invariance, it is convenient to separate the center-of-mass motion and to introduce relative coordinates $X = \left(mx_0 + \sum_{i=1}^N x_i\right)/(m+N)$, $y_i = x_i - x_0$ for $1 \le i \le N$ in the usual way. With their aid we can formally write the operator H in (2.1.1) as $H = H_{\mathrm{cm}} + \frac{m+1}{2m} H_{\mathrm{rel}}$, where $H_{\mathrm{cm}} = -(2(m+N))^{-1}\Delta_X$ and

$$H_{\mathrm{rel}} = -\sum_{i=1}^N \Delta_{y_i} - \frac{2}{m+1} \sum_{1\le i<j\le N} \nabla_{y_i} \cdot \nabla_{y_j} + \tilde{\gamma} \sum_{i=1}^N \delta(y_i) \tag{2.2.1}$$

for $\tilde{\gamma} = 2m\gamma/(m+1)$. The latter operator acts on purely anti-symmetric functions of N variables only.

The formal expression (2.2.1) can be given a meaning in terms of a suitable quadratic form [11, 15, 21], which will be introduced in the next subsection.

2.2.1 Quadratic Form and Stability

The model under consideration here is defined via a quadratic form F_α as follows. For $\mu > 0$ and $q_i \in \mathbb{R}^3$, $1 \le i \le N$, let

$$G(q_1, \dots, q_N) := \left(\sum_{i=1}^{N} q_i^2 + \frac{2}{m+1} \sum_{1\le i<j\le N} q_i \cdot q_j + \mu \right)^{-1} \tag{2.2.2}$$

The quadratic form F_α has the domain

$$D(F_\alpha) = \left\{ u \in L^2_{\mathrm{as}}(\mathbb{R}^{3N}) \mid u = w + G\xi, w \in H^1_{\mathrm{as}}(\mathbb{R}^{3N}), \xi \in H^{1/2}_{\mathrm{as}}(\mathbb{R}^{3(N-1)}) \right\} \tag{2.2.3}$$

where $G\xi$ is short for the function with Fourier transform

$$\widehat{G\xi}(q_1, \dots, q_N) = G(q_1, \dots, q_N) \sum_{i=1}^{N} (-1)^{i+1} \hat{\xi}(q_1, \dots, q_{i-1}, q_{i+1}, \dots, q_N) \tag{2.2.4}$$

and the subscript "as" indicates functions that are antisymmetric under permutations. For $u \in D(F_\alpha)$, we have

$$\begin{aligned} F_\alpha(u) = &\left\langle w \middle| -\sum_{i=1}^{N} \Delta_i - \frac{2}{m+1} \sum_{1\le i<j\le N} \nabla_i \cdot \nabla_j + \mu \middle| w \right\rangle - \mu \|u\|^2_{L^2(\mathbb{R}^{3N})} \\ &+ N \left(\alpha \|\xi\|^2_{L^2(\mathbb{R}^{3(N-1)})} + T_{\mathrm{diag}}(\xi) + T_{\mathrm{off}}(\xi) \right) \end{aligned} \tag{2.2.5}$$

where

$$\begin{aligned} T_{\mathrm{diag}}(\xi) &:= \int_{\mathbb{R}^{3(N-1)}} |\hat{\xi}(s, \vec{q})|^2 L(s, \vec{q}) \, \mathrm{d}s \, \mathrm{d}\vec{q} \\ T_{\mathrm{off}}(\xi) &:= (N-1) \int_{\mathbb{R}^{3N}} \hat{\xi}^*(s, \vec{q}) \hat{\xi}(t, \vec{q}) G(s, t, \vec{q}) \, \mathrm{d}s \, \mathrm{d}t \, \mathrm{d}\vec{q} \end{aligned} \tag{2.2.6}$$

We introduced $\vec{q} := (q_1, \dots, q_{N-2})$ for short, and the function L is given by

$$L(q_1, \dots, q_{N-1}) := 2\pi^2 \left(\frac{m(m+2)}{(m+1)^2} \sum_{i=1}^{N-1} q_i^2 + \frac{2m}{(m+1)^2} \sum_{1\le i<j\le N-1} q_i \cdot q_j + \mu \right)^{1/2} \tag{2.2.7}$$

Note that since $G\xi \notin H^1(\mathbb{R}^{3N})$ for $\xi \neq 0$, the decomposition of u as $u = w + G\xi$ is unique. Moreover, while w depends on μ, ξ is independent of the choice of μ.

Clearly $T_{\mathrm{diag}}(\xi)$ is bounded above and below by $\|\xi\|^2_{H^{1/2}(\mathbb{R}^{3(N-1)})}$, and also $T_{\mathrm{off}}(\xi)$ is bounded in $H^{1/2}(\mathbb{R}^{3(N-1)})$ (see Sect. 2.3). One readily checks that both $D(F_\alpha)$ and $F_\alpha(u)$ are actually independent of μ for $\mu > 0$, even though $T_{\mathrm{diag}}(\xi)$ and $T_{\mathrm{off}}(\xi)$ depend on μ. The domain $D(F_\alpha)$ is also independent of $\alpha \in \mathbb{R}$. Moreover, under the scaling $u \to u_\lambda(\,\cdot\,) = \lambda^{3N/2} u(\lambda\,\cdot\,)$ for $\lambda > 0$, F_α changes as $F_\alpha(u_\lambda) = \lambda^2 F_{\lambda^{-1}\alpha}(u)$. In particular, F_0 is homogeneous of order 2 under scaling.

The quadratic form F_α can be obtained as a limit of a suitably regularized version of (2.2.1), see [15] and [11, Appendix A]. As we shall see in the next subsection, the parameter α equals $-2\pi^2/a$, where a denotes the scattering length of the pair interaction. We note that other choices for quadratic forms are possible in the unitary case $\alpha = 0$ for small mass m, see [12].

To state our main result, we define, for any $m > 0$,

$$\Lambda(m) = \sup_{s,K\in\mathbb{R}^3, Q>0} \frac{s^2+Q^2}{\pi^2(1+m)} \ell_m(s,K,Q)^{-1/2} \int_{\mathbb{R}^3} \frac{1}{t^2} \ell_m(t,K,Q)^{-1/2} \times \frac{|(s+AK)\cdot(t+AK)|}{\left[(s+AK)^2+(t+AK)^2+\frac{m}{1+m}(Q^2+AK^2)\right]^2 - \left[\frac{2}{(1+m)}(s+AK)\cdot(t+AK)\right]^2} \, dt \tag{2.2.8}$$

where $A := (2+m)^{-1}$ and

$$\ell_m(s,K,Q) := \left(\frac{m}{(m+1)^2}(s+K)^2 + \frac{m}{m+1}(s^2+Q^2)\right)^{1/2} \tag{2.2.9}$$

A somewhat simpler, equivalent expression for $\Lambda(m)$, involving only the supremum over two positive parameters, will be given in Section 2.7. We shall show in Section 2.6 that $\Lambda(m)$ is finite, and satisfies the upper bound

$$\Lambda(m) \leq \frac{4(1+m)^2(2+4m+m^2)^{3/2}}{\sqrt{2}\pi\,[m(m+2)]^3} \tag{2.2.10}$$

Note that (2.2.10) implies, in particular, that $\lim_{m\to\infty}\Lambda(m) = 0$.

Our first main result is the following:

Theorem 2.2.1. *For any $\xi \in H^{1/2}_{\mathrm{as}}(\mathbb{R}^{3(N-1)})$, $\mu > 0$ and $N \geq 2$,*

$$T_{\mathrm{off}}(\xi) \geq -\Lambda(m) T_{\mathrm{diag}}(\xi) \tag{2.2.11}$$

In particular, if m is such that $\Lambda(m) < 1$, then F_α is closed and bounded from below by

$$F_\alpha(u) \geq \begin{cases} 0 & \text{for } \alpha \geq 0 \\ -\left(\frac{\alpha}{2\pi^2(1-\Lambda(m))}\right)^2 \|u\|^2_{L^2(\mathbb{R}^{3N})} & \text{for } \alpha < 0 \end{cases} \tag{2.2.12}$$

for all $u \in D(F_\alpha)$.

We note that (2.2.12) follows immediately from (2.2.11) in combination with the simple estimate $T_{\mathrm{diag}}(\xi) \geq 2\pi^2\sqrt{\mu}\|\xi\|^2_{L^2(\mathbb{R}^{3(N-1)})}$. For $\alpha < 0$, one simply chooses $\mu = \alpha^2(2\pi^2(1-\Lambda(m))^{-2}$, using the independence of $F_\alpha(u)$ of μ. As a closed and bounded from below quadratic form, F_α gives rise to a unique self-adjoint operator [57, Thm. VIII.15] for $\Lambda(m) < 1$. We shall describe it in detail in the next subsection.

The lower bound (2.2.12) is sharp as $m \to \infty$. For $\alpha < 0$, $-(\alpha/2\pi^2)^2$ equals the binding energy of the two-particle problem with point interactions. As $m \to \infty$, only one of the fermions can be bound, hence the ground state energy becomes independent of N in that limit.

We emphasize that in contrast to the previous work [11, 13] we prove a bound on the critical mass that is independent of N and, in particular, does not grow as N gets large. Also the lower bound (2.2.12) is independent of N.

We shall prove Theorem 2.2.1 in Section 2.4 below. The right side of (2.2.10) turns out to be less than 1 for $m \geq 1.76$, and hence stability holds in that region. For $m = 1$, it equals about 2.47, however, and is larger than 1 as a result of the rather crude bounds leading to (2.2.10).

In Section 2.7 we evaluate $\Lambda(m)$ numerically and show that it satisfies $\Lambda(1) < 1$. In fact, from the numerics we shall see that $\Lambda(m) < 1$ if $m \geq 0.36$ (see Fig. 2.1). Recall that F_α is known to be unbounded from below [11, Thm. 2.2] for any $N \geq 2$ for $m \leq 0.0735$. In particular, the critical mass for stability satisfies $0.0735 < m^* < 0.36$.

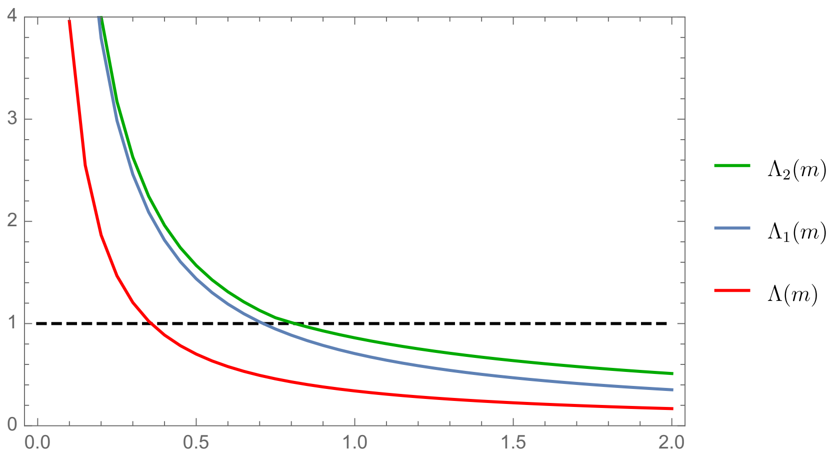

Figure 2.1: Numerical evaluation of $\Lambda(m)$ defined in (2.2.8). In the region $\Lambda(m) < 1$, we prove stability of the system. Asymptotically, $\Lambda(m) \approx 1/(2\sqrt{2}m)$ for large m (and in fact, approximately within a few percent in the whole region $m \gtrsim 1$). For $\Lambda_1(m) < 1$, we prove that the domain of the operator Γ in (2.2.13) equals $H^1_{\text{as}}(\mathbb{R}^{3(N-1)})$. Moreover, for $\Lambda_2(m) < 1$ the boundary condition in (2.2.18) implies that for every function in the domain of H_α one has $\xi \in H^{3/2}_{\text{as}}(\mathbb{R}^{3(N-1)})$.

2.2.2 Hamiltonian

For $\Lambda(m) < 1$, Theorem 2.2.1 implies that

$$T_{\text{diag}}(\xi) + T_{\text{off}}(\xi) = \langle \xi | \Gamma \xi \rangle \tag{2.2.13}$$

defines a positive selfadjoint operator Γ on $L^2_{\text{as}}(\mathbb{R}^{3(N-1)})$, with domain $D(\Gamma) \subset H^{1/2}_{\text{as}}(\mathbb{R}^{3(N-1)})$. In fact,

$$\Gamma \geq (1 - \Lambda(m))\, L \geq (1 - \Lambda(m))\, 2\pi^2 \sqrt{\mu} \tag{2.2.14}$$

where L is short for the multiplication operator in momentum space defined by (2.2.7).

It is not difficult to see that $H^1_{\text{as}}(\mathbb{R}^{3(N-1)}) \subset D(\Gamma)$ (see Sect. 2.3), but this inclusion could possibly be strict. In fact, it was shown in [46, 47] in the case $N = 2$ that Γ is not selfadjoint on H^1 for certain small m, but admits a one-parameter family of semi-bounded self-adjoint extensions. In contrast, the following theorem implies that $D(\Gamma) = H^1_{\text{as}}(\mathbb{R}^{3(N-1)})$ for larger m, more precisely for $\Lambda_1(m) < 1$, which is slightly more restrictive than our regime of stability, $\Lambda(m) < 1$.

To state our result, we define, analogously to (2.2.8), for $\beta \geq 0$ and $m > 0$,

$$\Lambda_\beta(m) = \sup_{s,K\in\mathbb{R}^3, Q>0} \frac{s^2 + Q^2}{\pi^2(1+m)} \int_{\mathbb{R}^3} \frac{1}{t^2} \left(\frac{\ell_m(s,K,Q)^{(\beta-1)/2}}{\ell_m(t,K,Q)^{(\beta+1)/2}} + \frac{\ell_m(t,K,Q)^{(\beta-1)/2}}{\ell_m(s,K,Q)^{(\beta+1)/2}} \right)$$
$$\times \frac{|(s+AK)\cdot(t+AK)|}{\left[(s+AK)^2 + (t+AK)^2 + \frac{m}{1+m}(Q^2 + AK^2)\right]^2 - \left[\frac{2}{(1+m)}(s+AK)\cdot(t+AK)\right]^2}\, \mathrm{d}t \tag{2.2.15}$$

Note that the integrand in (2.2.15) is increasing and convex in β, hence $\Lambda_\beta(m)$ is, as a supremum over such functions, also increasing and convex. We have $\Lambda_\beta(m) \geq \Lambda_0(m) = 2\Lambda(m)$. We shall show in Section 2.6 that $\Lambda_\beta(m)$ is finite for $\beta < 3$ and satisfies $\lim_{m\to\infty}\Lambda_\beta(m) = 0$. In particular, from the convexity it then follows that $\Lambda_\beta(m)$ is continuous in β for $0 \le \beta < 3$.

Theorem 2.2.2. *For any $\xi \in H^1_{\mathrm{as}}(\mathbb{R}^{3(N-1)})$, $\mu > 0$ and $N \ge 2$,*

$$\|\Gamma\xi\|^2_{L^2(\mathbb{R}^{3(N-1)})} \ge (1 - \Lambda_1(m))\,\|L\xi\|^2_{L^2(\mathbb{R}^{3(N-1)})} \tag{2.2.16}$$

In particular, if $\Lambda_1(m) < 1$, then $D(\Gamma) = D(L) = H^1_{\mathrm{as}}(\mathbb{R}^{3(N-1)})$. More generally, for $0 \le \beta \le 2$,

$$\|L^{(\beta-1)/2}\Gamma\xi\|^2_{L^2(\mathbb{R}^{3(N-1)})} \ge \left(1 - \Lambda_\beta(m)\right)\|L^{(\beta+1)/2}\xi\|^2_{L^2(\mathbb{R}^{3(N-1)})} \tag{2.2.17}$$

for all $\xi \in H^{(\beta+1)/2}_{\mathrm{as}}(\mathbb{R}^{3(N-1)})$.

The proof of Theorem 2.2.2 will be given in Section 2.5. A numerical evaluation of $\Lambda_\beta(m)$ yields $\Lambda_1(m) < 1$ for $m \ge 0.72$, while $\Lambda_2(m) < 1$ for $m \ge 0.82$ (see Fig. 2.1).

In terms of $D(\Gamma)$, the self-adjoint operator H_α defined by the quadratic form F_α in (2.2.5) can be constructed in a straightforward way following the analogous construction in the two-dimensional case in [15, Sect. 5] (see also [11,21,46,47,66]). The result is

$$D(H_\alpha) = \left\{u \in L^2_{\mathrm{as}}(\mathbb{R}^{3N}) \mid u = w + G\xi, w \in H^2_{\mathrm{as}}(\mathbb{R}^{3N}), \xi \in D(\Gamma), w\restriction_{y_N=0} = (2\pi)^{-3/2}(-1)^{N+1}(\alpha+\Gamma)\xi\right\} \tag{2.2.18}$$

and H_α acts on $u \in D(H_\alpha)$ as

$$(H_\alpha + \mu)\,u = \left(-\sum_{i=1}^N \Delta_{y_i} - \frac{2}{m+1}\sum_{1\le i<j\le N}\nabla_{y_i}\cdot\nabla_{y_j} + \mu\right)w \tag{2.2.19}$$

Note that as an H^2-function, w has an L^2-restriction to the hyperplane $y_N = 0$, and the last identity in (2.2.18) has to be understood as an identity of functions in $L^2_{\mathrm{as}}(\mathbb{R}^{3(N-1)})$. In fact, the restriction of the H^2-function w to the hyperplane $y_N = 0$ is an $H^{1/2}$ function, and hence we conclude that for any $u \in D(H_\alpha)$, the corresponding ξ satisfies $\Gamma\xi \in H^{1/2}$. The last part of Theorem 2.2.2 thus implies that for $\Lambda_2(m) < 1$, ξ is necessarily in $H^{3/2}$.

The last identity in (2.2.18) encodes the boundary condition satisfied by functions $u \in D(H_\alpha)$ at the origin. To see this, consider the behavior of the function $G\xi$ as $y_N \to 0$ or, equivalently, the integral of (2.2.4) over q_N in a large ball. A short calculation using (2.2.4) shows that

$$\begin{aligned}
&\lim_{K\to\infty}\int_{|q_N|<K}\left(\widehat{G\xi}(q_1,\ldots,q_N) - \frac{1}{q_N^2}(-1)^{N+1}\hat\xi(q_1,\ldots q_{N-1})\right)\mathrm{d}q_N \\
&= \int_{\mathbb{R}^3}\left(G(q_1,\ldots,q_N)\sum_{i=1}^{N-1}(-1)^{i+1}\hat\xi(q_1,\ldots,q_{i-1},q_{i+1},\ldots,q_N)\right)\mathrm{d}q_N \\
&\quad + (-1)^{N+1}\hat\xi(q_1,\ldots q_{N-1})\lim_{K\to\infty}\int_{|q_N|<K}\left(G(q_1,\ldots,q_N) - \frac{1}{q_N^2}\right)\mathrm{d}q_N \\
&= (-1)^N\widehat{\Gamma\xi}(q_1,\ldots,q_{N-1})
\end{aligned} \tag{2.2.20}$$

where we have used that

$$L(q_1,\ldots,q_{N-1}) = -\lim_{K\to\infty}\int_{|q_N|<K}\left(G(q_1,\ldots,q_N) - \frac{1}{q_N^2}\right)\mathrm{d}q_N \tag{2.2.21}$$

We conclude that the boundary condition in (2.2.18) implies that any $u \in D(H_\alpha)$ has the asymptotic behavior

$$\int_{|q_N|<K} \hat{u}(q_1, \ldots, q_N)\, \mathrm{d}q_N \approx (4\pi K + \alpha)\,(-1)^{N+1}\hat{\xi}(q_1, \ldots, q_{N-1}) \quad \text{as } K \to \infty. \tag{2.2.22}$$

In particular, u diverges as $2\pi^2/|y_N| + \alpha$ as $|y_N| \to 0$, and hence α is to be interpreted as $\alpha = -2\pi^2/a$ with a the scattering length of the point interaction. A precise formulation of this divergence in configuration space will be given in Proposition 1 in the next subsection.

As in the case of the corresponding quadratic form, H_α is independent of the parameter μ used in its construction. Under a unitary scaling of the form $U_\lambda\psi(\,\cdot\,) = \lambda^{3(N+1)/2}\psi(\lambda\,\cdot\,)$, it transforms as $U_\lambda^{-1} H_\alpha U_\lambda = \lambda^2 H_{\lambda^{-1}\alpha}$. Note that in contrast to $D(F_\alpha)$, the domain $D(H_\alpha)$ *does* depend on α.

2.2.3 Tan Relations

In [62–64], Tan derived a number of identities that should hold for any system of particles with point interactions (see also the review [7] and the references there). These can be experimentally tested, see [30,54,55,60,69]. In this section, we shall present a rigorous version of the Tan relations for the Hamiltonian H_α constructed in the last subsection. The analysis in this section does not actually use the self-adjointness and analogous results also hold for the general $N + M$ system, irrespective of its stability and the self-adjointness of the corresponding H_α. We shall work with the assumption $\xi \in H^1$, however, which is guaranteed to be the case for $\Lambda_1(m) < 1$, by Theorem 2.2.2.

In order to state the results, we have to re-introduce the center-of-mass motion. The Hilbert space for the $N + 1$ system is thus $L^2(\mathbb{R}^3) \otimes L^2_{\mathrm{as}}(\mathbb{R}^{3N})$, and the form domain of the corresponding quadratic form, which we denote by $\mathcal{F}_\alpha$, equals

$$D(\mathcal{F}_\alpha) = \left\{\psi = \phi + \mathcal{G}\xi \mid \phi \in H^1(\mathbb{R}^3) \otimes H^1_{\mathrm{as}}(\mathbb{R}^{3N}), \xi \in H^{1/2}(\mathbb{R}^3) \otimes H^{1/2}_{\mathrm{as}}(\mathbb{R}^{3(N-1)})\right\} \tag{2.2.23}$$

where

$$\mathcal{G}(k_0, k_1, \ldots, k_N) := \left(\frac{1}{2m}k_0^2 + \frac{1}{2}\sum_{i=1}^N k_i^2 + \mu\right)^{-1}, \tag{2.2.24}$$

$\mathcal{G}\xi$ is short for the function with Fourier transform

$$\widehat{\mathcal{G}\xi}(k_0, k_1, \ldots, k_N) = \mathcal{G}(k_0, k_1, \ldots, k_N) \sum_{i=1}^N (-1)^{i+1}\hat{\xi}(k_0 + k_i, k_1, \ldots, k_{i-1}, k_{i+1}, \ldots, k_N) \tag{2.2.25}$$

and, compared to (2.2.3), we have absorbed a factor $\frac{m+1}{2m}$ into the definition of ξ for simplicity. For $\psi \in D(\mathcal{F}_\alpha)$, we have

$$\begin{aligned} \mathcal{F}_\alpha(\psi) = &\left\langle \phi \left| -\frac{1}{2m}\Delta_{x_0} - \frac{1}{2}\sum_{i=1}^N \Delta_{x_i} + \mu \right| \phi \right\rangle - \mu\, \|\psi\|^2_{L^2(\mathbb{R}^{3(N+1)})} \\ &+ N\left(\frac{2m}{m+1}\alpha\, \|\xi\|^2_{L^2(\mathbb{R}^{3N})} + \mathcal{T}_{\mathrm{diag}}(\xi) + \mathcal{T}_{\mathrm{off}}(\xi)\right) \end{aligned} \tag{2.2.26}$$

where

$$\mathcal{T}_{\mathrm{diag}}(\xi) := \int_{\mathbb{R}^{3N}} |\hat{\xi}(k_0, k_1, \vec{k})|^2 \mathcal{L}(k_0, k_1, \vec{k})\, \mathrm{d}k_0\, \mathrm{d}k_1\, \mathrm{d}\vec{k}$$
$$\mathcal{T}_{\mathrm{off}}(\xi) := (N-1) \int_{\mathbb{R}^{3(N+1)}} \hat{\xi}^*(k_0 + s, t, \vec{k}) \hat{\xi}(k_0 + t, s, \vec{k}) \mathcal{G}(k_0, s, t, \vec{k})\, \mathrm{d}k_0\, \mathrm{d}s\, \mathrm{d}t\, \mathrm{d}\vec{k} \tag{2.2.27}$$

and we used $\vec{k} = (k_2, \ldots, k_{N-1})$ for short. The function $\mathcal{L}$ is given by

$$\mathcal{L}(k_0, k_1, \ldots, k_{N-1}) := 2\pi^2 \left(\frac{2m}{m+1}\right)^{3/2} \left(\frac{k_0^2}{2(m+1)} + \frac{1}{2}\sum_{i=1}^{N-1} k_i^2 + \mu\right)^{1/2} \tag{2.2.28}$$

Theorem 2.2.1 implies that

$$\mathcal{T}_{\mathrm{off}}(\xi) \geq -\Lambda(m) \mathcal{T}_{\mathrm{diag}}(\xi) \qquad \text{for all } \xi \in H^{1/2}(\mathbb{R}^3) \otimes H^{1/2}_{\mathrm{as}}(\mathbb{R}^{3(N-1)}). \tag{2.2.29}$$

To see this, one can either mimic the proof of Theorem 2.2.1, or one simply argues as follows. Displaying the dependence on μ explicitly via a superscript in the expressions for $T_{\mathrm{diag/off}}$ and $\mathcal{T}_{\mathrm{diag/off}}$ in (2.2.6) and (2.2.27), respectively, it is straightforward to check that

$$\mathcal{T}^{\mu}_{\mathrm{diag/off}}(\xi) = \frac{2m}{m+1} \int_{\mathbb{R}^3} T^{\tilde{\mu}_P}_{\mathrm{diag/off}}(\eta_P)\, \mathrm{d}P \tag{2.2.30}$$

where $\tilde{\mu}_P = \frac{2m}{m+1}(\mu + \frac{P^2}{2(m+N)})$ and

$$\hat{\eta}_P(q_1, \ldots, q_{N-1}) = \hat{\xi}\left(\tfrac{m+1}{m+N} P - \sum_{j=1}^{N-1} q_j, q_1 + \tfrac{1}{m+N} P, \ldots, q_{N-1} + \tfrac{1}{m+N} P\right) \tag{2.2.31}$$

which is in $H^{1/2}_{\mathrm{as}}(\mathbb{R}^{3(N-1)})$ for almost every $P \in \mathbb{R}^3$. Since the bound (2.2.11) is uniform in μ, (2.2.29) follows.

Analogously to the discussion in the previous subsection, for $\Lambda(m) < 1$ the quadratic form $\mathcal{T}_{\mathrm{diag}}(\xi) + \mathcal{T}_{\mathrm{off}}(\xi)$ defines a positive self-adjoint operator $\tilde{\Gamma}$ on $L^2(\mathbb{R}^3) \otimes L^2_{\mathrm{as}}(\mathbb{R}^{3(N-1)})$. Explicitly, $\tilde{\Gamma}$ acts as

$$\begin{aligned}
&\widehat{\tilde{\Gamma}\xi}(k_0, k_1, \ldots, k_{N-1}) \\
&\quad = \mathcal{L}(k_0, k_1, \ldots, k_{N-1}) \hat{\xi}(k_0, k_1, \ldots, k_{N-1}) \\
&\qquad + \sum_{j=1}^{N-1} (-1)^{j+1} \int_{\mathbb{R}^3} \mathcal{G}(k_0 - s, s, k_1, \ldots, k_{N-1}) \hat{\xi}(k_0 + k_j - s, s, k_1, \ldots, k_{j-1}, k_{j+1}, \ldots, k_{N-1})\, \mathrm{d}s
\end{aligned} \tag{2.2.32}$$

Theorem 2.2.2 implies that the domain $D(\tilde{\Gamma})$ equals $H^1(\mathbb{R}^3) \otimes H^1_{\mathrm{as}}(\mathbb{R}^{3(N-1)})$ in the case $\Lambda_1(m) < 1$. The domain of the self-adjoint operator $\mathcal{H}_\alpha$ corresponding to the quadratic form $\mathcal{F}_\alpha$ is given by those $\psi \in D(\mathcal{F}_\alpha)$ where $\phi \in H^2(\mathbb{R}^3) \otimes H^2_{\mathrm{as}}(\mathbb{R}^{3N})$, $\xi \in D(\tilde{\Gamma})$ and the boundary condition

$$\phi \upharpoonright_{x_N = x_0} = \frac{(-1)^{N+1}}{(2\pi)^{3/2}} \left(\frac{2m\alpha}{m+1} + \tilde{\Gamma}\right) \xi \tag{2.2.33}$$

is satisfied. The Hamiltonian $\mathcal{H}_\alpha$ acts as

$$(\mathcal{H}_\alpha + \mu)\,\psi = \left(-\frac{1}{2m}\Delta_{x_0} - \frac{1}{2}\sum_{i=1}^{N}\Delta_{x_i} + \mu\right)\phi \tag{2.2.34}$$

It commutes with translations and rotations, and transforms under scaling in the same way as discussed for H_α at the end of the previous subsection.

The connection between the boundary condition (2.2.33) and the asymptotic behavior of $\psi \in D(\mathcal{H}_\alpha)$ as $|x_N - x_0| \to 0$ is explored in the following proposition, whose proof will be given in Section 2.8.

Proposition 1. *For any $\psi \in D(\mathcal{H}_\alpha)$ with $\xi \in H^1(\mathbb{R}^{3N})$, we have*

$$\begin{aligned}\psi\left(R + \tfrac{r}{1+m}, x_1, \ldots, x_{N-1}, R - \tfrac{mr}{1+m}\right) = \left(\frac{2\pi^2}{|r|} + \alpha\right)\frac{2m}{m+1}\frac{(-1)^{N+1}}{(2\pi)^{3/2}}\xi(R, x_1, \ldots x_{N-1})\\ + \upsilon(R, x_1, \ldots, x_{N-1}, r)\end{aligned} \tag{2.2.35}$$

with $\upsilon(\,\cdot\,, r) \in L^2(\mathbb{R}^{3N})$ for all $r \in \mathbb{R}^3$, and $\lim_{r\to 0}\|\upsilon(\,\cdot\,, r)\|_{L^2(\mathbb{R}^{3N})} = 0$.

Proposition 1 immediately implies a two-term asymptotics for the two-particle density

$$\rho(r) = N\int_{\mathbb{R}^{3N}}\left|\psi\left(R + \tfrac{r}{1+m}, x_1, \ldots, x_{N-1}, R - \tfrac{mr}{1+m}\right)\right|^2 \mathrm{d}R\,\mathrm{d}x_1\cdots\mathrm{d}x_{N-1} \tag{2.2.36}$$

as $r \to 0$. In fact, ρ satisfies

$$\rho(r) = \frac{\pi}{2}\left(\frac{1}{|r|^2} - \frac{2}{|r|a}\right)C + g(r) \quad \text{with} \quad \lim_{r\to 0}|rg(r)| = 0 \tag{2.2.37}$$

where $a = -2\pi^2/\alpha$ denotes the scattering length and

$$C = \left(\frac{2m}{m+1}\right)^2 N\|\xi\|^2_{L^2(\mathbb{R}^{3N})} \tag{2.2.38}$$

In the physics literature, C is called the *contact* [62–64]. It turns out to play a crucial role in various other relevant quantities, as we shall demonstrate now.

For general $\psi \in L^2(\mathbb{R}^3)\otimes L^2_{\mathrm{as}}(\mathbb{R}^{3N})$, the momentum densities of the mass m (spin up) particle $n_\uparrow(k)$ and of the mass 1 (spin-down) particles $n_\downarrow(k)$ are defined as

$$n_\uparrow(k) = \int_{\mathbb{R}^{3N}}|\hat{\psi}(k, k_1, \ldots, k_N)|^2\,\mathrm{d}k_1\cdots\mathrm{d}k_N\ ,\ n_\downarrow(k) = N\int_{\mathbb{R}^{3N}}|\hat{\psi}(k_0, k, k_2, \ldots, k_N)|^2\,\mathrm{d}k_0\,\mathrm{d}k_2\cdots\mathrm{d}k_N \tag{2.2.39}$$

Our rigorous formulation of the Tan relation for the energy is as follows.

Theorem 2.2.3. *For $\psi \in D(\mathcal{H}_\alpha)$ with $\xi \in H^1(\mathbb{R}^{3N})$, let C be given in* (2.2.38)*, and let*

$$p_\uparrow = \frac{2m}{m+1}\|\xi\|^{-2}_{L^2(\mathbb{R}^{3N})}\int_{\mathbb{R}^{3N}}k_1|\hat{\xi}(k_1, \ldots, k_N)|^2\,\mathrm{d}k_1\cdots\mathrm{d}k_N \quad , \quad p_\downarrow = \frac{1}{m}p_\uparrow. \tag{2.2.40}$$

Then

$$k \mapsto k^2 n_\uparrow(k) - \frac{C}{|k-p_\uparrow|^2} \in L^1(\mathbb{R}^3) \quad \textit{and} \quad k \mapsto k^2 n_\downarrow(k) - \frac{C}{|k-p_\downarrow|^2} \in L^1(\mathbb{R}^3) \tag{2.2.41}$$

and we have the identity

$$\langle\psi|\mathcal{H}_\alpha\psi\rangle = \int_{\mathbb{R}^3} \left[\frac{1}{2m}\left(k^2 n_\uparrow(k) - \frac{C}{|k-p_\uparrow|^2}\right) + \frac{1}{2}\left(k^2 n_\downarrow(k) - \frac{C}{|k-p_\downarrow|^2}\right)\right] \mathrm{d}k - \frac{m+1}{2m} C\alpha \tag{2.2.42}$$

Since C, $p_\uparrow$ and $p_\downarrow$ are uniquely determined by the momentum densities via (2.2.41), Eq. (2.2.42) expresses the energy solely in terms of the momentum densities. The set of possible momentum densities arising from wave functions $\psi \in D(\mathcal{H}_\alpha)$ is not known, however, and can be expected to depend in a complicated way on both α and N.

The contact C thus determines the asymptotic behavior of both $n_\uparrow(k)$ and $n_\downarrow(k)$, via $n_\uparrow(k) \approx n_\downarrow(k) \approx C|k|^{-4}$ for large $|k|$. In fact, up to terms decaying faster than $|k|^{-5}$, we have for large $|k|$

$$n_\uparrow(k) + n_\downarrow(k) \approx \frac{C}{|k|^2|k-p_\uparrow|^2} + \frac{C}{|k|^2|k-p_\downarrow|^2} \approx \frac{C}{|k-P|^4} \tag{2.2.43}$$

for $P = \frac{1}{2}(p_\uparrow + p_\downarrow) = \|\xi\|^{-2}_{L^2(\mathbb{R}^{3N})} \int_{\mathbb{R}^{3N}} k_1 |\hat{\xi}(k_1,\dots,k_N)|^2 \, \mathrm{d}k_1 \dots \mathrm{d}k_N$. Note also that due to the fact that $\lim_{K\to\infty} \int_{|k|<K} (|k|^{-2} - |k-p|^{-2})\, \mathrm{d}k = 0$ for any $p \in \mathbb{R}^3$, one can rewrite the identity (2.2.42) as

$$\langle\psi|\mathcal{H}_\alpha\psi\rangle = \lim_{K\to\infty} \int_{|k|<K} \left[\frac{k^2}{2m}\left(n_\uparrow(k) - \frac{C}{|k|^4}\right) + \frac{k^2}{2}\left(n_\downarrow(k) - \frac{C}{|k|^4}\right)\right] \mathrm{d}k - \frac{m+1}{2m} C\alpha \tag{2.2.44}$$

For any stationary state, the contact C can be computed as the derivative of the energy with respect to α, by the Feynman-Hellmann principle. In fact, for *fixed* ψ (and hence fixed ξ),

$$\frac{\partial}{\partial\alpha}\mathcal{F}_\alpha(\psi) = \frac{m+1}{2m} C \tag{2.2.45}$$

Note that it is important to use the quadratic form formulation here, as the domain of $\mathcal{H}_\alpha$ depends on α and hence ψ cannot be fixed when taking the derivative of $\langle\psi|\mathcal{H}_\alpha\psi\rangle$ with respect to α. Note also the minus sign in front of the last term in (2.2.42); a naive derivative of (2.2.42) would give the wrong sign!

The L^1-property (2.2.41) claimed in Theorem 2.2.3 does not make use of the boundary condition (2.2.33) satisfied by $\psi \in D(\mathcal{H}_\alpha)$ and holds more generally, in fact. The identity (2.2.42) only holds for ψ satisfying (2.2.33), however; i.e., it holds for all functions ψ in the domain of $\mathcal{H}_\alpha$. (As already mentioned in the beginning of this section, self-adjointness of $\mathcal{H}_\alpha$ on this domain is not actually needed here. In particular, Theorem 2.2.3 holds for all $m > 0$.)

The equations (2.2.37), (2.2.41), (2.2.42) and (2.2.45) can be interpreted as a rigorous formulation of the Tan relations introduced in [62–64]. There is actually one more relation, a virial type theorem. It is an immediate consequence of the relation $U_\lambda^{-1}\mathcal{H}_\alpha U_\lambda = \lambda^2 \mathcal{H}_{\lambda^{-1}\alpha}$ for scaling the variables by $\lambda > 0$ and we shall not discuss it further here.

The proof of Theorem 2.2.3 will be given in Section 2.9.

2.3 Preliminaries

Before giving the proof of the results in the previous section, we collect here a few auxiliary facts that will be used in the proofs.

Lemma 2.3.1. *The operator σ on $L^2(\mathbb{R}^3)$ with integral kernel*

$$\sigma(s,t) = (s^2+1)^{(\beta-1)/4}(t^2+1)^{-(\beta+1)/4}\frac{1}{s^2+t^2+\lambda s\cdot t+1} \tag{2.3.1}$$

is bounded for $-2 < \lambda < 2$ and $-2 < \beta < 2$.

Proof. We use the Schur test in the form

$$\|\sigma\| \leq \frac{1}{2}\sup_s h(s)\int_{\mathbb{R}^3} h(t)^{-1}\left(|\sigma(s,t)| + |\sigma(t,s)|\right)\,\mathrm{d}t \tag{2.3.2}$$

for any positive function h, which is a consequence of the Cauchy-Schwarz inequality. Since $|\lambda| < 2$, a pointwise estimate of the kernel reduces the problem to the case $\lambda = 0$. Choosing $h(t) = (t^2+1)^\gamma$ one easily checks that the right side of (2.3.2) is finite if and only if $(1+|\beta|)/4 < \gamma < (5-|\beta|)/4$. □

In the special case $\beta = 0$, Lemma 2.3.1 can be used to show that, for some $c > 0$, $|T_{\mathrm{off}}(\xi)| \leq c(N-1)T_{\mathrm{diag}}(\xi)$ for all $\xi \in H^{1/2}_{\mathrm{as}}(\mathbb{R}^{3(N-1)})$. In particular, F_α is well-defined on its domain (2.2.3). Similarly, $\|L^{(\beta-1)/2}\Gamma\xi\|_{L^2(\mathbb{R}^{3(N-1)})}$ is finite for $\xi \in H^{(\beta+1)/2}_{\mathrm{as}}(\mathbb{R}^{3(N-1)})$ for $0 \leq \beta < 2$. For $\beta = 1$, this implies that the domain of Γ contains $H^1_{\mathrm{as}}(\mathbb{R}^{3(N-1)})$.

Lemma 2.3.2. *The operator σ on $L^2(\mathbb{R}^3)$ with integral kernel*

$$\sigma(s,t) = \left(\frac{(s^2+\nu)^{(\beta-1)/4}}{(t^2+\nu)^{(\beta+1)/4}} + \frac{(t^2+\nu)^{(\beta-1)/4}}{(s^2+\nu)^{(\beta+1)/4}}\right)\frac{1}{s^2+t^2+\lambda s\cdot t+1} \tag{2.3.3}$$

is bounded and non-negative for $-2 < \beta < 2$, $\nu \geq 1/2$ and $-2 < \lambda \leq 0$.

Proof. Boundedness follows immediately from Lemma 2.3.1. For $\beta = 0$, positivity can be deduced from the integral representation

$$\left(t^2+s^2+\lambda s\cdot t+1\right)^{-1} = \int_0^\infty e^{-r(1+\lambda/2)t^2}e^{-r(1+\lambda/2)s^2}e^{r\lambda(t-s)^2/2}e^{-r}\,\mathrm{d}r\,, \tag{2.3.4}$$

noting that $-2 < \lambda \leq 0$ and that the Gaussian has a positive Fourier transform. We are thus left with proving positivity for $\beta \neq 0$. Without loss of generality, we may assume $\beta > 0$, since σ is invariant under the transformation $\beta \to -\beta$. To this aim, we use

$$x^{-\beta/2} = c_\beta\int_0^\infty \frac{1}{x+r}r^{-\beta/2}\,\mathrm{d}r \tag{2.3.5}$$

with $c_\beta = \pi^{-1}\sin\left(\frac{\pi}{2}\beta\right)$ for $x > 0$ and $0 < \beta < 2$ to rewrite the kernel as

$$\sigma(s,t) = c_\beta(s^2+\nu)^{(\beta-1)/4}(t^2+\nu)^{(\beta-1)/4}\int_0^\infty\left(\frac{1}{s^2+\nu+r} + \frac{1}{t^2+\nu+r}\right)\frac{r^{-\beta/2}}{s^2+t^2+\lambda s\cdot t+1}\,\mathrm{d}r \tag{2.3.6}$$

Let us rewrite the integrand further as

$$r^{-\beta/2}\frac{1}{s^2+\nu+r}\frac{1}{t^2+\nu+r}\frac{s^2+t^2+2(\nu+r)}{s^2+t^2+\lambda s\cdot t+1}$$
$$= r^{-\beta/2}\frac{1}{s^2+\nu+r}\frac{1}{t^2+\nu+r}\left(1+\frac{2(\nu+r)-1-\lambda s\cdot t}{s^2+t^2+\lambda s\cdot t+1}\right) \tag{2.3.7}$$

Using again (2.3.4), as well as $2(\nu+r)\geq 1$ and $\lambda\leq 0$, we see that (2.3.7) defines a non-negative operator. This completes the proof. □

Lemma 2.3.3. *Consider the bounded operator σ on $L^2(\mathbb{R}^3)$ with integral kernel given by* (2.3.3) *for $-2<\beta<2$, $\nu\geq 1/2$ and $0\leq\lambda<2$. Its positive and negative parts are the operators with kernels*

$$\sigma_+(s,t) = \frac{1}{2}\left(\sigma(s,t)+\sigma(s,-t)\right)$$
$$\sigma_-(s,t) = -\frac{1}{2}\left(\sigma(s,t)-\sigma(s,-t)\right) \tag{2.3.8}$$

respectively.

Proof. Let R denote the reflection operator $(R\varphi)(s)=\varphi(-s)$ for $\varphi\in L^2(\mathbb{R}^3)$. The operators R and σ clearly commute. Moreover, the product σR equals the operator with integral kernel (2.3.3) and λ replaced by $-\lambda$, which was shown to be non-negative in Lemma 2.3.2. One readily checks that this implies that the positive and negative parts of σ are given by

$$\sigma_\pm = \pm\frac{1}{2}\sigma\,(1\pm R)\ , \tag{2.3.9}$$

respectively. In fact, clearly $\sigma_+\sigma_-=\sigma_-\sigma_+=0$, and $\sigma_\pm=\frac{1}{2}\sigma R(1\pm R)$, which is a product of two commuting nonnegative operators. □

2.4 Proof of Theorem 2.2.1

We assume $N\geq 3$ and define, for fixed $\vec{q}\in\mathbb{R}^{3(N-2)}$ and $-2<\beta<2$, an operator τ^β on $L^2(\mathbb{R}^3)$ via the quadratic form

$$\langle\varphi|\tau^\beta|\varphi\rangle = \frac{1}{2}\int_{\mathbb{R}^6}\varphi^*(s)\varphi(t)\left(\frac{L(s,\vec{q})^{(\beta-1)/2}}{L(t,\vec{q})^{(\beta+1)/2}}+\frac{L(t,\vec{q})^{(\beta-1)/2}}{L(s,\vec{q})^{(\beta+1)/2}}\right)G(s,t,\vec{q})\,\mathrm{d}s\,\mathrm{d}t \tag{2.4.1}$$

where L and G are defined in (2.2.7) and (2.2.2), respectively. Let $K:=\sum_{i=1}^{N-2}q_i$, and recall that $A=1/(m+2)$. The following observation is key to our further investigation. We shall need it here for $\beta=0$ only, but state it more generally for later use in the proof of Theorem 2.2.2.

Lemma 2.4.1. *The operator τ^β defined in* (2.4.1) *is bounded on $L^2(\mathbb{R}^3)$. Its positive and negative parts, $\tau^\beta_\pm$, are the operators with integral kernels*

$$\tau^\beta_+(s,t;\vec{q}) = \frac{1}{4}\left(\frac{L(s,\vec{q})^{(\beta-1)/2}}{L(t,\vec{q})^{(\beta+1)/2}}+\frac{L(t,\vec{q})^{(\beta-1)/2}}{L(s,\vec{q})^{(\beta+1)/2}}\right)\left(G(s,t,\vec{q})+G(s,-t-2AK,\vec{q})\right)$$
$$\tau^\beta_-(s,t;\vec{q}) = -\frac{1}{4}\left(\frac{L(s,\vec{q})^{(\beta-1)/2}}{L(t,\vec{q})^{(\beta+1)/2}}+\frac{L(t,\vec{q})^{(\beta-1)/2}}{L(s,\vec{q})^{(\beta+1)/2}}\right)\left(G(s,t,\vec{q})-G(s,-t-2AK,\vec{q})\right) \tag{2.4.2}$$

respectively.

Proof. Let $Q^2 := \sum_{i=1}^{N-2} q_i^2$, and define $\lambda := 2/(m+1)$. A simple calculation shows that

$$G(s - AK, t - AK, \vec{q})^{-1} = t^2 + s^2 + \lambda s \cdot t + C \tag{2.4.3}$$

where

$$C = C(\vec{q}) = \frac{m}{m+1}\left(AK^2 + Q^2\right) + \mu \tag{2.4.4}$$

Similarly,

$$L(s - AK, \vec{q}) = 2\pi^2 \left(\frac{m(m+2)}{(m+1)^2}s^2 + C\right)^{1/2} \tag{2.4.5}$$

In particular, after a unitary translation by AK, the operator τ^β becomes the operator σ with integral kernel

$$\begin{aligned}\sigma(s,t) = \frac{m+1}{4\pi^2}&\left(\frac{\left[m(m+2)s^2 + (m+1)^2C\right]^{(\beta-1)/4}}{\left[m(m+2)t^2 + (m+1)^2C\right]^{(\beta+1)/4}} + \frac{\left[m(m+2)t^2 + (m+1)^2C\right]^{(\beta-1)/4}}{\left[m(m+2)s^2 + (m+1)^2C\right]^{(\beta+1)/4}}\right) \\ &\times \left(t^2 + s^2 + \lambda s \cdot t + C\right)^{-1}\end{aligned} \tag{2.4.6}$$

After a simple rescaling of the variables by $\sqrt{C}$, this is exactly of the form (2.3.3), with $\nu = (m+1)^2/(m(m+2)) > 1/2$ (in fact, > 1). Hence boundedness of σ follows from Lemma 2.3.1. Moreover, Lemma 2.3.3 applies, which states that the positive and negative parts of σ are given by

$$\sigma_\pm = \pm\frac{1}{2}\sigma\,(1 \pm R)\ , \tag{2.4.7}$$

where R denotes reflection. Undoing the unitary translation by AK, this leads to the statement of the lemma. □

For $\xi \in H^{1/2}_{\mathrm{as}}(\mathbb{R}^{3(N-1)})$, we define $\varphi \in L^2_{\mathrm{as}}(\mathbb{R}^{3(N-1)})$ by $\varphi(s,\vec{q}) = L(s,\vec{q})^{1/2}\hat{\xi}(s,\vec{q})$. Then $T_{\mathrm{diag}}(\xi) = \|\varphi\|^2_{L^2(\mathbb{R}^{3(N-1)})}$, and

$$\begin{aligned}T_{\mathrm{off}}(\xi) &= (N-1)\int_{\mathbb{R}^{3N}} \varphi^*(s,\vec{q})\varphi(t,\vec{q})L(s,\vec{q})^{-1/2}L(t,\vec{q})^{-1/2}G(s,t,\vec{q})\,\mathrm{d}s\,\mathrm{d}t\,\mathrm{d}\vec{q} \\ &\geq -(N-1)\int_{\mathbb{R}^{3N}} \varphi^*(s,\vec{q})\varphi(t,\vec{q})\tau^0_-(s,t;\vec{q})\,\mathrm{d}s\,\mathrm{d}t\,\mathrm{d}\vec{q}\end{aligned} \tag{2.4.8}$$

where we simply dropped the positive part of the operator τ^0 appearing on the right side. Its negative part, τ^0_-, is explicitly identified in Lemma 2.4.1. To proceed, we use the fact that φ is antisymmetric. We introduce

$$\tilde{\tau}_-(s,\vec{q},t,\vec{\ell}) = \tau^0_-(s,t;\vec{q})\delta(\vec{q} - \vec{\ell}) \tag{2.4.9}$$

for $\vec{\ell} \in \mathbb{R}^{3(N-2)}$, and rewrite the term on the right side of (2.4.8) as

$$\begin{aligned}&(N-1)\int_{\mathbb{R}^{3N}} \varphi^*(s,\vec{q})\varphi(t,\vec{q})\tau^0_-(s,t;\vec{q})\,\mathrm{d}s\,\mathrm{d}t\,\mathrm{d}\vec{q} \\ &= \sum_{i=0}^{N-2}\int_{\mathbb{R}^{6(N-1)}} \varphi^*(s,\vec{q})\varphi(t,\vec{\ell})\tilde{\tau}_-(q_i,\hat{q}_i,\ell_i,\hat{\ell}_i)\,\mathrm{d}s\,\mathrm{d}t\,\mathrm{d}\vec{q}\,\mathrm{d}\vec{\ell}\end{aligned} \tag{2.4.10}$$

where $\hat{q}_i = (q_1, \ldots, q_{i-1}, s, q_{i+1}, \ldots, q_{N-2})$ and $\hat{\ell}_i = (\ell_1, \ldots, \ell_{i-1}, t, \ell_{i+1}, \ldots, \ell_{N-2})$ for $1 \leq i \leq N-2$, as well as $q_0 = s$, $\hat{q}_0 = \vec{q}$, $\ell_0 = t$, $\hat{\ell}_0 = \vec{\ell}$. To bound this last expression, we use the Schwarz inequality, as in (2.3.2), to obtain

$$(2.4.10) \leq \|\varphi\|^2_{L^2(\mathbb{R}^{3(N-1)})} \sup_{s,\vec{q}} h(s,\vec{q}) \sum_{i=0}^{N-2} \int_{\mathbb{R}^{3(N-1)}} h(t,\vec{\ell})^{-1} |\tilde{\tau}_-(q_i, \hat{q}_i, \ell_i, \hat{\ell}_i)| \, \mathrm{d}t \, \mathrm{d}\vec{\ell} \tag{2.4.11}$$

for any positive function h. Assume that h is symmetric with respect to permutations. Inserting the special structure (2.4.9), the expression on the right side of (2.4.11) then equals

$$\|\varphi\|^2_{L^2(\mathbb{R}^{3(N-1)})} \sup_{s,\vec{q}} h(s,\vec{q}) \sum_{i=0}^{N-2} \int_{\mathbb{R}^3} h(t,\hat{q}_i)^{-1} |\tau^0_-(q_i, t; \hat{q}_i)| \, \mathrm{d}t \tag{2.4.12}$$

We shall choose $h(s,\vec{q}) = s^2 \prod_{j=1}^{N-2} q_j^2$ in (2.4.12). The resulting bound is then

$$\begin{aligned}(2.4.10) &\leq \|\varphi\|^2_{L^2(\mathbb{R}^{3(N-1)})} \sup_{s,\vec{q}} \sum_{i=0}^{N-2} \int_{\mathbb{R}^3} \frac{q_i^2}{t^2} |\tau^0_-(q_i, t; \hat{q}_i)| \, \mathrm{d}t \\ &\leq \|\varphi\|^2_{L^2(\mathbb{R}^{3(N-1)})} \sup_{s,\vec{q}} \left(s^2 + Q^2\right) \max_{0 \leq i \leq N-2} \int_{\mathbb{R}^3} \frac{1}{t^2} |\tau^0_-(q_i, t; \hat{q}_i)| \, \mathrm{d}t \end{aligned} \tag{2.4.13}$$

where we again use the notation $Q^2 = \sum_{i=1}^{N-2} q_i^2$, as in the proof of Lemma 2.4.1. Since for any $1 \leq i \leq N-2$, $s^2 + Q^2$ is symmetric under exchange of s and q_i, we can drop the maximum over i when taking the supremum over s and $\vec{q}$, and simply take $i = 0$ (or any other value of i, in fact). We thus arrive at

$$(2.4.10) \leq \|\varphi\|^2_{L^2(\mathbb{R}^{3(N-1)})} \sup_{s,\vec{q}} \left(s^2 + Q^2\right) \int_{\mathbb{R}^3} \frac{1}{t^2} |\tau^0_-(s, t; \vec{q})| \, \mathrm{d}t \tag{2.4.14}$$

To complete the proof of (2.2.11), we need to show that the term multiplying $\|\varphi\|^2_{L^2(\mathbb{R}^{3(N-1)})} = T_{\mathrm{diag}}(\xi)$ on the right side of (2.4.14) is bounded by $\Lambda(m)$. Recall the explicit expression of $\tau^0_-(s,t;\vec{q})$, given in (2.4.2) above. We have

$$\begin{aligned}|\tau^0_-(s,t;\vec{q})| = {} & \frac{1}{\pi^2(1+m)} \left(\frac{m}{(m+1)^2}(s+K)^2 + \frac{m}{m+1}(s^2+Q^2) + \mu \right)^{-1/4} \\ & \times \left(\frac{m}{(m+1)^2}(t+K)^2 + \frac{m}{m+1}(t^2+Q^2) + \mu \right)^{-1/4} \\ & \times \frac{|(s+AK)\cdot(t+AK)|}{\left[(s+AK)^2 + (t+AK)^2 + \frac{m}{1+m}(Q^2 + AK^2) + \mu\right]^2 - \left[\frac{2}{(1+m)}(s+AK)\cdot(t+AK)\right]^2}\end{aligned} \tag{2.4.15}$$

For an upper bound, we can replace μ by 0. Moreover, we can replace the supremum over $\vec{q} \in \mathbb{R}^{3(N-2)}$ by a supremum over all $Q > 0$ and $K \in \mathbb{R}^3$. This yields (2.2.11).

To complete the proof of Theorem 2.2.1, we have to show that F_α is closed for $\Lambda(m) < 1$. This was already proved in [11, Thm. 2.1], we include the proof here for completeness. Given a sequence $u_n \in D(F_\alpha)$ with $\|u_n - u_m\|_{L^2(\mathbb{R}^{3N})} \to 0$ and $F_\alpha(u_n - u_m) \to 0$ as $n, m \to \infty$, we need to show that there exists a $u \in D(F_\alpha)$ with $\lim_{n\to\infty} \|u_n - u\|_{L^2(\mathbb{R}^{3N})} = 0$ and $\lim_{n\to\infty} F_\alpha(u_n - u) = 0$. We choose any $\mu > 0$ for $\alpha \geq 0$, and $\mu > \alpha^2(2\pi(1 - \Lambda(m))^{-2}$ for $\alpha < 0$. For such a choice, writing $u_n = w_n + G\xi_n$, the bound (2.2.11) implies that $\|w_n - w_m\|_{H^1(\mathbb{R}^{3N})} \to 0$ and $\|\xi_n - \xi_m\|_{H^{1/2}(\mathbb{R}^{3(N-1)})} \to 0$ as $n, m \to \infty$, and hence $w_n \to w$ and $\xi_n \to \xi$ for some w and ξ, respectively, in the corresponding norms. Since $\|G(\xi_n - \xi_m)\|_{L^2(\mathbb{R}^{3N})} \leq \text{const}\|\xi_n - \xi_m\|_{L^2(\mathbb{R}^{3(N-1)})}$, u_n converges to $u = w + G\xi$ in $L^2(\mathbb{R}^{3N})$. Moreover, since $|F_\alpha(u_n - u)|$ is bounded from above by $\text{const}(\|w_n - w\|^2_{H^1(\mathbb{R}^{3N})} + \|\xi_n - \xi\|^2_{H^{1/2}(\mathbb{R}^{3(N-1)})})$ (compare with the remark after Lemma 2.3.1 in Section 2.3), the result follows. □

Remark 2.4.2. *It is worth pointing out that the antisymmetry of the wave functions enters our proof of stability in three different ways. The first two concern the very definition of the model. First, there are no point interactions among the N particles of mass* 1 *themselves, due to the antisymmetry which forces the wave functions to vanish at particle coincidences. Second, the term T_{off} in the definition (2.2.5) of the quadratic form F_α enters with a plus sign, while it would have a minus sign for bosons. This fact is crucial, as it allows to work with the negative part of the operator τ^0 in* (2.4.1) *instead of the positive part, which is larger. And third, we use the symmetry to replace the factor* $(N - 1)$ *by a sum over particles in* (2.4.10)*.*

This last step would also work for bosons, only the symmetry of the absolute value of the wave functions is important. For the first two points, however, the antisymmetry is crucial. In the bosonic case, there is instability for any $N \geq 2$ and any $0 < m < \infty$ [8,61,73] (a fact known as the Thomas effect [68]). While T_{off} can be bounded from below by $-T_{\text{diag}}$, as Theorem 2.2.1 shows, it is in fact known that $T_{\text{off}}(\xi) \leq T_{\text{diag}}(\xi)$ is false for suitable ξ for any m [11].

2.5 Proof of Theorem 2.2.2

Let us define the operator J by $\Gamma = L + J$, i.e., $T_{\text{off}}(\xi) = \langle\xi|J\xi\rangle$ for $\xi \in H^1_{\text{as}}(\mathbb{R}^{3(N-1)})$. For $0 \leq \beta < 2$, we have

$$\begin{aligned}\|L^{(\beta-1)/2}\Gamma\xi\|^2_{L^2(\mathbb{R}^{3(N-1)})} &= \|L^{(\beta+1)/2}\xi\|^2_{L^2(\mathbb{R}^{3(N-1)})} + \langle\xi|(JL^\beta + L^\beta J)\xi\rangle + \|L^{(\beta-1)/2}J\xi\|^2_{L^2(\mathbb{R}^{3(N-1)})} \\ &\geq \|L^{(\beta+1)/2}\xi\|^2_{L^2(\mathbb{R}^{3(N-1)})} + \langle\xi|(JL^\beta + L^\beta J)\xi\rangle \qquad (2.5.1)\end{aligned}$$

for all $\xi \in H^{(\beta+1)/2}_{\text{as}}(\mathbb{R}^{3(N-1)})$. The result (2.2.17) thus follows if we can show that

$$\langle\xi|(JL^\beta + L^\beta J)\xi\rangle \geq -\Lambda_\beta(m)\|L^{(\beta+1)/2}\xi\|^2_{L^2(\mathbb{R}^{3(N-1)})} \qquad (2.5.2)$$

With $\varphi = L^{(\beta+1)/2}\xi$ this reads, equivalently,

$$\langle\varphi|(L^{-(\beta+1)/2}JL^{(\beta-1)/2} + L^{(\beta-1)/2}JL^{-(\beta+1)/2})\varphi\rangle \geq -\Lambda_\beta(m)\|\varphi\|^2_{L^2(\mathbb{R}^{3(N-1)})} \qquad (2.5.3)$$

for all $\varphi \in L^2_{\text{as}}(\mathbb{R}^{3(N-1)})$. The left side equals

$$(N-1)\int_{\mathbb{R}^{3N}} \hat{\varphi}^*(s,\vec{q})\hat{\varphi}(t,\vec{q})\left(\frac{L(t,\vec{q})^{(\beta-1)/2}}{L(s,\vec{q})^{(\beta+1)/2}} + \frac{L(s,\vec{q})^{(\beta-1)/2}}{L(t,\vec{q})^{(\beta+1)/2}}\right)G(s,t,\vec{q})\,\mathrm{d}s\,\mathrm{d}t\,\mathrm{d}\vec{q} \qquad (2.5.4)$$

where $\vec{q} \in \mathbb{R}^{3(N-2)}$ and L and G are defined in (2.2.7) and (2.2.2), respectively.

The above integral over s and t, for fixed $\vec{q}$, is the expectation of (twice) the operator τ^β defined in (2.4.1). Lemma 2.4.1 identifies its negative and positive parts. Dropping the latter, we thus have

$$(2.5.4) \geq (N-1) \int_{\mathbb{R}^{3N}} \hat{\varphi}^*(s,\vec{q})\hat{\varphi}(t,\vec{q}) \left(\frac{L(t,\vec{q})^{(\beta-1)/2}}{L(s,\vec{q})^{(\beta+1)/2}} + \frac{L(s,\vec{q})^{(\beta-1)/2}}{L(t,\vec{q})^{(\beta+1)/2}} \right) \times \frac{1}{2} \left(G(s,t,\vec{q}) - G(s,-t-2AK,\vec{q}) \right) \mathrm{d}s\,\mathrm{d}t\,\mathrm{d}\vec{q} \tag{2.5.5}$$

The remainder of the proof proceeds in exactly the same way as in the proof of Theorem 2.2.1, Eqs. (2.4.9)–(2.4.14), and we shall not repeat it here. The result is (2.2.17), for any $0 \leq \beta < 2$. The limiting case $\beta = 2$ is then obtained by monotone convergence, using that $\Lambda_\beta(m)$ is convex and thus continuous in β. (Note that for $\beta = 2$, the left side of (2.2.17) need not be finite, a priori.) □

2.6 Upper Bound on $\Lambda_\beta(m)$

In this section we shall prove an upper bound on $\Lambda_\beta(m)$. While only the case $0 \leq \beta \leq 2$ is of interest here, our bound is actually valid for all $0 \leq \beta < 3$. We start with proving the bound (2.2.10) on $\Lambda(m)$. Recall the definitions of $\Lambda(m)$ and ℓ_m in (2.2.8) and (2.2.9), respectively, as well as $A = (2+m)^{-1}$. We shall use that

$$\ell_m(s,K,Q) \geq \frac{\sqrt{m(m+2)}}{m+1} |s + AK| \tag{2.6.1}$$

and that

$$\begin{aligned} &\left[(s+AK)^2 + (t+AK)^2 + \frac{m}{1+m}(Q^2 + AK^2) \right]^2 - \left[\frac{2}{(1+m)} (s+AK)\cdot(t+AK) \right]^2 \\ &\geq \frac{m(m+2)}{(1+m)^2} \left[(s+AK)^2 + (t+AK)^2 + \frac{m}{1+m}(Q^2+AK^2) \right]^2 \\ &\geq \frac{m(m+2)}{(1+m)^2} \left[\frac{m(2+m)}{2+4m+m^2}(s^2+t^2) + \frac{m}{1+m} Q^2 \right]^2 \end{aligned} \tag{2.6.2}$$

Together with the simple bound

$$|s+AK|^{1/2} |t+AK|^{1/2} \leq \sqrt{\frac{1}{2}(s+AK)^2 + \frac{1}{2}(t+AK)^2} \tag{2.6.3}$$

this gives

$$\begin{aligned} \Lambda(m) &\leq \frac{(1+m)^2}{\sqrt{2}\pi^2 \left[m(m+2) \right]^{3/2}} \sup_{s\in\mathbb{R}^3, Q>0} \int_{\mathbb{R}^3} \frac{1}{t^2} \frac{s^2+Q^2}{\left[\frac{m(2+m)}{2+4m+m^2}(s^2+t^2) + \frac{m}{1+m}Q^2 \right]^{3/2}} \mathrm{d}t \\ &= \frac{4(1+m)^2 (2+4m+m^2)^{3/2}}{\sqrt{2}\pi \left[m(m+2) \right]^3} \sup_{s\in\mathbb{R}^3, Q>0} \frac{s^2+Q^2}{s^2 + \frac{2+4m+m^2}{(2+m)(1+m)} Q^2} \end{aligned} \tag{2.6.4}$$

Since $2 + 4m + m^2 > (2 + m)(1 + m)$, the last supremum equals 1, and we obtain the bound (2.2.10).

The same strategy can be used to derive an upper bound on $\Lambda_\beta(m)$ in (2.2.15), for $\beta \le 1$. Instead of (2.6.3), one uses

$$|s + AK|^{(1+\beta)/2}|t + AK|^{(1-\beta)/2} + |s + AK|^{(1-\beta)/2}|t + AK|^{(1+\beta)/2} \le \sqrt{2(s + AK)^2 + 2(t + AK)^2} \quad (2.6.5)$$

(which follows from convexity of the exponential function, $xy \le \frac{1}{p}x^p + \frac{1}{q}y^q$ for $x, y \ge 0$, $p > 1$, $\frac{1}{p} + \frac{1}{q} = 1$), resulting in

$$\Lambda_\beta(m) \le \frac{4\sqrt{2}(1 + m)^2(2 + 4m + m^2)^{3/2}}{\pi\,[m(m + 2)]^3} \quad \text{for } \beta \le 1. \quad (2.6.6)$$

For $1 < \beta < 3$, we need an upper bound on ℓ_m, and we shall simply use

$$\ell_m(s, K, Q) \le \sqrt{(s + AK)^2 + \frac{m}{m + 1}(Q^2 + AK^2)} \quad (2.6.7)$$

For a lower bound, we shall use (2.6.1) for one power of ℓ_m, and

$$\ell_m(s, K, Q) \ge \sqrt{\frac{m}{m + 1}(s^2 + Q^2)} \quad (2.6.8)$$

for the remaining $\ell_m^{(\beta-1)/2}$. This leads to

$$\begin{aligned}\Lambda_\beta(m) &\le \frac{1}{\pi^2}\frac{(m + 1)^{(\beta+7)/4}}{m^{(\beta+5)/4}(2 + m)^{3/2}} \sup_{s\in\mathbb{R}^3, Q>0} \int_{\mathbb{R}^3} \frac{1}{t^2}\left(\frac{1}{|t|^{(\beta-1)/2}} + \frac{1}{(s^2 + Q^2)^{(\beta-1)/4}}\right) \\ &\qquad \times \frac{s^2 + Q^2}{\left[\frac{m(2+m)}{2+4m+m^2}(s^2 + t^2) + \frac{m}{1+m}Q^2\right]^{(7-\beta)/4}}\,\mathrm{d}t \\ &= \frac{4}{\pi}\frac{(m + 1)^{(\beta+7)/4}}{m^3(2 + m)^{(13-\beta)/4}}\left(2 + 4m + m^2\right)^{(7-\beta)/4}\left(\frac{2}{3 - \beta} + \frac{\sqrt{\pi}}{2}\frac{\Gamma((5 - \beta)/4)}{\Gamma((7 - \beta)/4)}\right) \quad (2.6.9)\end{aligned}$$

for $1 < \beta < 3$, where Γ denotes the gamma-function in the last expression. In particular, $\Lambda_\beta(m)$ is finite for $\beta < 3$, and decays at least like m^{-1} for large m.

2.7 Numerical Evaluation of $\Lambda_\beta(m)$

Recall the definition of $\Lambda(m)$ in (2.2.8). In order to obtain a numerical value for $\Lambda(m)$, it is convenient to simplify this expression a bit. As a first step, we claim that, given s, the supremum over K in (2.2.8) is attained at some K of the form $K = -bs$ for $0 \le b \le 1/A = 2 + m$. To see this, we substitute $\tilde{s} = s + AK$, $\tilde{t} = t + AK$, and rewrite (2.2.8) as

$$\begin{aligned}\Lambda(m) = \sup_{\tilde{s},K\in\mathbb{R}^3,Q>0} &\frac{(\tilde{s} - AK)^2 + Q^2}{\pi^2(1 + m)}\left(\frac{m(m + 2)}{(m + 1)^2}\tilde{s}^2 + \frac{m}{m + 1}(Q^2 + AK^2)\right)^{-1/4} \\ &\times \int_{\mathbb{R}^3} \frac{1}{(\tilde{t} - AK)^2}\left(\frac{m(m + 2)}{(m + 1)^2}\tilde{t}^2 + \frac{m}{m + 1}(Q^2 + AK^2)\right)^{-1/4} \\ &\times \frac{\left|\tilde{s}\cdot\tilde{t}\right|}{\left[\tilde{s}^2 + \tilde{t}^2 + \frac{m}{1+m}(Q^2 + AK^2)\right]^2 - \left[\frac{2}{(1+m)}\tilde{s}\cdot\tilde{t}\right]^2}\,\mathrm{d}\tilde{t} \quad (2.7.1)\end{aligned}$$

Since the term on the last line is invariant under the reflection $\tilde t \mapsto -\tilde t$, the integral above is equal to

$$\int_{\mathbb{R}^3} \frac{\tilde t^2 + A^2K^2}{(\tilde t^2 + A^2K^2)^2 - 4A^2(\tilde t \cdot K)^2} \left(\frac{m(m+2)}{(m+1)^2} \tilde t^2 + \frac{m}{m+1}(Q^2 + AK^2) \right)^{-1/4} \times \frac{\left|\tilde s \cdot \tilde t\right|}{\left[\tilde s^2 + \tilde t^2 + \frac{m}{1+m}(Q^2 + AK^2)\right]^2 - \left[\frac{2}{(1+m)} \tilde s \cdot \tilde t\right]^2} \, \mathrm{d}\tilde t \tag{2.7.2}$$

When optimizing over the orientation of $\tilde s$ and K, the very first factor after the supremum in (2.7.1) is clearly largest if $\tilde s$ and K are antiparallel. That the same is true for the integral (2.7.2) is the content of the following lemma, whose proof is an easy exercise.

Lemma 2.7.1. *Let f and g be measurable functions on $[-1, 1]$ that are non-negative, even, and increasing on $[0, 1]$. For $a, b \in \mathbb{S}^2$,*

$$\int_{\mathbb{S}^2} f(\omega \cdot a) g(\omega \cdot b) \, \mathrm{d}\omega \tag{2.7.3}$$

is largest if a and b are either parallel or antiparallel (as vectors in $\mathbb{R}^3$).

Proof. We can represent the functions f and g by their level sets, and write

$$(2.7.3) = \int_{\mathbb{S}^2 \times \mathbb{R}^2_+} \chi_{\{f>x\}}(\omega \cdot a) \chi_{\{g>y\}}(\omega \cdot b) \, \mathrm{d}\omega \, \mathrm{d}x \, \mathrm{d}y \tag{2.7.4}$$

The support of the function $\omega \mapsto \chi_{\{f>x\}}(\omega \cdot a)$ consists of the union of two spherical caps, centered at $\pm a$, respectively, and similarly for $\chi_{\{g>y\}}(\omega \cdot b)$. If $\pm a$ is parallel to b, the integral over $\mathbb{S}^2$ in (2.7.4) (for fixed x and y) is clearly largest, since one of the characteristic functions simply equals 1 on the support of the other in this case. This completes the proof. □

The angular part of the integral in (2.7.2) is exactly of the form (2.7.3). We thus conclude that we can restrict the supremum in (2.7.1) to the set where $K = -\kappa \tilde s$ for some $\kappa \geq 0$ or, equivalently, $K = -bs$ for some $0 \leq b = \kappa/(1 + \kappa A) \leq 1/A$.

To evaluate $\Lambda(m)$, we thus have to find the supremum over $\tilde s \in \mathbb{R}^3$, $\kappa \geq 0$ and $Q \geq 0$ of

$$\frac{\tilde s^2(1+\kappa A)^2 + Q^2}{\pi^2(1+m)} \left(\frac{m(m+2)}{(m+1)^2} \tilde s^2 + \frac{m}{m+1}(Q^2 + A\kappa^2 \tilde s^2) \right)^{-1/4} \times \int_{\mathbb{R}^3} \frac{\tilde t^2 + A^2\kappa^2\tilde s^2}{(\tilde t^2 + A^2\kappa^2\tilde s^2)^2 - 4A^2\kappa^2(\tilde t \cdot \tilde s)^2} \left(\frac{m(m+2)}{(m+1)^2} \tilde t^2 + \frac{m}{m+1}(Q^2 + A\kappa^2\tilde s^2) \right)^{-1/4} \times \frac{\left|\tilde s \cdot \tilde t\right|}{\left[\tilde s^2 + \tilde t^2 + \frac{m}{1+m}(Q^2 + A\kappa^2\tilde s^2)\right]^2 - \left[\frac{2}{(1+m)} \tilde s \cdot \tilde t\right]^2} \, \mathrm{d}\tilde t \tag{2.7.5}$$

After carrying out the angle integration, this becomes

$$2\frac{\tilde s^2(1+\kappa A)^2 + Q^2}{\pi(1+m)} \left(\frac{m(m+2)}{(m+1)^2} \tilde s^2 + \frac{m}{m+1}(Q^2 + A\kappa^2 \tilde s^2) \right)^{-1/4} \times \int_0^\infty \frac{t^2}{t^2 + A^2\kappa^2\tilde s^2} \left(\frac{m(m+2)}{(m+1)^2} t^2 + \frac{m}{m+1}(Q^2 + A\kappa^2\tilde s^2) \right)^{-1/4} \times \frac{|\tilde s| t}{\left[\tilde s^2 + t^2 + \frac{m}{1+m}(Q^2 + A\kappa^2\tilde s^2)\right]^2} \frac{\ln(1-\lambda_1) - \ln(1-\lambda_2)}{\lambda_2 - \lambda_1} \, \mathrm{d}t \tag{2.7.6}$$

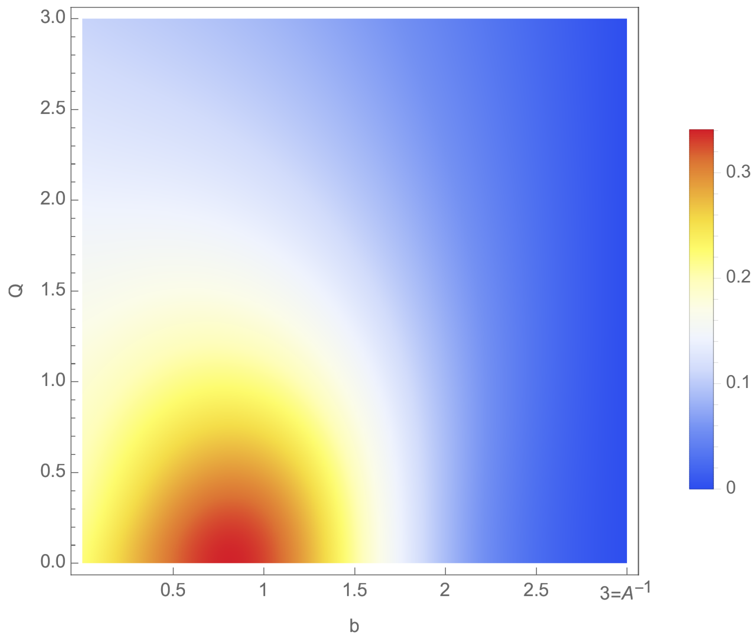

Figure 2.2: Numerical evaluation of the expression (2.7.6) (for $\tilde{s}^2 = 1$), whose maximal value is $\Lambda(1)$. The maximum is attained at $Q = 0$ and $b \approx 0.82$, and has a value $\Lambda(1) \approx 0.34$.

where

$$\lambda_1 = \frac{4A^2\kappa^2 t^2 \tilde{s}^2}{(t^2 + A^2\kappa^2\tilde{s}^2)^2} \quad , \qquad \lambda_2 = \frac{4}{(m+1)^2} \frac{t^2\tilde{s}^2}{(t^2 + \tilde{s}^2 + \frac{m}{m+1}(Q^2 + A\kappa^2\tilde{s}^2))^2} \tag{2.7.7}$$

By the overall scale invariance, we can set $\tilde{s}^2 = 1$, and hence we are left with two parameters to optimize over, $Q \geq 0$ and $\kappa \geq 0$ or, equivalently, $0 \leq b \leq 1/A = 2 + m$. It is not difficult to see that (2.7.6) tends to zero as $Q \to \infty$ (uniformly in b) and thus the optimization is effectively over a compact set. The result of a numerical integration of (2.7.6) in the case $m = 1$ is shown in Figure 2.2. The supremum is attained at $Q = 0$ and $b \approx 0.82$, and equals $\Lambda(1) \approx 0.34$. In particular, it is less than 1. Moreover, the numerical evaluation yields $\Lambda(m) < 1$ for all $m \geq 0.36$, i.e., the critical mass for stability is less than 0.36, as shown in Figure 2.1.

The same analysis applies to $\Lambda_\beta(m)$ in (2.2.15). For $\beta = 1$ and $\beta = 2$, the graph of these functions is plotted in Figure 2.1.

2.8 Proof of Proposition 1

Let $\psi \in D(\mathcal{H}_\alpha)$, and consider the partial Fourier transform

$$\eta(P, k_1, \ldots, k_{N-1}, r) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \hat{\psi}\left(\tfrac{m}{1+m}P + q, k_1, \ldots, k_{N-1}, \tfrac{1}{1+m}P - q\right) e^{ir\cdot q}\, \mathrm{d}q \tag{2.8.1}$$

With the aid of (2.2.25) and (2.2.28)–(2.2.33) we can write

$$\eta(P, k_1, \ldots, k_{N-1}, r) = \left(\frac{2\pi^2}{|r|} + \alpha\right) \frac{2m}{m+1} \frac{(-1)^{N+1}}{(2\pi)^{3/2}} \hat{\xi}(P, k_1, \ldots k_{N-1}) + \sum_{j=1}^{3} \kappa_j(P, k_1, \ldots, k_{N-1}, r) \tag{2.8.2}$$

where

$$\kappa_1(P, k_1, \ldots, k_{N-1}, r) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \hat{\phi}\left(\tfrac{m}{1+m}P + q, k_1, \ldots, k_{N-1}, \tfrac{1}{1+m}P - q\right)\left(e^{ir\cdot q} - 1\right) \mathrm{d}q \tag{2.8.3}$$

and

$$\begin{aligned} &\kappa_2(P, k_1, \ldots, k_{N-1}, r) \\ &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \mathcal{G}\left(\tfrac{m}{1+m}P + q, k_1, \ldots, k_{N-1}, \tfrac{1}{1+m}P - q\right)\left(e^{ir\cdot q} - 1\right) \\ &\quad \times \sum_{j=1}^{N-1} (-1)^{j+1} \hat{\xi}\left(\tfrac{m}{1+m}P + q + k_j, k_1, \ldots, k_{j-1}, k_{j+1} \ldots, k_{N-1}, \tfrac{1}{1+m}P - q\right) \mathrm{d}q \end{aligned} \tag{2.8.4}$$

Introducing the function $f(t) = t^{-1}(e^{-t} - 1 + t)$ for $t > 0$ we further have

$$\begin{aligned} &\kappa_3(P, k_1, \ldots, k_{N-1}, r) \\ &= \frac{(-1)^{N+1}}{(2\pi)^{3/2}} f\left(\frac{|r|}{2\pi^2}\frac{1+m}{2m}\mathcal{L}(P, k_1, \ldots, k_{N-1})\right)\mathcal{L}(P, k_1, \ldots, k_{N-1})\hat{\xi}(P, k_1, \ldots k_{N-1}) \end{aligned} \tag{2.8.5}$$

Since $\phi \in H^2(\mathbb{R}^{3(N+1)})$, one readily checks that $\lim_{r\to 0} \|\kappa_1(\,\cdot\,, r)\|_{L^2(\mathbb{R}^{3N})} = 0$. Moreover, since $\xi \in H^1(\mathbb{R}^{3N})$ by assumption, $\lim_{r\to 0} \|\kappa_3(\,\cdot\,, r)\|_{L^2(\mathbb{R}^{3N})} = 0$ by dominated convergence, using $\lim_{t\to 0} f(t) = 0$. The same holds true for κ_2 if we can show that

$$\int_{\mathbb{R}^3} \mathcal{G}\left(\tfrac{m}{1+m}P + q, k_1, \ldots, k_{N-1}, \tfrac{1}{1+m}P - q\right)\left|\hat{\xi}\left(\tfrac{m}{1+m}P + q + k_1, k_2, \ldots, k_{N-1}, \tfrac{1}{1+m}P - q\right)\right| \mathrm{d}q \tag{2.8.6}$$

is an $L^2(\mathbb{R}^{3N})$ function. For this purpose, pick a function $\nu \in L^2(\mathbb{R}^3) \otimes L^2_{\mathrm{as}}(\mathbb{R}^{3(N-1)})$ and integrate the expression (2.8.6) against $\nu(P, k_1, \ldots k_{N-1})$. After a change of integration variables, this gives

$$\int_{\mathbb{R}^{3(N+1)}} \nu(k_0 + k_N, k_1, \ldots, k_{N-1})\mathcal{G}(k_0, k_1, \ldots, k_N)\left|\hat{\xi}(k_0 + k_1, k_2, \ldots, k_N)\right| \mathrm{d}k_0\, \mathrm{d}k_1 \cdots \mathrm{d}k_N \tag{2.8.7}$$

Since $\xi \in H^1(\mathbb{R}^{3N})$ by assumption, Lemma 2.3.1 (for $\beta = 1$) implies that (2.8.7) is finite. This shows that also $\|\kappa_2(\,\cdot\,, r)\|_{L^2(\mathbb{R}^{3N})}$ goes to 0 as $r \to 0$, and thus completes the proof of Proposition 1. □

2.9 Proof of Theorem 2.2.3

We start with $n_\uparrow$. For $\psi = \phi + \mathcal{G}\xi \in D(\mathcal{H}_\alpha)$, we have

$$
\begin{aligned}
&k^2 n_\uparrow(k) - \frac{C}{|k-p_\uparrow|^2} \\
&= k^2 \int_{\mathbb{R}^{3N}} |\hat{\phi}(k,k_1,k_2,\vec{k})|^2 \, \mathrm{d}k_1 \, \mathrm{d}k_2 \, \mathrm{d}\vec{k} \\
&\quad - k^2 N(N-1) \int_{\mathbb{R}^{3N}} \mathcal{G}(k,k_1,k_2,\vec{k})^2 \hat{\xi}^*(k+k_1,k_2,\vec{k})\hat{\xi}(k+k_2,k_1,\vec{k}) \, \mathrm{d}k_1 \, \mathrm{d}k_2 \, \mathrm{d}\vec{k} \\
&\quad + N \int_{\mathbb{R}^{3N}} \left(k^2 \mathcal{G}(k,k_1,k_2,\vec{k})^2 - \left(\frac{2m}{m+1}\right)^2 \frac{1}{|k-p_\uparrow|^2} \right) |\hat{\xi}(k+k_1,k_2,\vec{k})|^2 \, \mathrm{d}k_1 \, \mathrm{d}k_2 \, \mathrm{d}\vec{k} \\
&\quad + 2k^2 N \operatorname{Re} \int_{\mathbb{R}^{3N}} \hat{\phi}^*(k,k_1,k_2,\vec{k}) \mathcal{G}(k,k_1,k_2,\vec{k}) \hat{\xi}(k+k_1,k_2,\vec{k}) \, \mathrm{d}k_1 \, \mathrm{d}k_2 \, \mathrm{d}\vec{k}
\end{aligned} \tag{2.9.1}
$$

where $\vec{k} \in \mathbb{R}^{3(N-2)}$, as before. We write the right side as $\sum_{j=1}^4 M_j^\uparrow(k)$, with $M_j^\uparrow$ corresponding to the term on the jth line on the right side. The first term $M_1^\uparrow$ is clearly in $L^1(\mathbb{R}^3)$. Using (2.2.24) the second term can be bounded as

$$
|M_2^\uparrow(k)| \le N(N-1) \int_{\mathbb{R}^{3N}} \frac{4m}{k_1^2+k_2^2} |\hat{\xi}(k+k_1,k_2,\vec{k})||\hat{\xi}(k+k_2,k_1,\vec{k})| \, \mathrm{d}k_1 \, \mathrm{d}k_2 \, \mathrm{d}\vec{k} \tag{2.9.2}
$$

After integrating over k and using the Cauchy-Schwarz inequality for the $(k,\vec{k})$ integration, we get

$$
\begin{aligned}
\int_{\mathbb{R}^3} |M_2^\uparrow(k)| \, \mathrm{d}k &\le N(N-1) \int_{\mathbb{R}^{3N}} \frac{4m}{k_1^2+k_2^2} \|\hat{\xi}(\,\cdot\,,k_1)\|_{L^2(\mathbb{R}^{3(N-1)})} \|\hat{\xi}(\,\cdot\,,k_2)\|_{L^2(\mathbb{R}^{3(N-1)})} \, \mathrm{d}k_1 \, \mathrm{d}k_2 \\
&\le 4mcN(N-1)^2 \|\xi\|^2_{H^{1/2}(\mathbb{R}^{3N})}
\end{aligned} \tag{2.9.3}
$$

where c equals the norm of the operator with integral kernel $|k_1|^{-1/2}|k_2|^{-1/2}(k_1^2+k_2^2)^{-1}$, which can easily be shown to be finite (and, in fact, equals $2\pi^2$ [21, Lemma 2.1]).

Next we shall consider $M_3^\uparrow(k)$, which we rewrite as

$$
M_3^\uparrow(k) = N \int_{\mathbb{R}^{3N}} \left(k^2 \mathcal{G}(k,k_1-k,k_2,\vec{k})^2 - \left(\frac{2m}{m+1}\right)^2 \frac{1}{|k-p_\uparrow|^2} \right) |\hat{\xi}(k_1,k_2,\vec{k})|^2 \, \mathrm{d}k_1 \, \mathrm{d}k_2 \, \mathrm{d}\vec{k} \tag{2.9.4}
$$

Since $\xi \in L^2(\mathbb{R}^{3N})$, $M_3^\uparrow$ is clearly in $L^1_{\mathrm{loc}}(\mathbb{R}^3)$ and we only have to investigate its behavior for large k. If we write

$$
k^2 \mathcal{G}(k,k_1-k,k_2,\vec{k})^2 - \left(\frac{2m}{m+1}\right)^2 \frac{1}{|k-p_\uparrow|^2} = \left(\frac{2m}{m+1}\right)^2 \frac{2}{|k|^4} k \cdot \left(\frac{2m}{m+1}k_1 - p_\uparrow\right) + R_\uparrow(k,k_1,k_2,\vec{k}) \tag{2.9.5}
$$

the first term on the right side gives zero after integration when inserted in (2.9.4), by the definition of $p_\uparrow$ in (2.2.40). That is,

$$
M_3^\uparrow(k) = N \int_{\mathbb{R}^{3N}} R_\uparrow(k,k_1,k_2,\vec{k}) |\hat{\xi}(k_1,k_2,\vec{k})|^2 \, \mathrm{d}k_1 \, \mathrm{d}k_2 \, \mathrm{d}\vec{k} \tag{2.9.6}
$$

Moreover, in the region where $|k|^2 \geq \mathrm{const}(\mu + p_\uparrow^2)$ we have

$$|R_\uparrow(k, k_1, k_2, \ldots, k_N)| \leq \mathrm{const}\frac{1}{|k|^3}\left(\mu + p_\uparrow^2 + \sum_{j=1}^N k_j^2\right)^{1/2} \min\left\{1, \frac{1}{|k|}\left(\mu + p_\uparrow^2 + \sum_{j=1}^N k_j^2\right)^{1/2}\right\} \quad (2.9.7)$$

for suitable constants. If we integrate $R_\uparrow$ over k in this region we thus obtain an expression that is bounded from above by $\mathrm{const}(\mu + p_\uparrow^2 + \sum_{j=1}^N k_j^2)^{1/2} \ln(1 + \mu + p_\uparrow^2 + \sum_{j=1}^N k_j^2)$, and we conclude, in particular, that $\|M_3^\uparrow\|_{L^1(\mathbb{R}^3)} \leq \mathrm{const}\|\xi\|^2_{H^1(\mathbb{R}^{3N})}$. Finally, using the simple pointwise bound

$$|M_4^\uparrow(k)| \leq 4mN\|\hat{\phi}(k, \cdot)\|_{L^2(\mathbb{R}^{3N})}\|\xi\|_{L^2(\mathbb{R}^{3N})} \quad (2.9.8)$$

and the assumption that $\phi \in H^2(\mathbb{R}^{3(N+1)})$, the Cauchy-Schwarz inequality readily implies that $M_4^\uparrow \in L^1(\mathbb{R}^3)$. This concludes the proof that $k^2 n_\uparrow(k) - C|k - p_\uparrow|^{-2}$ is integrable.

Similarly we have for $n_\downarrow$

$$\begin{aligned}
&k^2 n_\downarrow(k) - \frac{C}{|k - p_\downarrow|^2} = \sum_{j=1}^7 M_j^\downarrow(k) = \\
&= Nk^2 \int_{\mathbb{R}^{3N}} |\hat{\phi}(k_0, k, k_2, \vec{k})|^2 \,\mathrm{d}k_0\,\mathrm{d}k_2\,\mathrm{d}\vec{k} \\
&\quad - k^2 N(N-1)(N-2) \int_{\mathbb{R}^{3N}} \mathcal{G}(k_0, k, k_2, \ldots, k_N)^2 \hat{\xi}^*(k_0 + k_2, k, k_3, \ldots, k_N) \\
&\qquad\qquad \times \hat{\xi}(k_0 + k_3, k, k_2, k_4, \ldots, k_N)\,\mathrm{d}k_0\,\mathrm{d}k_2 \cdots \mathrm{d}k_N \\
&\quad - 2k^2 N(N-1) \int_{\mathbb{R}^{3N}} \mathcal{G}(k_0, k, k_2, \vec{k})^2 \hat{\xi}^*(k_0 + k, k_2, \vec{k})\hat{\xi}(k_0 + k_2, k, \vec{k})\,\mathrm{d}k_0\,\mathrm{d}k_2\,\mathrm{d}\vec{k} \\
&\quad + k^2 N(N-1) \int_{\mathbb{R}^{3N}} \mathcal{G}(k_0, k, k_2, \vec{k})^2 |\hat{\xi}(k_0 + k_2, k, \vec{k})|^2\,\mathrm{d}k_0\,\mathrm{d}k_2\,\mathrm{d}\vec{k} \\
&\quad + N \int_{\mathbb{R}^{3N}} \left(k^2 \mathcal{G}(k_0, k, k_2, \vec{k})^2 - \left(\frac{2m}{m+1}\right)^2 \frac{1}{|k - p_\downarrow|^2}\right)|\hat{\xi}(k_0 + k, k_2, \vec{k})|^2\,\mathrm{d}k_0\,\mathrm{d}k_2\,\mathrm{d}\vec{k} \\
&\quad + 2k^2 N\,\mathrm{Re} \int_{\mathbb{R}^{3N}} \hat{\phi}^*(k_0, k, k_2, \vec{k})\mathcal{G}(k_0, k, k_2, \vec{k})\hat{\xi}(k_0 + k, k_2, \vec{k})\,\mathrm{d}k_0\,\mathrm{d}k_2\,\mathrm{d}\vec{k} \\
&\quad + 2k^2 N(N-1)\,\mathrm{Re} \int_{\mathbb{R}^{3N}} \hat{\phi}^*(k_0, k, k_2, \vec{k})\mathcal{G}(k_0, k, k_2, \vec{k})\hat{\xi}(k_0 + k_2, k, \vec{k})\,\mathrm{d}k_0\,\mathrm{d}k_2\,\mathrm{d}\vec{k}
\end{aligned} \quad (2.9.9)$$

The terms $M_1^\downarrow$, $M_2^\downarrow$, $M_3^\downarrow$, $M_5^\downarrow$ and $M_6^\downarrow$ can be treated in the same way as the analogous terms in (2.9.1) above. Eq. (2.9.6) holds with $M_5^\downarrow$ in place of $M_3^\uparrow$ with $R_\uparrow$ replaced by

$$R_\downarrow(k, k_1, k_2, \vec{k}) = k^2 \mathcal{G}(k_1 - k, k, k_2, \vec{k})^2 - \left(\frac{2m}{m+1}\right)^2 \frac{1}{|k - p_\downarrow|^2} - \left(\frac{2m}{m+1}\right)^2 \frac{2}{|k|^4} k \cdot \left(\frac{2}{m+1} k_1 - p_\downarrow\right) \quad (2.9.10)$$

which also satisfies the bound (2.9.7). The expression $M_4^\downarrow$ equals

$$M_4^\downarrow(k) = k^2 N(N-1) \int_{\mathbb{R}^{3N}} \mathcal{G}(k_0 - k_2, k, k_2, \vec{k})^2 |\hat{\xi}(k_0, k, \vec{k})|^2\,\mathrm{d}k_0\,\mathrm{d}k_2\,\mathrm{d}\vec{k} \quad (2.9.11)$$

Performing the integration over k_2, one readily checks that

$$M_4^\downarrow(k) \leq \mathrm{const}|k|N(N-1) \int_{\mathbb{R}^{3N}} |\hat{\xi}(k_0, k, \vec{k})|^2\,\mathrm{d}k_0\,\mathrm{d}\vec{k} \quad (2.9.12)$$

which is in $L^1(\mathbb{R}^3)$ since $\xi \in H^{1/2}(\mathbb{R}^{3N})$. Finally, using Cauchy-Schwarz in $(k, k_2, \vec{k})$,

$$\int_{\mathbb{R}^3} |M_7^{\downarrow}(k)|\, \mathrm{d}k \le 4N(N-1)\|\xi\|_{L^2(\mathbb{R}^{3N})} \int_{\mathbb{R}^3} \|\hat{\phi}(k_0, \cdot)\|_{L^2(\mathbb{R}^{3N})}\, \mathrm{d}k_0 \tag{2.9.13}$$

which is finite for $\phi \in H^2(\mathbb{R}^{3(N-1)})$, as remarked above. We conclude, therefore, that also $k^2 n_{\downarrow}(k) - C|k - p_{\downarrow}|^{-2}$ is integrable.

Since all the terms in (2.9.1) and (2.9.9) are integrable, we can do the integration over k term by term. For all the terms except $M_3^{\uparrow}$ and $M_5^{\downarrow}$, we have actually shown that the L^1-property holds even if the respective integrands are replaced by their absolute value, and hence we can freely use Fubini's theorem for these terms. In the form (2.9.6) (and the analogous expression for $M_5^{\downarrow}$) the same applies to $M_3^{\uparrow}$ and $M_5^{\downarrow}$, in fact.

For the norm of ψ, we shall write

$$\begin{aligned}
\|\psi\|^2_{L^2(\mathbb{R}^{3(N+1)})} &= \sum_{j=1}^{4} n_j \\
&= \|\phi\|^2_{L^2(\mathbb{R}^{3(N+1)})} + 2\,\mathrm{Re}\langle\phi|\mathcal{G}\xi\rangle \\
&\quad - N(N-1)\int_{\mathbb{R}^{3N}} \mathcal{G}(k_0, k_1, k_2, \vec{k})^2 \hat{\xi}^*(k_0 + k_1, k_2, \vec{k})\hat{\xi}(k_0 + k_2, k_1, \vec{k})\, \mathrm{d}k_0\, \mathrm{d}k_1\, \mathrm{d}k_2\, \mathrm{d}\vec{k} \\
&\quad + N\int_{\mathbb{R}^{3N}} \mathcal{G}(k_0, k_1, k_2, \vec{k})^2 |\hat{\xi}(k_0 + k_1, k_2, \vec{k})|^2\, \mathrm{d}k_0\, \mathrm{d}k_1\, \mathrm{d}k_2\, \mathrm{d}\vec{k}
\end{aligned} \tag{2.9.14}$$

We have

$$\int_{\mathbb{R}^3} \left(\frac{1}{2m} M_1^{\uparrow}(k) + \frac{1}{2} M_1^{\downarrow}(k)\right) \mathrm{d}k + \mu n_1 = \left\langle \phi \left| -\frac{1}{2m}\Delta_{x_0} - \frac{1}{2}\sum_{i=1}^{N} \Delta_{x_i} + \mu \right| \phi \right\rangle \tag{2.9.15}$$

and

$$\int_{\mathbb{R}^3} \left[\frac{1}{2m} M_2^{\uparrow}(k) + \frac{1}{2}\left(M_2^{\downarrow}(k) + M_3^{\downarrow}(k)\right)\right] \mathrm{d}k + \mu n_3 = -N\mathcal{T}_{\mathrm{off}}(\xi) \tag{2.9.16}$$

Moreover, we claim that

$$\int_{\mathbb{R}^3} \left[\frac{1}{2m} M_3^{\uparrow}(k) + \frac{1}{2}\left(M_4^{\downarrow}(k) + M_5^{\downarrow}(k)\right)\right] \mathrm{d}k + \mu n_4 = -N\mathcal{T}_{\mathrm{diag}}(\xi) \tag{2.9.17}$$

To see this, note that we can replace $M_3^{\uparrow}(k)$ by its symmetrized version $\frac{1}{2}(M_3^{\uparrow}(k) + M_3^{\uparrow}(-k))$, and likewise for $M_5^{\downarrow}$. Then (2.9.17) follows from the fact that

$$\begin{aligned}
\int_{\mathbb{R}^3} \Bigg(&\frac{1}{4m}\left(R_{\uparrow}(k, k_1, \ldots, k_N) + R_{\uparrow}(-k, k_1, \ldots, k_N)\right) + \frac{1}{4}\left(R_{\downarrow}(k, k_1, \ldots, k_N) + R_{\downarrow}(-k, k_1, \ldots, k_N)\right) \\
&+ \frac{1}{2}\sum\nolimits_{j=2}^{N} k_j^2 \mathcal{G}(k_1 - k, k, k_2, \ldots, k_N)^2 \Bigg) \mathrm{d}k = -\mathcal{L}(k_1, \ldots, k_N)
\end{aligned} \tag{2.9.18}$$

which, in turn, uses that

$$\int_{\mathbb{R}^3} \left(\frac{2}{|k|^2} - \frac{1}{|k-p|^2} - \frac{1}{|k+p|^2}\right) \mathrm{d}k = 0 \tag{2.9.19}$$

for any $p \in \mathbb{R}^3$ (which can be proved, e.g., by computing the Fourier transform). Finally,

$$\begin{aligned}&\int_{\mathbb{R}^3}\left[\frac{1}{2m}M_4^{\uparrow}(k)+\frac{1}{2}\left(M_6^{\downarrow}(k)+M_7^{\downarrow}(k)\right)\right]\mathrm{d}k+\mu n_2\\&=2N\,\mathrm{Re}\int\hat{\phi}^*(k_0,k_1-k_0,k_2,\vec{k})\hat{\xi}(k_1,k_2,\vec{k})\,\mathrm{d}k_0\,\mathrm{d}k_1\,\mathrm{d}k_2\,\mathrm{d}\vec{k}\end{aligned}\tag{2.9.20}$$

In Fourier space, the boundary condition (2.2.33) satisfied by ϕ reads

$$\int\hat{\phi}(k_0,k_1-k_0,k_2,\vec{k})\,\mathrm{d}k_0=\left(\frac{2m}{m+1}\alpha\hat{\xi}+\widehat{\Gamma\xi}\right)(k_1,k_2,\vec{k})\tag{2.9.21}$$

and hence

$$(2.9.20)=2N\left(\mathcal{T}_{\mathrm{diag}}(\xi)+\mathcal{T}_{\mathrm{off}}(\xi)+\frac{2m}{m+1}\alpha\|\xi\|^2_{L^2(\mathbb{R}^{3N})}\right)\tag{2.9.22}$$

A combination of (2.9.15), (2.9.16), (2.9.17), (2.9.22) with (2.2.26) establishes (2.2.42) and thus completes the proof of Theorem 2.2.3. □

Remark 2.9.1. *The proof of Theorem 2.2.3 does not actually make use of the assumption* $\xi \in H^1(\mathbb{R}^{3N})$*, it is only used that*

$$\int_{\mathbb{R}^{3N}}\left(1+\sum_{j=1}^{N}|k_j|^2\right)^{1/2}\ln\left(2+\sum_{j=1}^{N}|k_j|^2\right)|\hat{\xi}(k_1,\ldots,k_N)|^2\,\mathrm{d}k_1\cdots\mathrm{d}k_N<\infty\tag{2.9.23}$$

By Theorem 2.2.2, this is actually the case if $\Lambda_0(m)=2\Lambda(m)<1$ *(instead of* $\Lambda_1(m)<1$*) since then, by continuity,* $\Lambda_\beta(m)<1$ *for some* $\beta>0$*, and hence* $\xi\in H^{(1+\beta)/2}(\mathbb{R}^{3N})$.

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CHAPTER 3

Energy contribution of a point interacting impurity in a Fermi gas

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Abstract

We give a bound on the ground state energy of a system of N non-interacting fermions in a three dimensional cubic box interacting with an impurity particle via point interactions. We show that the change in energy compared to the system in the absence of the impurity is bounded in terms of the gas density and the scattering length of the interaction, independently of N. Our bound holds as long as the ratio of the mass of the impurity to the one of the gas particles is larger than a critical value $m^{**} \approx 0.36$, which is the same regime for which we recently showed stability of the system.

3.1 Introduction

Quantum systems of particles interacting with forces of very short range allow for an idealized description in terms of point interactions. The latter are characterized by a single number, the scattering length. Originally point interactions were introduced in the 1930s to model nuclear interactions [5, 6, 19, 68, 72], but later they were also successfully applied to many other areas of physics, like polarons (see [40] and references there) or cold atomic gases [74].

It was already known to Thomas [68] that the spectrum of a bosonic many-particle system depends strongly on the range of the interactions, and that an idealized point-interacting system with more than two particles is inherently unstable, i.e., the energy is not bounded from below. This collapse can be counteracted by the Pauli principle for fermions with two species (e.g., spin states). In this paper we are interested in the impurity problem where there is only one particle for one of the species.

Given $N \geq 1$ fermions of one type with mass 1 and one particle of another type with mass $m > 0$, a model of point interactions gives a meaning to the formal expression

$$-\frac{1}{2m}\Delta_y - \frac{1}{2}\sum_{i=1}^{N}\Delta_{x_i} + \gamma\sum_{i=1}^{N}\delta(x_i - y) \tag{3.1.1}$$

for $\gamma \in \mathbb{R}$. We note that because of the antisymmetry constraint on the wavefunctions there are only interactions between particles of different species. The expression (3.1.1) is ill-defined in $d \geq 2$ dimensions since $H^1(\mathbb{R}^d)$, the form domain of the Laplacian, contains discontinuous functions for which the meaning of the δ-function as a potential is unclear. In the following we restrict our attention to the case $d = 3$, but we note that also two-dimensional systems exhibit interesting behavior [15, 16, 27, 28, 35]. For $d \geq 4$ there are no point interactions as the Laplacian restricted to functions supported away from the hyperplanes of interactions is essentially self-adjoint.

A mathematically precise meaning to (3.1.1) in three dimensions was given in [15, 20, 45] and we will work with the model introduced there. Our analysis will start from this well-defined model, but we note that the question whether the model can be obtained as a limit of Schrödinger operators with genuine interaction potentials of shrinking support is still open. (See, however, [1] for the case $N = 1$, and [3] for models in one dimension.)

In this paper we study the energy contribution of the point-interacting impurity. We confine the $N + 1$ particles to a box $(0, L)^3$ and investigate the ground state energy of the system. In particular, our goal is the show that at given mean particle density $\bar{\rho} = N/L^3$, the difference between the ground state energies of the interacting and the non-interacting system is bounded independently of the system size.

Previous work on this model was mostly concerned with stability and hence studied the model without confinement. For example, it is possible to analyze the 2 + 1 model, i.e,. two fermions of one kind and one impurity of another kind, in great detail [4, 11–13, 15, 45–48]. It turns out that the mass of the impurity plays an important role for stability. It was shown in [11] that for the 2 + 1 system there is a critical mass $m^* \approx 0.0735$ such that the system is stable for $m \geq m^*$ and unstable otherwise. This critical mass does not depend on the strength of the interaction, i.e., the scattering length.

Building on these results it was shown in [50] that a similar statement holds for the $N + 1$ system. In particular, it was proven that there is a critical mass $m^{**} \approx 0.36$ such that the system is stable for all $m \geq m^{**}$, independently of N. This bound is presumably not sharp and stability is still open for $m \in [m^*, m^{**})$. Recently also the stability of the 2 + 2 system was proved in a suitable mass range [53]. The general case with $N + M$ particles still poses an open problem, however.

In all cases where stability of the system was established, the ground state energy in infinite volume is actually zero in case the scattering length is negative, and there are no bound states. For positive scattering length there are bound states, but one still expects that only a finite number of particles can bind to the impurity. In particular, the ground state energy of the $N + 1$ system is bounded from below independently of N [50]. Intuitively one would expect that if one confines the system to a box in order to have a non-zero mean particle density, the interaction with the impurity should again only affect a finite number of particles, and hence the *energy change* compared to the non-interacting system should be $O(1)$, independently of N. This is what we prove here. We note that it is sufficient to derive a lower bound on the ground state energy, as point interactions are always attractive, i.e., they lower the energy.

Even for regular interaction potentials, it is highly non-trivial to show that an impurity causes only an $O(1)$ change to the energy of a non-interacting Fermi gas. For fixed, i.e., non-dynamical impurities, this was established in [24] as a consequence of a positive density version of the Lieb-Thirring inequality. The result in [24] applies to systems in infinite volume, as well as to systems in a box with periodic boundary conditions. In the appendix we provide an extension to Dirichlet boundary conditions, since this result will be an essential ingredient in our proof.

Compared to [24] we face here two additional difficulties: the impurity is dynamic and has a finite mass, and the interaction with the gas particles is through singular point interactions. Besides the methods of [24] and [50], a key ingredient in our analysis is a proof of an IMS type formula for the quadratic form defining the model, which allows for a localization of the particles into regions close and far away from the impurity. It has the same form as the IMS formula for regular Schrödinger operators (see [14, Thm. 3.2]), but is much harder to prove.

3.1.1 The point interaction model

We consider a system of N fermions of mass 1, interacting with another particle of mass $m > 0$. Let

$$H_0^N = -\frac{1}{2m}\Delta_0 - \frac{1}{2}\sum_{i=1}^{N}\Delta_i \tag{3.1.2}$$

be the non-interacting part of the Hamiltonian, acting on $L^2(\mathbb{R}^3) \otimes L^2_{\mathrm{as}}(\mathbb{R}^{3N})$, where L^2_{as} denotes the totally antisymmetric functions in $\otimes^N L^2(\mathbb{R}^3)$. The $N+1$ coordinates we denote by $x_0, x_1, \ldots, x_N \in \mathbb{R}^3$ and throughout this paper we will use the notation $\vec{x} = (x_1, \ldots, x_N)$. If we want to exclude a set of coordinates labeled by $A \subseteq \{1, \ldots, N\}$ we use $\hat{x}_A = (x_i)_{i\notin A}$ and for short $\hat{x}_i = \hat{x}_{\{i\}}$. If we want to restrict to certain coordinates we write $\vec{x}_A = (x_i)_{i\in A}$.

For $\mu > 0$, we define G_μ as the resolvent of H_0^N in momentum space, i.e.,

$$G_\mu(k_0, \vec{k}) := \left(\frac{1}{2m}k_0^2 + \frac{1}{2}\vec{k}^2 + \mu\right)^{-1}. \tag{3.1.3}$$

We denote by $F_{\alpha,N}$ the quadratic form used in [11,50] describing point interactions between N fermions and the impurity. Its domain is given by

$$D(F_{\alpha,N}) = \left\{\psi = \phi_\mu + G_\mu\xi \mid \phi_\mu \in H^1(\mathbb{R}^3) \otimes H^1_{\mathrm{as}}(\mathbb{R}^{3N}), \xi \in H^{1/2}(\mathbb{R}^3) \otimes H^{1/2}_{\mathrm{as}}(\mathbb{R}^{3(N-1)})\right\} \tag{3.1.4}$$

where $G_\mu\xi$ is defined via its Fourier transform (denoted by a $\hat{\cdot}$) as

$$\widehat{G_\mu\xi}(k_0, \vec{k}) = G_\mu(k_0, \vec{k})\sum_{i=1}^{N}(-1)^{i+1}\hat{\xi}(k_0 + k_i, \hat{k}_i). \tag{3.1.5}$$

The space $H^1_{\mathrm{as}}(\mathbb{R}^{3N})$ contains all totally antisymmetric functions in $H^1(\mathbb{R}^{3N})$. For a given $\psi \in D(F_{\alpha,N})$ and $\mu > 0$, the splitting $\psi = \phi_\mu + G_\mu\xi$ is unique. We point out that while ϕ_μ depends on the choice of μ, ξ is independent of μ. We will call ϕ_μ the regular part and ξ the singular part of ψ. Note that $D(F_{\alpha,N})$ is independent of the choice of μ, and so is the quadratic form $F_{\alpha,N}$ defined as

$$F_{\alpha,N}(\psi) := \left\langle\phi_\mu \left| H_0^N + \mu \right| \phi_\mu\right\rangle - \mu\,\|\psi\|^2_{L^2(\mathbb{R}^{3(N+1)})} + T_{\alpha,\mu,N}(\xi) \tag{3.1.6}$$

$$T_{\alpha,\mu,N}(\xi) := N\left(\frac{2m}{m+1}\alpha\,\|\xi\|^2_{L^2(\mathbb{R}^{3N})} + T^{\mu,N}_{\mathrm{dia}}(\xi) + T^{\mu,N}_{\mathrm{off}}(\xi)\right) \tag{3.1.7}$$

where

$$T_{\text{dia}}^{\mu,N}(\xi) := \int_{\mathbb{R}^{3N}} |\hat{\xi}(\vec{k})|^2 L_{\mu,N}(\vec{k})\, \mathrm{d}\vec{k} \tag{3.1.8}$$

$$T_{\text{off}}^{\mu,N}(\xi) := (N-1)\int_{\mathbb{R}^{3(N+1)}} \hat{\xi}^*(k_0+k_1,\hat{k}_1)\hat{\xi}(k_0+k_2,\hat{k}_2)G_\mu(k_0,\vec{k})\, \mathrm{d}k_0\, \mathrm{d}\vec{k} \tag{3.1.9}$$

$$L_{\mu,N}(\vec{k}) := 2\pi^2\left(\frac{2m}{m+1}\right)^{3/2}\left(\frac{k_1^2}{2(m+1)}+\frac{1}{2}\hat{k}_1^2+\mu\right)^{1/2}. \tag{3.1.10}$$

The quadratic form $F_{\alpha,N}$ describes N fermions interacting with an impurity particle via point interactions with scattering length $a = -2\pi^2/\alpha$, with $\alpha \in \mathbb{R}$. The non-interacting system is recovered in the limit $\alpha \to +\infty$.

Notation. Throughout the paper we will use the following notation. We define the relation $\lesssim$ by

$$x \lesssim y \iff \exists C > 0\colon x \leq Cy \tag{3.1.11}$$

where C is independent of x and y. In the obvious way we define $\gtrsim$. In case that $x \lesssim y$ and $y \lesssim x$ we write $x \sim y$.

3.2 Main result for confined wavefunctions

Let us assume that $\operatorname{supp}\psi \subseteq B^{N+1}$, where $B = (0,L)^3$ for some $L > 0$. The mean particle density will be denoted by $\rho = N/L^3$. Let E_N^D be the ground state energy of $-\frac{1}{2}\sum_{i=1}^N \Delta_i$ for wavefunctions in $H^1_{\text{as}}(\mathbb{R}^{3N})$ with Dirichlet boundary conditions on ∂B. It equals the sum of the lowest N eigenvalues of the Dirichlet Laplacian on B, and it is easy to see that

$$E_N^D \sim N\rho^{2/3}. \tag{3.2.1}$$

A natural question is how the interactions affect this energy. From [50, Thm. 2.1] we know that there is a mass-dependent constant $\Lambda(m)$ [50, Eq. (2.8)], given in Eq. (3.4.53) below, such that if $\Lambda(m) < 1$ then $F_{\alpha,N}$ is bounded from below independently of N by

$$\frac{F_{\alpha,N}(\psi)}{\|\psi\|_2^2} \geq \frac{m+1}{2m}\begin{cases} 0 & \alpha \geq 0 \\ -\left(\dfrac{\alpha}{2\pi^2(1-\Lambda(m))}\right)^2 & \text{otherwise.}\end{cases} \tag{3.2.2}$$

(The additional factor $(m+1)/(2m)$ compared to [50, Thm. 2.1] results from the separation of the center-of-mass motion used in [50].) It was also shown in [50] that $\Lambda(m) < 1$ if $m > m^{**} \approx 0.36$.

For particles confined to the box B with mean density ρ we can show that under the condition $\Lambda(m) < 1$ the correction to E_N^D is small, i.e., it is $O(1)$ independently of N. Our main result is the following.

Theorem 3.2.1. *Let $\psi \in D(F_{\alpha,N})$, supported in $(0,L)^{3(N+1)}$, with $\|\psi\| = 1$. Let $\rho = NL^{-3}$, and assume that $\Lambda(m) < 1$. Then*

$$F_{\alpha,N}(\psi) \geq E_N^D - \mathit{const}\left(\frac{\rho^{2/3}}{(1-\Lambda(m))^{9/2}} + \frac{\alpha_-^2}{(1-\Lambda(m))^2}\right) \tag{3.2.3}$$

where the constant is independent of ψ, m, N, L and α, and α_- denotes the negative part of α, i.e., $\alpha_- = \frac{1}{2}(|\alpha| - \alpha)$.

Thm. 3.2.1 shows that the presence of the impurity affects the ground state energy by a term that is bounded independently of N. The bound (3.2.3) is an extension of (3.2.2) in the sense that if we take $L \to \infty$ in (3.2.3) we recover (3.2.2) up to the value of the constant.

Remark. *For $\alpha \to \infty$ one would expect that the optimal lower bound converges to the ground state energy of the non-interacting Hamiltonian H_0^N with Dirichlet boundary conditions. This is not the case for* (3.2.3) *which is independent of α for $\alpha \geq 0$.*

Using various types of trial states the ground state energy of point-interacting systems is extensively discussed in the physics literature (see [40] and references there). We note that with this method it is only possible to derive upper bounds, while Thm. 3.2.1 gives a lower bound on the ground state energy.

3.2.1 Proof outline

For the proof of Theorem 3.2.1 we first prove in Section 3.3 an IMS type formula, which allows to localize the impurity in a small box, of side length ℓ independent of L. In a second step we localize all of the remaining particles to be either close to the impurity or separated from it. Doing this we partly violate the antisymmetry constraint on the wavefunctions, which makes it necessary to first extend the quadratic form $F_{\alpha,N}$ to $\tilde{F}_{\alpha,N}$. The latter does not require the antisymmetry, but coincides with $F_{\alpha,N}$ on $D(F_{\alpha,N})$.

In Section 3.4 we give a rough lower bound on the energy in case the wavefunction is compactly supported in a box $(0,\ell)^3$. This lower bound is of the order $N^{5/3}/\ell^2$, as expected, but with a non-sharp prefactor. We shall introduce a quadratic form $F_{\alpha,N}^{\text{per}}$ with periodic boundary conditions and show that it is equivalent to $F_{\alpha,N}$ for confined wavefunctions. The reason we work with periodic boundary conditions instead of Dirichlet ones is that it allows to perform explicit computations in momentum space.

Because the ground state energy of the confined non-interacting N-particle system is strictly positive, we are allowed to choose μ negative in the definition of $F_{\alpha,N}^{\text{per}}$. Applying the method of [50] then leads to the lower bound on $F_{\alpha,N}^{\text{per}}$ in Theorem 3.4.1. The downside of working with $F_{\alpha,N}^{\text{per}}$ will be that because of the discrete nature of momentum space for periodic functions, we have to work with sums instead of integrals, and the difference between the sum and the integral versions will have to be carefully controlled.

In Section 3.5 we give the proof of Theorem 3.2.1. Using the IMS formula of Prop. 2, we localize the particles either in a small box with side length $\ell \sim \rho^{-1/3}$ containing the impurity, or in the large complement. In the small box we use Theorem 3.4.1 for a lower bound, whereas in the large complement we use Theorem 3.A.3, which is a version of the positive density Lieb-Thirring inequality in [24] adapted to our setting of Dirichlet boundary conditions, and which is proved in the appendix. This allows us to improve the rough bound of Thm. 3.4.1 and show Thm. 3.2.1.

3.3 Properties of the quadratic form

In this section we will first extend the quadratic form $F_{\alpha,N}$ to functions that are not required to be antisymmetric in the last N variables. Afterwards we shall discuss how the splitting

$\psi = \phi_\mu + G_\mu \xi$ is affected when multiplying ψ by a smooth function (which need not be symmetric under permutations). This will be utilized in the last part of this section where an IMS formula for the (extended) quadratic form is shown.

3.3.1 Extension to functions without symmetry

To prove our main theorem, we want to localize the particles in different subsets of the cube $B = (0, L)^3$. Hence it is necessary to extend the quadratic form $F_{\alpha,N}$ by removing the antisymmetry constraint. To this aim we define

$$D(\tilde{F}_{\alpha,N}) = \left\{ \psi = \phi_\mu + \sum_{i=1}^{N} G_\mu \xi_i \mid \phi_\mu \in H^1(\mathbb{R}^{3(N+1)}), \xi_i \in H^{1/2}(\mathbb{R}^{3N}) \; \forall\, i, 1 \le i \le N \right\} \tag{3.3.1}$$

where

$$\widehat{G_\mu \xi_i}(k_0, \vec{k}) = G_\mu(k_0, \vec{k}) \hat{\xi}_i(k_0 + k_i, \hat{k}_i)\,. \tag{3.3.2}$$

The quadratic form $\tilde{F}_{\alpha,N}$ is defined as

$$\tilde{F}_{\alpha,N}(\psi) := \left\langle \phi_\mu \left| H_0^N + \mu \right| \phi_\mu \right\rangle - \mu \, \|\psi\|^2_{L^2(\mathbb{R}^{3(N+1)})} + \tilde{T}_{\alpha,\mu,N}(\vec{\xi}) \tag{3.3.3}$$

$$\tilde{T}_{\alpha,\mu,N}(\vec{\xi}) := \frac{2m}{m+1} \alpha \sum_{i=1}^{N} \|\xi_i\|^2_{L^2(\mathbb{R}^{3N})} + \tilde{T}^{\mu,N}_{\mathrm{dia}}(\vec{\xi}) + \tilde{T}^{\mu,N}_{\mathrm{off}}(\vec{\xi}) \tag{3.3.4}$$

where $\vec{\xi} = (\xi_i)_{i=1}^N$ and

$$\tilde{T}^{\mu,N}_{\mathrm{dia}}(\vec{\xi}) := \sum_{i=1}^{N} \int_{\mathbb{R}^{3N}} |\hat{\xi}_i(\vec{k})|^2 L_{\mu,N}(\vec{k}) \, \mathrm{d}\vec{k} \tag{3.3.5}$$

$$\tilde{T}^{\mu,N}_{\mathrm{off}}(\vec{\xi}) := - \sum_{\substack{i \neq j \\ 1 \le i,j \le N}} \int_{\mathbb{R}^{3(N+1)}} \hat{\xi}_i^*(k_0 + k_i, \hat{k}_i) \hat{\xi}_j(k_0 + k_j, \hat{k}_j) G_\mu(k_0, \vec{k}) \, \mathrm{d}k_0 \, \mathrm{d}\vec{k}\,. \tag{3.3.6}$$

Each ξ_i in (3.3.2) corresponds to a function supported on the hyperplane $x_0 = x_i$. The only overlap between hyperplanes for $i \neq j$ is on the set $x_i = x_0 = x_j$, which implies that $\sum_{i=1}^N \hat{\xi}_i(k_0 + k_i, \hat{k}_i)$ has a unique decomposition into $(\xi_i)_{i=1}^N$, and thus the splitting $\psi = \phi_\mu + \sum_{i=1}^N G_\mu \xi_i$ is unique. To stress the dependence on ψ, we will sometimes use the notation ϕ_μ^ψ and ξ_i^ψ below.

In the case that ψ is antisymmetric in the last N coordinates, the uniqueness of the decomposition $\psi = \phi_\mu + \sum_{i=1}^N G_\mu \xi_i$ shows that there exists a function $\xi \in H^{1/2}(\mathbb{R}^3) \otimes H^{1/2}_{\mathrm{as}}(\mathbb{R}^{3(N-1)})$ such that $\xi_i = (-1)^{i+1} \xi$, and hence $\sum_{i=1}^N G_\mu \xi_i = G_\mu \xi$, defined in (3.1.5). Furthermore we have

$$\tilde{T}^{\mu,N}_{\mathrm{dia}}(\vec{\xi}) = N T^{\mu,N}_{\mathrm{dia}}(\xi), \qquad \tilde{T}^{\mu,N}_{\mathrm{off}}(\vec{\xi}) = N T^{\mu,N}_{\mathrm{off}}(\xi) \tag{3.3.7}$$

in this case, which shows that $\tilde{F}_{\alpha,N}(\psi) = F_{\alpha,N}(\psi)$ for ψ antisymmetric in the last N coordinates. In particular, $\tilde{F}_{\alpha,N}$ is an extension of $F_{\alpha,N}$, and for a lower bound it therefore suffices to work with $\tilde{F}_{\alpha,N}$.

In the following, it will be convenient to introduce the notation

$$\tilde{\nabla} := \left(\frac{1}{\sqrt{2m}} \nabla_0, \frac{1}{\sqrt{2}} \nabla_1, \ldots, \frac{1}{\sqrt{2}} \nabla_N \right) \tag{3.3.8}$$

as well as

$$H_\mu := H_0^N + \mu = -\tilde{\nabla}^2 + \mu\,. \tag{3.3.9}$$

3.3.2 Localization of wavefunctions

An important ingredient in the proof of Theorem 3.2.1 will be to localize the particles. For this purpose we will study in this subsection how the splitting $\psi = \phi_\mu^\psi + \sum_{i=1}^N G_\mu \xi_i^\psi$ is affected when multiplying ψ by a smooth function.

Lemma 3.3.1. *For $J \in C^\infty(\mathbb{R}^{3(N+1)})$ bounded and with bounded derivatives, we define $J\vec{\xi} = (J\xi_i)_{i=1}^N$ by*

$$(J\xi_i)(x_i, \hat{x}_i) = J(x_i, \vec{x})\xi_i(x_i, \hat{x}_i)\,. \tag{3.3.10}$$

Then $\xi_i \mapsto [J, G_\mu]\xi_i := JG_\mu\xi_i - G_\mu J\xi_i$ is a bounded map from $L^2(\mathbb{R}^{3N})$ to $H^1(\mathbb{R}^{3(N+1)})$. In particular

$$\xi_i^{J\psi} = J\xi_i^\psi \tag{3.3.11}$$

and the regular part $\phi_\mu^{J\psi}$ of $J\psi$ is given by

$$\phi_\mu^{J\psi} = J\phi_\mu^\psi + \sum_{i=1}^N [J, G_\mu]\xi_i^\psi\,. \tag{3.3.12}$$

Remark. *We clarify that J acts on functions on $\mathbb{R}^{3(N+1)}$, and in particular on ϕ_μ^ψ and $G_\mu\xi_i^\psi$, as a multiplication operator, whereas on functions in $L^2(\mathbb{R}^{3N})$ it acts as in* (3.3.10). *Hence the commutator $[J, G_\mu]$ has no meaning here independently of its application on $\vec{\xi}$, and is only used as a convenient notation.*

Proof. We first argue that $[J, G_\mu]\xi_i^\psi \in H^1(\mathbb{R}^{3(N+1)})$ implies (3.3.11) and (3.3.12). We have

$$J\psi - \sum_{i=1}^N G_\mu J\xi_i^\psi = J\phi_\mu^\psi + \sum_{i=1}^N [J, G_\mu]\xi_i^\psi\,. \tag{3.3.13}$$

Since $J\phi_\mu^\psi$ and $[J, G_\mu]\xi_i^\psi$ are in $H^1(\mathbb{R}^{3(N+1)})$, the uniqueness of the decomposition of $J\psi$ into regular and singular parts implies (3.3.11) and (3.3.12).

It remains to show that $[J, G_\mu]\xi_i \in H^1(\mathbb{R}^{3(N+1)})$ for $\xi_i \in L^2(\mathbb{R}^{3N}$. In order to do so, we shall in fact show that

$$[J, G_\mu]\xi_i = H_\mu^{-1}[H_0^N, J]G_\mu\xi_i = H_\mu^{-1}(-2\tilde{\nabla}\cdot(\tilde{\nabla}J) - (\tilde{\nabla}^2 J))G_\mu\xi_i\,, \tag{3.3.14}$$

where we used the notation introduced in (3.3.8) and (3.3.9). From (3.3.14) the H^1 property readily follows, using that

$$\left\|G_\mu\xi_i\right\|^2_{L^2(\mathbb{R}^{3(N+1)})} = \int_{\mathbb{R}^{3(N+1)}} G_\mu(k_0, \vec{k})^2 |\hat{\xi}_i(k_0 + k_i, \hat{k}_i)|^2 \,\mathrm{d}k_0\,\mathrm{d}\vec{k} \lesssim \left(\frac{m}{m+1}\right)^{3/2} \mu^{-1/2}\, \|\xi_i\|^2_{L^2(\mathbb{R}^{3N})}\,. \tag{3.3.15}$$

In the last step we did an explicit integration over $\frac{1}{m+1}k_0 - \frac{m}{m+1}k_i$, the variable canonically conjugate to $x_0 - x_i$.

In order to show (3.3.14), we note that since J is smooth, $H_\mu^{-1}JH_\mu$ is a bounded operator. In the sense of distributions, we have

$$\left(H_\mu G_\mu \xi_i\right)(x_0, \vec{x}) = \xi_i(x_i, \hat{x}_i)\delta(x_0 - x_i) \tag{3.3.16}$$

and hence $H_\mu^{-1} J H_\mu G_\mu \xi_i = G_\mu J \xi_i$. In particular,

$$[J, G_\mu]\xi_i = \left(J - H_\mu^{-1} J H_\mu\right) G_\mu \xi_i \tag{3.3.17}$$

which indeed equals (3.3.14). This completes the proof of the lemma. □

Corollary 3.3.2. *Assume that $\psi \in D(\tilde{F}_{\alpha,N})$ satisfies* $\operatorname{supp}\psi \subseteq \Omega_0 \times \cdots \times \Omega_N$, *where $\Omega_j \subseteq \mathbb{R}^3$ for $0 \le j \le N$. Then*

$$\operatorname{supp}\xi_i^\psi \subseteq (\Omega_0 \cap \Omega_i) \times \Omega_1 \times \cdots \times \Omega_{i-1} \times \Omega_{i+1} \times \cdots \times \Omega_N\,. \tag{3.3.18}$$

Proof. Let $J \in C^\infty(\mathbb{R}^{3(N+1)})$ such that $J(x_0, \vec{x}) = 1$ for $(x_0, \vec{x}) \in \Omega_0 \times \cdots \times \Omega_N$. Using Lemma 3.3.1 we get that

$$\xi_i^\psi(x_0, \hat{x}_i) = \xi_i^{J\psi}(x_0, \hat{x}_i) = J(x_i, \vec{x})\xi_i^\psi(x_i, \hat{x}_i)\,. \tag{3.3.19}$$

Since this holds for all J with the above property, the claim follows. □

3.3.3 Alternative representation of the singular part

The following Lemma gives an alternative representation of the singular part of the quadratic form, defined in (3.3.4). It will turn out to be useful in the proof of the IMS formula in the next subsection.

Lemma 3.3.3. *For $\vec{\xi} = (\xi_i)_{i=1}^N$ with $\xi_i \in H^{1/2}(\mathbb{R}^{3N})$, the function*

$$\mathcal{I}(\nu) := \left\| \sum_{i=1}^N G_\nu \xi_i \right\|^2_{L^2(\mathbb{R}^{3(N+1)})} - \pi^2 \left(\frac{2m}{m+1}\right)^{3/2} \frac{1}{\sqrt{\nu}} \sum_{i=1}^N \|\xi_i\|^2_{L^2(\mathbb{R}^{3N})} \tag{3.3.20}$$

is integrable on $[\mu, \infty)$ for any $\mu > 0$, and we have

$$\tilde{T}_{\alpha,\mu,N}(\vec{\xi}) = \left(\frac{2m}{m+1}\alpha + 2\pi^2 \left(\frac{2m}{m+1}\right)^{3/2} \sqrt{\mu}\right) \sum_{i=1}^N \|\xi_i\|^2_{L^2(\mathbb{R}^{3N})} - \int_\mu^\infty \mathrm{d}\nu\, \mathcal{I}(\nu)\,. \tag{3.3.21}$$

Proof. For any $1 \le i \le N$, we have

$$\begin{aligned} \|G_\nu \xi_i\|^2_{L^2(\mathbb{R}^{3(N+1)})} &= \int_{\mathbb{R}^{3(N+1)}} G_\nu(k_0, \vec{k})^2 |\hat{\xi}_i(k_0 + k_i, \hat{k}_i)|^2 \,\mathrm{d}k_0 \,\mathrm{d}\vec{k} = \\ &= \left(\frac{2m}{m+1}\right)^{3/2} \int_{\mathbb{R}^{3N}} \frac{\pi^2}{\sqrt{\frac{k_i^2}{2(1+m)} + \frac{1}{2}\hat{k}_i^2 + \nu}} |\hat{\xi}_i(k_i, \hat{k}_i)|^2 \,\mathrm{d}k_0 \,\mathrm{d}\vec{k}\,. \end{aligned} \tag{3.3.22}$$

In particular,

$$\|G_\nu \xi_i\|^2_{L^2(\mathbb{R}^{3(N+1)})} - \left(\frac{2m}{m+1}\right)^{3/2} \frac{\pi^2}{\sqrt{\nu}} \|\xi_i\|^2_{L^2(\mathbb{R}^{3N})} \le 0 \tag{3.3.23}$$

and we have

$$\begin{aligned} &- \int_\mu^\infty \mathrm{d}\nu \left(\|G_\nu \xi_i\|^2_{L^2(\mathbb{R}^{3(N+1)})} - \left(\frac{2m}{m+1}\right)^{3/2} \frac{\pi^2}{\sqrt{\nu}} \|\xi_i\|^2_{L^2(\mathbb{R}^{3N})} \right) \\ &= \int_{\mathbb{R}^{3N}} |\hat{\xi}_i(\vec{k})|^2 L_{\mu,N}(\vec{k}) \,\mathrm{d}\vec{k} - 2\pi^2 \left(\frac{2m}{m+1}\right)^{3/2} \sqrt{\mu}\, \|\xi_i\|^2_{L^2(\mathbb{R}^{3N})}\,. \end{aligned} \tag{3.3.24}$$

For the terms $i \neq j$, on the other hand, we have

$$\int_\mu^\infty \mathrm{d}\nu \, \langle G_\nu \xi_i | G_\nu \xi_j \rangle = \int_\mu^\infty \mathrm{d}\nu \int_{\mathbb{R}^{3(N+1)}} \hat{\xi}_i^*(k_0 + k_i, \hat{k}_i) \hat{\xi}_j(k_0 + k_j, \hat{k}_j) G_\nu(k_0, \vec{k})^2 \, \mathrm{d}k_0 \, \mathrm{d}\vec{k}$$
$$= \int_{\mathbb{R}^{3(N+1)}} \hat{\xi}_i^*(k_0 + k_i, \hat{k}_i) \hat{\xi}_j(k_0 + k_j, \hat{k}_j) G_\mu(k_0, \vec{k}) \, \mathrm{d}k_0 \, \mathrm{d}\vec{k} \, . \tag{3.3.25}$$

Here the exchange of the order of integration is justified by Fubini's theorem, since the integrand in the first line on the right is absolutely integrable for $\xi_i \in H^{1/2}$. This completes the proof. □

3.3.4 IMS formula

In this subsection we will prove the following Lemma.

Proposition 2. *Given $M \geq 1$ and $(J_i)_{i=1}^M$ with $J_i \in C^\infty(\mathbb{R}^{3(N+1)})$ and $\sum_{i=1}^M J_i^2 = 1$, we have*

$$\tilde{F}_{\alpha,N}(\psi) = \sum_{i=1}^M \tilde{F}_{\alpha,N}(J_i\psi) - \sum_{i=1}^M \left\| (\tilde{\nabla} J_i)\psi \right\|^2 \tag{3.3.26}$$

for all $\psi \in D(\tilde{F}_{\alpha,N})$.

Proof. By using the polarization identity, we can extend $\tilde{F}_{\alpha,N}$ to a sesquilinear form, denoted as $\tilde{F}_{\alpha,N}(\psi_1, \psi_2)$. It suffices to prove that

$$\tilde{F}_{\alpha,N}(J^2\psi, \psi) + \tilde{F}_{\alpha,N}(\psi, J^2\psi) - 2\tilde{F}_{\alpha,N}(J\psi, J\psi) = -2 \left\| (\tilde{\nabla} J)\psi \right\|^2 \tag{3.3.27}$$

for smooth functions J, since then

$$\tilde{F}_{\alpha,N}(\psi) = \frac{1}{2} \sum_{i=1}^M \left(\tilde{F}_{\alpha,N}(J_i^2\psi, \psi) + \tilde{F}_{\alpha,N}(\psi, J_i^2\psi) \right) \overset{(3.3.27)}{=} \sum_{i=1}^M \tilde{F}_{\alpha,N}(J_i\psi, J_i\psi) - \sum_{i=1}^M \left\| (\tilde{\nabla} J_i)\psi \right\|^2 \, . \tag{3.3.28}$$

Recall the definition $H_\mu = H_0^N + \mu$. The left side of (3.3.27) equals

$$\langle \phi_\mu^{J^2\psi} | H_\mu | \phi_\mu^\psi \rangle + \langle \phi_\mu^\psi | H_\mu | \phi_\mu^{J^2\psi} \rangle - 2 \langle \phi_\mu^{J\psi} | H_\mu | \phi_\mu^{J\psi} \rangle$$
$$+ \tilde{T}_{\alpha,\mu,N}(\vec{\xi}^{J^2\psi}, \vec{\xi}^\psi) + \tilde{T}_{\alpha,\mu,N}(\vec{\xi}^\psi, \vec{\xi}^{J^2\psi}) - 2\tilde{T}_{\alpha,\mu,N}(\vec{\xi}^{J\psi}, \vec{\xi}^{J\psi}) \tag{3.3.29}$$

where we introduced the sesquilinear form $\tilde{T}_{\alpha,\mu,N}(\vec{\xi}_1, \vec{\xi}_2)$ corresponding to the quadratic form (3.3.4). We use Lemma 3.3.1 to identify the regular and singular parts of the various wavefunctions. For the quadratic form $\tilde{T}_{\alpha,\mu,N}$, we utilize the representation (3.3.21), which together with (3.3.11) implies that

$$\tilde{T}_{\alpha,\mu,N}(\vec{\xi}^{J^2\psi}, \vec{\xi}^\psi) + \tilde{T}_{\alpha,\mu,N}(\vec{\xi}^\psi, \vec{\xi}^{J^2\psi}) - 2\tilde{T}_{\alpha,\mu,N}(\vec{\xi}^{J\psi}, \vec{\xi}^{J\psi})$$
$$= \int_\mu^\infty \mathrm{d}\nu \sum_{i,j=1}^N \left(2\langle G_\nu J\xi_i^\psi | G_\nu J\xi_j^\psi \rangle - \langle G_\nu J^2\xi_i^\psi | G_\nu \xi_j^\psi \rangle - \langle G_\nu \xi_i^\psi | G_\nu J^2 \xi_j^\psi \rangle \right) \, . \tag{3.3.30}$$

Since $G_\nu J\xi_i^\psi = H_\nu^{-1} J H_\nu G_\nu \xi^\psi$, as shown in the proof of Lemma 3.3.1, we can rewrite the terms in the integrand as

$$\begin{aligned} &2\langle G_\nu J\xi_i^\psi | G_\nu J \xi_j^\psi\rangle - \langle G_\nu J^2 \xi_i^\psi | G_\nu \xi_j^\psi\rangle - \langle G_\nu \xi_i^\psi | G_\nu J^2 \xi_j^\psi\rangle \\ &= \left\langle G_\nu \xi_i^\psi \left| 2H_\nu J H_\nu^{-2} J H_\nu - H_\nu^{-1} J^2 H_\nu - H_\nu J^2 H_\nu^{-1} \right| G_\nu \xi_j^\psi \right\rangle . \end{aligned} \tag{3.3.31}$$

Using that $(\partial/\partial\nu) G_\nu \xi_i^\psi = -H_\nu^{-1} G_\nu \xi_i^\psi$ as well as $[J,[H_\nu, J]] = 2|\tilde\nabla J|^2$, one readily checks that this further equals

$$(3.3.31) = -2\frac{\partial}{\partial \nu} \left\langle G_\nu \xi_i^\psi \left| [J, H_\nu] H_\nu^{-1} [H_\nu, J] - |\tilde\nabla J|^2 \right| G_\nu \xi_j^\psi \right\rangle . \tag{3.3.32}$$

The operator $A_\nu := [J,H_\nu]H_\nu^{-1}[H_\nu,J] - |\tilde\nabla J|^2$ is bounded, uniformly in ν for $\nu \geq \mu > 0$. Since $\|G_\nu \xi_i^\psi\|_2 \to 0$ as $\nu \to \infty$, we have $\lim_{\nu\to\infty} \langle G_\nu \xi_i^\psi | A_\nu | G_\nu \xi_j^\psi\rangle = 0$. In particular, from (3.3.30)–(3.3.32) we conclude that

$$\begin{aligned} &\tilde T_{\alpha,\mu,N}(\vec\xi^{J^2\psi}, \vec\xi^\psi) + \tilde T_{\alpha,\mu,N}(\vec\xi^\psi, \vec\xi^{J^2\psi}) - 2\tilde T_{\alpha,\mu,N}(\vec\xi^{J\psi}, \vec\xi^{J\psi}) \\ &= \sum_{i,j=1}^N \left(2\left\langle G_\mu \xi_i^\psi \left| [J, H_\mu] H_\mu^{-1} [H_\mu, J] \right| G_\mu \xi_j^\psi \right\rangle - 2\langle G_\mu \xi_i^\psi | |\tilde\nabla J|^2 G_\mu \xi_j^\psi\rangle \right) . \end{aligned} \tag{3.3.33}$$

For the regular part, we use (3.3.12) to rewrite the first line in (3.3.29) as

$$\begin{aligned} &\langle \phi_\mu^{J^2\psi} | H_\mu | \phi_\mu^\psi\rangle + \langle \phi_\mu^\psi | H_\mu | \phi_\mu^{J^2\psi}\rangle - 2\langle \phi_\mu^{J\psi} | H_\mu | \phi_\mu^{J\psi}\rangle \\ &= -2\langle \phi_\mu^\psi | |\tilde\nabla J|^2 \phi_\mu^\psi\rangle - 2\sum_{i,j=1}^N \langle [J, G_\mu]\xi_i^\psi | H_\mu | [J, G_\mu]\xi_j^\psi\rangle \\ &\quad - 4\,\mathrm{Re} \sum_{i=1}^N \langle [J, G_\mu]\xi_i^\psi | H_\mu | J\phi_\mu^\psi\rangle + 2\,\mathrm{Re}\sum_{i=1}^N \langle [J^2, G_\mu]\xi_i^\psi | H_\mu | \phi_\mu^\psi\rangle . \end{aligned} \tag{3.3.34}$$

The second term on the right side equals $-2\sum_{i,j=1}^N \left\langle G_\mu \xi_i^\psi \left| [J, H_\mu] H_\mu^{-1} [H_\mu, J] \right| G_\mu \xi_j^\psi \right\rangle$, as (3.3.14) shows. Also the last line in (3.3.34) can be evaluated with the aid of (3.3.14), with the result that

$$\begin{aligned} &- 4\,\mathrm{Re} \sum_{i=1}^N \langle [J, G_\mu]\xi_i^\psi | H_\mu | J\phi_\mu^\psi\rangle + 2\,\mathrm{Re}\sum_{i=1}^N \langle [J^2, G_\mu]\xi_i^\psi | H_\mu | \phi_\mu^\psi\rangle \\ &= -4\,\mathrm{Re}\sum_{i=1}^N \langle G_\mu \xi_i^\psi | |\tilde\nabla J|^2 \phi_\mu^\psi\rangle . \end{aligned} \tag{3.3.35}$$

In combination, (3.3.33), (3.3.34) and (3.3.35) imply the desired identity (3.3.27). This completes the proof of the lemma. □

3.4 A rough bound

In this section we give a rough lower bound on the ground state energy of $F_{\alpha,N}$ when restricted to wavefunctions $\psi \in D(F_{\alpha,N})$ that are supported in B^{N+1} with $B = (0,\ell)^3$ for some $\ell > 0$.

This lower bound has the desired scaling in N and ℓ, i.e., it is proportional to $N^{5/3}\ell^{-2}$, but with a non-sharp prefactor. For its proof, we will first reformulate the problem using periodic boundary conditions, and then apply the methods previously introduced in [50] to show stability in infinite space.

The statement of the following theorem involves three positive constants c_T, c_L and c_Λ, which are independent of m, N, ℓ and α and which will be defined later. In particular, c_T is defined in Eq. (3.4.44), c_L in Eq. (3.4.84) and c_Λ in Lemma 3.4.8.

Theorem 3.4.1. *Let* $\psi \in D(F_{\alpha,N})$ *with* $\|\psi\| = 1$ *and* $\operatorname{supp}\psi \subseteq (0,\ell)^{3(N+1)}$ *or some* $\ell > 0$. *Given* $m > 0$ *and* $\kappa > 0$ *such that*

$$1 - \kappa/c_T > \Lambda(m) \tag{3.4.1}$$

let $N_0 = N_0(m,\kappa)$ *be defined as*

$$N_0(m,\kappa) = \left((1-\kappa/c_T - \Lambda(m))\,\frac{m(1-\kappa/c_T)^2}{c_\Lambda}\right)^{-9/2}. \tag{3.4.2}$$

For $N > N_0$ *we have*

$$F_{\alpha,N}(\psi) \geq \kappa N^{5/3}\ell^{-2} - \frac{1}{4\pi^4}\frac{m+1}{2m}\frac{[\alpha - c_L\ell^{-1}]_-^2}{(1-\kappa/c_T-\Lambda(m))^2(1-(N_0/N)^{2/9})^2}\,. \tag{3.4.3}$$

We note that this result gives a lower bound only for particle numbers $N > N_0(m,\kappa)$. In the case that $N \leq N_0$, we can still use (3.2.2), however.

The remainder of this section contains the proof of Theorem 3.4.1. An important role will be played by a reformulation using periodic boundary conditions. We will start by introducing the functional $\tilde{F}^{\mathrm{per}}_{\alpha,N}$ which is defined for periodic functions. In Lemma 3.4.3 we will show that it is in fact equivalent to the original quadratic form $\tilde{F}_{\alpha,N}$ when applied to wavefunctions with compact support in B^{N+1}. Working with periodic boundary conditions comes with the inconvenience of having to work with sums, rather than with integrals, in momentum space. In particular, this makes the explicit form of the singular part of $\tilde{F}^{\mathrm{per}}_{\alpha,N}$ rather complicated; we shall compare it with the singular part of $\tilde{F}_{\alpha,N}$ in Lemma 3.4.5 and bound the difference. It comes with the big advantage of allowing us to choose μ negative, however, which will be essential to show a positive lower bound to the energy. We shall use the method of [50] which gives positivity of the singular part of $F^{\mathrm{per}}_{\alpha,N}$ for $\mu \geq -\kappa N^{5/3}\ell^{-2}$ for small enough κ, under a condition of the form $\tilde{\Lambda}(m,\kappa) < 1$. In Lemmas 3.4.6–3.4.8, we investigate the difference between $\tilde{\Lambda}(m,\kappa)$ and $\Lambda(m)$. In the last subsection we combine these results to prove Theorem 3.4.1.

3.4.1 Periodic boundary conditions

Given $\psi \in D(\tilde{F}_{\alpha,N})$ such that $\operatorname{supp}\psi \subseteq B^{N+1}$, we extend ψ to a periodic function ψ^{per}, defined as

$$\psi^{\mathrm{per}}(x_0,\ldots,x_N) = \psi(\tau(x_0),\ldots,\tau(x_N)) \tag{3.4.4}$$

with

$$\tau(x) = (\tau(x^1),\tau(x^2),\tau(x^3)), \qquad \tau(s) := \inf\left((s+\ell\mathbb{Z})\cap\mathbb{R}_+\right) \quad \text{for } s\in\mathbb{R}. \tag{3.4.5}$$

In the following we shall rewrite the functional $\tilde{F}_{\alpha,N}(\psi)$ in terms of ψ^{per}. Compared to Dirichlet boundary conditions, periodic ones have the advantage that one can work easily in the associated momentum space, similar to the unconfined case. For this purpose, we define the lattice in momentum space as

$$\mathbb{L} := \frac{2\pi}{\ell}\mathbb{Z}^3 . \tag{3.4.6}$$

The function ψ^{per} is then determined by its Fourier coefficients $\hat{\psi}^{\mathrm{per}}(k_0, \vec{k})$, which can be viewed as a function $\mathbb{L}^{N+1} \to \mathbb{C}$.

Corollary 3.3.2 implies that $\operatorname{supp}\xi_i \subseteq B^N$ for all $1 \le i \le N$. Hence we can extend it in a similar way as ψ to a periodic function ξ^{per}. In momentum space we can write it as $\hat{\xi}^{\mathrm{per}} : \mathbb{L}^N \to \mathbb{C}$. For periodic functions, $G_\mu \psi^{\mathrm{per}}$ does not make sense anymore, but instead choosing G_μ^{per} as the resolvent of the non-interacting Hamiltonian with periodic boundary conditions allows us to define $G_\mu^{\mathrm{per}}\xi_i^{\mathrm{per}}$ by the Fourier coefficients

$$\widehat{G_\mu^{\mathrm{per}}\xi_i^{\mathrm{per}}}(k_0, \vec{k}) = G_\mu(k_0, \vec{k})\hat{\xi}_i^{\mathrm{per}}(k_0 + k_i, \hat{k}_i) . \tag{3.4.7}$$

In order to motivate the quadratic form introduced below, we note that the expression $L_{\mu,N}(\vec{k})$ in (3.1.10) originates from the limit

$$L_{\mu,N}(\vec{k}) = \lim_{R\to\infty}\left(\frac{8\pi m R}{m+1} - \int_{|t|\le R} \frac{1}{\tilde{H}_0(k_1, t, \hat{k}_1) + \mu}\,\mathrm{d}t\right) \tag{3.4.8}$$

where $\tilde{H}_0$ is the non-interacting Hamiltonian in momentum space, expressed in terms of center-of-mass and relative coordinates for the pair (k_0, k_1), i.e.,

$$\tilde{H}_0(s, t, \hat{k}_1) := \hat{H}_0^N\left(\frac{m}{m+1}s + t, \frac{1}{m+1}s - t, \hat{k}_1\right) = \frac{1}{2(m+1)}s^2 + \frac{1+m}{2m}t^2 + \frac{1}{2}\hat{k}_1^2 . \tag{3.4.9}$$

More generally, we have

Lemma 3.4.2. *Let τ be a non-negative function in $C_0^\infty(\mathbb{R}^3)$ such that $\hat{\tau}(0) = 1, \hat{\tau}(p) \ge 0$ for all $p \in \mathbb{R}^3$ and*

$$\int_{\mathbb{R}^3} |t|^{-2}\tau(t)\,\mathrm{d}t = 4\pi . \tag{3.4.10}$$

Then

$$L_{\mu,N}(\vec{k}) = \lim_{R\to\infty}\left[\frac{8\pi m R}{m+1} - \int_{\mathbb{R}^3} \frac{1}{\tilde{H}_0(k_1, t, \hat{k}_1) + \mu}\hat{\tau}(t/R)\,\mathrm{d}t\right] . \tag{3.4.11}$$

Proof. Let $\gamma = \frac{1}{2(m+1)}k_1^2 + \frac{1}{2}\hat{k}_1^2 + \mu$. Using (3.4.10) we observe that (3.4.11) is equivalent to

$$\lim_{R\to\infty}\int_{\mathbb{R}^3} \frac{\gamma}{\left(\left(\frac{1+m}{2m}\right)t^2 + \gamma\right)\left(\frac{1+m}{2m}\right)t^2}\hat{\tau}(t/R)\,\mathrm{d}t = L_{\mu,N}(\vec{k}) . \tag{3.4.12}$$

Since $\hat{\tau}(0) = 1$ and $\hat{\tau}(t) \le 1$ for all other t, the result follows from dominated convergence. □

When replacing integrals by sums, we have to keep in mind that a change of coordinates from (k_0, k_1) to $s = k_0 + k_1$ and $t = \frac{m}{m+1}k_1 - \frac{1}{m+1}k_0$ changes the domain over which we have to take the sums. Whereas $s \in \mathbb{L}$ we have to sum for a fixed s the variable t over $\mathbb{L}^s := \mathbb{L} + \frac{ms}{m+1}$. Let τ be chosen as in Lemma 3.4.2, and define

$$L^{\mathrm{per}}_{\mu,N}(\vec{k}) := \lim_{R\to\infty}\left(\frac{8\pi mR}{m+1} - \left(\frac{2\pi}{\ell}\right)^3 \sum_{p\in\mathbb{L}^{k_1}} \frac{1}{\tilde{H}_0(k_1, p, \hat{k}_1) + \mu}\hat{\tau}(p/R)\right). \tag{3.4.13}$$

We shall see below that this definition is actually independent of τ. For us it will be important that τ has compact support, hence a sharp cut-off in momentum space would not be suitable.

We shall now define $\tilde{F}^{\mathrm{per}}_{\alpha,N}$ with domain

$$D(\tilde{F}^{\mathrm{per}}_{\alpha,N}) = \left\{\psi^{\mathrm{per}} = \phi^{\mathrm{per}}_\mu + \sum_{i=1}^N G^{\mathrm{per}}_\mu \xi^{\mathrm{per}}_i \mid \phi^{\mathrm{per}}_\mu \in H^1_{\mathrm{per}}(B^{N+1}),\ \xi^{\mathrm{per}}_i \in H^{1/2}_{\mathrm{per}}(B^N)\ \forall\, i, 1 \le i \le N\right\}, \tag{3.4.14}$$

where $H^1_{\mathrm{per}}(B^{N+1})$ and $H^{1/2}_{\mathrm{per}}(B^N)$ denotes the spaces of functions defined by Fourier coefficients in $\ell^2(\mathbb{L}, (1 + p^2))^{\otimes(N+1)}$ and $\ell^2(\mathbb{L}, (1 + p^2)^{1/2})^{\otimes N}$ respectively. The quadratic form is given by

$$\tilde{F}^{\mathrm{per}}_{\alpha,N}(\psi^{\mathrm{per}}) := \int_{B^{N+1}} \left(|\tilde{\nabla}\phi^{\mathrm{per}}_\mu|^2 + \mu|\phi^{\mathrm{per}}_\mu|^2\right) - \mu\,\|\psi^{\mathrm{per}}\|^2_{L^2(B^{N+1})} + \tilde{T}^{\mathrm{per}}_{\alpha,\mu,N}(\vec{\xi}^{\mathrm{per}}) \tag{3.4.15}$$

$$\tilde{T}^{\mathrm{per}}_{\alpha,\mu,N}(\vec{\xi}^{\mathrm{per}}) := \sum_{i=1}^N \frac{2m}{m+1}\alpha\left\|\xi^{\mathrm{per}}_i\right\|^2_{L^2(B^N)} + \tilde{T}^{\mathrm{per},\mu,N}_{\mathrm{dia}}(\vec{\xi}^{\mathrm{per}}) + \tilde{T}^{\mathrm{per},\mu,N}_{\mathrm{off}}(\vec{\xi}^{\mathrm{per}}) \tag{3.4.16}$$

where $\vec{\xi}^{\mathrm{per}} = (\xi^{\mathrm{per}}_i)^N_{i=1}$, $\tilde{\nabla}$ is defined in (3.3.8), and the singular parts of the quadratic form are given by

$$\tilde{T}^{\mathrm{per},\mu,N}_{\mathrm{dia}}(\vec{\xi}^{\mathrm{per}}) := \sum_{i=1}^N \left(\frac{2\pi}{\ell^3}\right)^{3N} \sum_{\vec{k}\in\mathbb{L}^N} |\hat{\xi}^{\mathrm{per}}_i(\vec{k})|^2 L^{\mathrm{per}}_{\mu,N}(\vec{k}) \tag{3.4.17}$$

$$\tilde{T}^{\mathrm{per},\mu,N}_{\mathrm{off}}(\vec{\xi}^{\mathrm{per}}) := -\sum_{\substack{i\neq j\\ 1\le i,j\le N}} \left(\frac{2\pi}{\ell^3}\right)^{3(N+1)} \sum_{k_0\in\mathbb{L},\vec{k}\in\mathbb{L}^N} \hat{\xi}^{\mathrm{per}*}_j(k_0 + k_j, \hat{k}_j)\hat{\xi}^{\mathrm{per}}_i(k_0 + k_i, \hat{k}_i)G_\mu(k_0, \vec{k}). \tag{3.4.18}$$

We also define $F^{\mathrm{per}}_{\alpha,N}$ as the restriction of $\tilde{F}^{\mathrm{per}}_{\alpha,N}$ to functions antisymmetric in the last N coordinates. Further we define $T^{\mathrm{per},\mu,N}_{\mathrm{dia}}$, $T^{\mathrm{per},\mu,N}_{\mathrm{off}}$ and $T^{\mathrm{per}}_{\alpha,\mu,N}$ in the natural way similar to $T^{\mu,N}_{\mathrm{dia}}$, $T^{\mu,N}_{\mathrm{off}}$ and $T_{\alpha,\mu,N}$ originating from $\tilde{T}^{\mu,N}_{\mathrm{dia}}$, $\tilde{T}^{\mu,N}_{\mathrm{off}}$ and $\tilde{T}_{\alpha,\mu,N}$, respectively (compare with (3.1.7) and (3.3.7)).

Lemma 3.4.3. *Let $\psi \in D(\tilde{F}_{\alpha,N})$ be such that* $\operatorname{supp}\psi \subseteq B^{N+1}$. *Then*

$$\tilde{F}^{\mathrm{per}}_{\alpha,N}(\psi^{\mathrm{per}}) = \tilde{F}_{\alpha,N}(\psi). \tag{3.4.19}$$

Proof. Recall the splitting of ψ into its regular and singular parts, and similarly for ψ^{per}:

$$\psi = \phi_\mu + \sum_i G_\mu\xi_i\,, \quad \psi^{\mathrm{per}} = \phi^{\mathrm{per}}_\mu + \sum_i G^{\mathrm{per}}_\mu \xi^{\mathrm{per}}_i\,. \tag{3.4.20}$$

Recall also the definition (3.3.9). In the sense of distributions we can apply H_μ to ϕ_μ, and in particular $H_\mu\phi_\mu \in H^{-1}(\mathbb{R}^{3(N+1)})$ as $\phi_\mu \in H^1(\mathbb{R}^{3(N+1)})$. In this sense we can write the regular part of $\tilde{F}_{\alpha,N}$ as $\langle\phi_\mu|H_\mu\phi_\mu\rangle$. Because $\operatorname{supp}\psi \subseteq B^{N+1}$ we have $\varepsilon := \operatorname{dist}(\operatorname{supp}\psi, \partial B) > 0$. Let χ be a smooth cutoff function such that $\chi(x) = 1$ if $x \in B_0 = [\varepsilon/2, \ell - \varepsilon/2]^3$ and $\chi(x) = 0$ if $x \in B^c$. As $\operatorname{supp}(H_\mu G_\mu \xi) \subseteq B_0^{N+1}$ and $\operatorname{supp}\psi \subseteq B_0^{N+1}$ also $\operatorname{supp}(H_\mu\phi_\mu) \subseteq B_0^{N+1}$, and therefore

$$\langle\phi_\mu|H_\mu\phi_\mu\rangle = \langle\chi\phi_\mu|H_\mu\phi_\mu\rangle\,. \tag{3.4.21}$$

We use the identity $\chi\phi_\mu = \chi\phi_\mu^{\text{per}} + \chi\sum_{i=1}^N G_\mu^{\text{per}}\xi_i^{\text{per}} - \chi\sum_{i=1}^N G_\mu\xi_i$ as well as the fact that $H_\mu\phi_\mu = H_\mu\phi_\mu^{\text{per}}$ on B_0^{N+1} to obtain

$$\begin{aligned}(3.4.21) &= \langle\chi\phi_\mu^{\text{per}}|H_\mu\phi_\mu^{\text{per}}\rangle + \sum_{i=1}^N \langle\chi(G_\mu^{\text{per}}\xi_i^{\text{per}} - G_\mu\xi_i)|H_\mu\phi_\mu^{\text{per}}\rangle \\ &= \int_{B^{N+1}} \left(|\tilde\nabla\phi_\mu^{\text{per}}|^2 + \mu|\phi_\mu^{\text{per}}|^2\right) + \sum_{i=1}^N \langle\chi(G_\mu^{\text{per}}\xi_i^{\text{per}} - G_\mu\xi_i)|H_\mu\phi_\mu^{\text{per}}\rangle\,. \end{aligned} \tag{3.4.22}$$

Note that $H_\mu\chi(G_\mu^{\text{per}}\xi_i^{\text{per}} - G_\mu\xi_i)$ is supported on $B \setminus B_0$, and ψ^{per} vanishes on this set. Hence

$$\sum_{i=1}^N \langle\chi(G_\mu^{\text{per}}\xi_i^{\text{per}} - G_\mu\xi_i)|H_\mu\phi_\mu^{\text{per}}\rangle = -\sum_{i,j=1}^N \langle G_\mu^{\text{per}}\xi_i^{\text{per}} - G_\mu\xi_i|\chi H_\mu G_\mu^{\text{per}}\xi_j^{\text{per}}\rangle\,. \tag{3.4.23}$$

We claim that (3.4.23) is equal to the difference $\tilde{T}^{\text{per}}_{\alpha,\mu,N}(\vec\xi^{\text{per}}) - \tilde{T}_{\alpha,\mu,N}(\vec\xi)$. Let τ be given as in Lemma 3.4.2. We approximate the distribution $(\chi H_\mu G_\mu^{\text{per}}\xi_j^{\text{per}})(x_0,\vec x) = \xi_j(x_j,\hat x_j)\delta(x_j - x_0)$ by the sequence of functions $(\xi_j\tau_R)(x_0,\vec x) = \xi_j((mx_j + x_0)/(1+m), \hat x_j)\tau_R(x_j - x_0)$ with $\tau_R(x) = R^3\tau(Rx)$. We assume that R is large enough such that τ_R is supported in a ball of radius $\varepsilon/2$, and hence $\xi_j\tau_R$ is supported in B^{N+1}. Because $G_\mu^{\text{per}}\xi_i^{\text{per}} - G_\mu\xi_i$ is actually a smooth function, as $H_\mu(G_\mu^{\text{per}}\xi_i^{\text{per}} - G_\mu\xi_i) = 0$ on B^{N+1}, we conclude that (3.4.23) is equal to

$$(3.4.23) = -\lim_{R\to\infty}\sum_{i,j=1}^N \langle G_\mu^{\text{per}}\xi_i^{\text{per}} - G_\mu\xi_i|\xi_j\tau_R\rangle\,. \tag{3.4.24}$$

For the terms with $i \neq j$, we can use dominated convergence in momentum space to conclude that

$$\lim_{R\to\infty}\sum_{i\neq j} \langle G_\mu^{\text{per}}\xi_i^{\text{per}} - G_\mu\xi_i|\xi_j\tau_R\rangle = \tilde{T}_{\text{off}}^{\mu,N}(\vec\xi) - \tilde{T}_{\text{off}}^{\text{per},\mu,N}(\vec\xi^{\text{per}})\,. \tag{3.4.25}$$

For the terms with $i = j$, we can further write

$$\begin{aligned}&\sum_{i=1}^N \langle G_\mu^{\text{per}}\xi_i^{\text{per}} - G_\mu\xi_i|\xi_i\tau_R\rangle \\ &= \sum_{i=1}^N \left(\langle G_\mu^{\text{per}}\xi_i^{\text{per}}|\xi_i\tau_R\rangle - \frac{8\pi mR}{m+1}\|\xi_i\|_2^2\right) - \sum_{i=1}^N \left(\langle G_\mu\xi_i|\xi_i\tau_R\rangle - \frac{8\pi mR}{m+1}\|\xi_i\|_2^2\right)\,. \end{aligned} \tag{3.4.26}$$

Lemma 3.4.2 implies that the limit of the last two terms exists, is independent of the choice of τ and is equal to $\tilde{T}_{\text{dia}}^{\mu,N}(\vec\xi)$. Because also (3.4.23) does not depend on τ we conclude that

$$\lim_{R\to\infty}\sum_{i=1}^N \left(\langle G_\mu^{\text{per}}\xi_i^{\text{per}}|\xi_i\tau_R\rangle - \frac{8\pi mR}{m+1}\|\xi_i\|_2^2\right) \tag{3.4.27}$$

exists and is independent of τ. Comparing with (3.4.13) and (3.4.17), we see that it actually equals $\tilde{T}^{\mathrm{per},\mu,N}_{\mathrm{dia}}(\vec{\xi}^{\mathrm{per}})$. Combining the above, we obtain

$$\langle\phi_\mu|H_\mu\phi_\mu\rangle = \int_{B^{N+1}} \left(|\tilde{\nabla}\phi_\mu^{\mathrm{per}}|^2 + \mu|\phi_\mu^{\mathrm{per}}|^2\right) + \tilde{T}^{\mathrm{per}}_{\alpha,\mu,N}(\vec{\xi}^{\mathrm{per}}) - \tilde{T}_{\alpha,\mu,N}(\vec{\xi})\,. \tag{3.4.28}$$

This completes the proof of the lemma. □

For fermions, described by wavefunctions ψ^{per} that are antisymmetric in the last N variables, the expression $G_\mu^{\mathrm{per}}\xi^{\mathrm{per}}$ in (3.4.7) is also well defined for negative μ as long as $\mu > -E^{\mathrm{per}}_{N-1}$, where E^{per}_{N-1} denotes the ground state energy of the non-interacting Hamiltonian for $N-1$ fermions with periodic boundary conditions on ∂B. (Note than $G_\mu\xi$, on the other hand, is only defined for $\mu > 0$.) The following lemma shows that for such μ the quadratic form $F^{\mathrm{per}}_{\alpha,N}$ is actually independent of μ.

Lemma 3.4.4. *For $\psi \in D(F^{\mathrm{per}}_{\alpha,N})$, the expression $F^{\mathrm{per}}_{\alpha,N}(\psi^{\mathrm{per}})$ is well-defined and independent of μ as long as $\mu > -E^{\mathrm{per}}_{N-1}$.*

Proof. We first note that $G_\mu^{\mathrm{per}}\xi^{\mathrm{per}}$ is well defined for $\mu > -E^{\mathrm{per}}_{N-1}$, because of the antisymmetry of ξ^{per} in the last $N-1$ variables, which implies that $N-1$ of the variables $(k_1,\ldots,k_N)$ in $G_\mu(k_0,\vec{k})$ in (3.4.7) are actually different. For $\nu,\mu > -E^{\mathrm{per}}_{N-1}$ we have

$$\phi_\mu^{\mathrm{per}} = \phi_\nu^{\mathrm{per}} + G_\nu^{\mathrm{per}}\xi^{\mathrm{per}} - G_\mu^{\mathrm{per}}\xi^{\mathrm{per}}\,. \tag{3.4.29}$$

Using the resolvent identity, we see that the regular part of the quadratic form satisfies

$$\begin{aligned}\int_{B^{N+1}} \left(|\tilde{\nabla}\phi_\mu^{\mathrm{per}}|^2 + \mu|\phi_\mu^{\mathrm{per}}|^2\right) &= \int_{B^{N+1}} \left(|\tilde{\nabla}\phi_\nu^{\mathrm{per}}|^2 + \nu|\phi_\nu^{\mathrm{per}}|^2\right) + (\mu-\nu)\left\|\phi_\nu^{\mathrm{per}}\right\|^2 \\ &\quad + 2(\mu-\nu)\,\mathrm{Re}\langle G_\nu^{\mathrm{per}}\xi^{\mathrm{per}}|\phi_\nu^{\mathrm{per}}\rangle + (\mu-\nu)\langle G_\nu^{\mathrm{per}}\xi^{\mathrm{per}}|G_\nu^{\mathrm{per}}\xi^{\mathrm{per}} - G_\mu^{\mathrm{per}}\xi^{\mathrm{per}}\rangle\,.\end{aligned} \tag{3.4.30}$$

A straightforward computation using the definitions (3.4.13)–(3.4.16) shows that

$$T^{\mathrm{per}}_{\alpha,\mu,N}(\xi^{\mathrm{per}}) - T^{\mathrm{per}}_{\alpha,\nu,N}(\xi^{\mathrm{per}}) = (\mu-\nu)\langle G_\nu^{\mathrm{per}}\xi^{\mathrm{per}}|G_\mu^{\mathrm{per}}\xi^{\mathrm{per}}\rangle\,. \tag{3.4.31}$$

Combining both statements yields the desired identity

$$\begin{aligned}&\int_{B^{N+1}} \left(|\tilde{\nabla}\phi_\mu^{\mathrm{per}}|^2 + \mu|\phi_\mu^{\mathrm{per}}|^2\right) - \mu\,\|\psi^{\mathrm{per}}\|^2 + T^{\mathrm{per}}_{\alpha,\mu,N}(\xi^{\mathrm{per}}) \\ &= \int_{B^{N+1}} \left(|\tilde{\nabla}\phi_\nu^{\mathrm{per}}|^2 + \nu|\phi_\nu^{\mathrm{per}}|^2\right) - \nu\,\|\psi^{\mathrm{per}}\|^2 + T^{\mathrm{per}}_{\alpha,\nu,N}(\xi^{\mathrm{per}})\,.\end{aligned} \tag{3.4.32}$$

□

3.4.2 Approximation by integrals

In the previous subsection we have shown that the original and the periodic formulations of the energy functionals, $\tilde{F}_{\alpha,N}$ and $\tilde{F}^{\mathrm{per}}_{\alpha,N}$, agree if applied to functions ψ compactly supported in B^{N+1}. One complication in the periodic form is that $L^{\mathrm{per}}_{\mu,N}$ is not given as explicitly as $L_{\mu,N}$. The following lemma gives a bound on the difference.

Lemma 3.4.5. *Given μ and $\vec{q}$ such that*

$$Q_\mu^2 := \frac{1}{2}\sum_{i=2}^{N} q_i^2 + \mu > 0 \tag{3.4.33}$$

we have

$$|L^{\text{per}}_{\mu,N}(q_1,\hat{q}_1) - L_{\mu,N}(q_1,\hat{q}_1)| \le c'_L \frac{1}{Q_\mu^2 \ell^3} \tag{3.4.34}$$

where the constant c'_L is independent of $N, \vec{q}, m, \ell$ and μ.

Proof. We recall the definitions of $L_{\mu,N}$ and $L^{\text{per}}_{\mu,N}$ for some arbitrary τ fulfilling the requirements of Lemma 3.4.2:

$$\begin{aligned} L_{\mu,N}(\vec{q}) &= -\lim_{R\to\infty}\left(\int \frac{1}{\tilde{H}_0(q_1,s,\hat{q}_1)+\mu}\hat{\tau}(s/R)\,\mathrm{d}s - \frac{8\pi m R}{m+1}\right) \\ L^{\text{per}}_{\mu,N}(\vec{q}) &= -\lim_{R\to\infty}\left(\left(\frac{2\pi}{\ell}\right)^3 \sum_{s\in\mathbb{L}^{q_1}} \frac{1}{\tilde{H}_0(q_1,s,\hat{q}_1)+\mu}\hat{\tau}(s/R) - \frac{8\pi m R}{m+1}\right) \end{aligned} \tag{3.4.35}$$

with $\tilde{H}_0$ defined in (3.4.9). For simplicity we assume that q_1 is such that $\mathbb{L}^{q_1} = \mathbb{L}$ but all other cases work analogously as a shift in momentum space only introduces a phase factor in configuration space, which vanishes when taking absolute values. In the following we denote $f_\infty(s) = (\tilde{H}_0(q_1,s,\hat{q}_1)+\mu)^{-1}$ and $f_R(s) = f_\infty(s)\hat{\tau}(s/R)$ and suppress the dependence on $\vec{q}$ for simplicity.

We can express the difference between the Riemann sum and the integral using Poisson's summation formula

$$\left(\frac{2\pi}{\ell}\right)^3 \sum_{s\in\mathbb{L}} f_R(s) - \int_{\mathbb{R}^3} f_R(s)\,\mathrm{d}s = \frac{(2\pi)^3}{\ell^3}\sum_{s\in\mathbb{L}} f_R(s) - (2\pi)^{3/2}\hat{f}_R(0) = (2\pi)^{3/2}\sum_{\substack{z\in\ell\mathbb{Z}^3\\ z\neq 0}} \hat{f}_R(z)\,. \tag{3.4.36}$$

For short we write $\gamma := \frac{1}{2(1+m)}q_1^2 + \frac{1}{2}\hat{q}_1^2 + \mu$, which is bounded from below by Q_μ^2 and hence is positive, by our assumption (3.4.33). The function f_∞ and its Fourier transform are given by

$$f_\infty(t) = \frac{1}{\frac{1+m}{2m}t^2 + \gamma}, \quad \hat{f}_\infty(z) = \sqrt{\frac{\pi}{2}}\frac{2m}{1+m}\frac{e^{-\left(\frac{2m}{m+1}\right)^{1/2}\sqrt{\gamma}|z|}}{|z|}\,. \tag{3.4.37}$$

Moreover,

$$\hat{f}_R(z) = (2\pi)^{-3/2}(R^3\tau(R\,\cdot\,) * \hat{f}_\infty)(z)\,. \tag{3.4.38}$$

We will show that $\hat{f}_R(s)$ is summable over $\ell\mathbb{Z}^3\setminus\{0\}$. In fact for $|z| \gtrsim \ell$,

$$\begin{aligned} (2\pi)^{3/2}|\hat{f}_R(z)| &= \int_{\mathbb{R}^3} R^3\tau(Rw)\hat{f}_\infty(z-w)\,\mathrm{d}w \\ &\le \int_{|w|>|z|/2} R^3\tau(Rw)\hat{f}_\infty(z-w)\,\mathrm{d}w + \int_{|z-w|>|z|/2} R^3\tau(Rw)\hat{f}_\infty(z-w)\,\mathrm{d}w \\ &\le \hat{f}_\infty(z/2)\int R^3\tau(Rw)\,\mathrm{d}w = \hat{f}_\infty(z/2) \end{aligned} \tag{3.4.39}$$

where we assumed that R is large enough such that $\tau(Rw) = 0$ for $|w| > |z|/2$, and used that $\int \tau = 1$, which was required by Lemma 3.4.2. As $\hat{f}_\infty$ is summable over $\ell\mathbb{Z}^3 \setminus \{0\}$ we get by dominated convergence that

$$\lim_{R\to\infty} \sum_{z\in\ell\mathbb{Z}^3\setminus\{0\}} |\hat{f}_R(z)| = \sum_{z\in\ell\mathbb{Z}^3\setminus\{0\}} \hat{f}_\infty(z)\,. \tag{3.4.40}$$

We bound the sum over $\hat{f}_\infty(|z|)$ by

$$\sum_{z\in\ell\mathbb{Z}^3\setminus\{0\}} \hat{f}_\infty(z) = \sum_{n\in\mathbb{Z}^3\setminus\{0\}} \sqrt{\frac{\pi}{2}} \frac{2m}{1+m} \frac{e^{-\left(\frac{2m}{m+1}\right)^{1/2}\sqrt{\gamma}\ell|n|}}{\ell|n|} \lesssim \frac{1}{\gamma\ell^3} \tag{3.4.41}$$

using

$$\sum_{n\in\mathbb{Z}^3\setminus\{0\}} e^{-\eta|n|}/|n| \lesssim \sum_{n\in\mathbb{N}} ne^{-\eta n} = \frac{e^{-\eta}}{(1-e^{-\eta})^2} \le \frac{1}{\eta^2} \tag{3.4.42}$$

for $\eta = (2m/(m+1))^{1/2}\sqrt{\gamma}\ell$. Combining (3.4.36), (3.4.40) and (3.4.41) and using that $\gamma \ge Q_\mu^2$, we conclude that

$$\lim_{R\to\infty} \left| \frac{(2\pi)^3}{\ell^3} \sum_{s\in\mathbb{L}} f_R(s) - \int_{\mathbb{R}^3} f_R(s)\,\mathrm{d}s \right| \le \frac{c_L'}{\gamma\ell^3} \le \frac{c_L'}{Q_\mu^2\ell^3} \tag{3.4.43}$$

for some constant $c_L' > 0$. This completes the proof of the lemma. □

3.4.3 Bound on the singular parts

The strategy for obtaining a lower bound on $F^{\mathrm{per}}_{\alpha,N}$ is to find a μ such that $T^{\mathrm{per}}_{\alpha,\mu,N} \ge 0$, in which case we obtain the lower bound $F^{\mathrm{per}}_{\alpha,N}(\psi^{\mathrm{per}}) \ge -\mu\|\psi^{\mathrm{per}}\|^2$. Hence we want to choose μ as negative as possible. We shall use the method of [50], which yields the desired positivity of $T^{\mathrm{per}}_{\alpha,\mu,N}$ (for large enough m) as long as $\mu \ge -\kappa N^{5/3}\ell^{-2}$ for κ small enough. (More precisely, $-\mu$ will be equal to the right side of (3.4.3).)

If we define $Q^2 = \frac{1}{2}\sum_{i=2}^N q_i^2$ for $N > 2$, we observe that there exists a constant $c_T > 0$ such that

$$Q^2 \ge c_T N^{5/3}\ell^{-2} \tag{3.4.44}$$

if all $q_i \in \mathbb{L}$ are different, as required by the antisymmetry constraint. (We note that in comparison with [50] Q^2 is defined with an additional factor $1/2$ here.) From now on we restrict μ to satisfy $\mu \ge -\kappa N^{5/3}\ell^{-2}$ for some $\kappa < c_T$. This implies that

$$Q_\mu^2 = Q^2 + \mu \ge (1-\kappa/c_T)Q^2 \ge (c_T-\kappa)N^{5/3}\ell^{-2}\,. \tag{3.4.45}$$

In particular, Lemma 3.4.5 yields the bound

$$T^{\mathrm{per},\mu,N}_{\mathrm{dia}}(\xi^{\mathrm{per}}) \ge \left(\frac{2\pi}{\ell}\right)^{3N} \sum_{\vec{q}\in\mathbb{L}^N} L_{\mu,N}(\vec{q})|\hat{\xi}^{\mathrm{per}}(\vec{q})|^2 - \frac{1}{N^{5/3}\ell}\frac{c_L'}{c_T-\kappa}\|\xi^{\mathrm{per}}\|_2^2 \tag{3.4.46}$$

on the diagonal term of the singular part of $F^{\mathrm{per}}_{\alpha,N}$. Following the same steps as in [50] we can obtain the following lower bound for the off-diagonal term.

Proposition 3. *Assume that* $\mu \geq -\kappa N^{5/3}\ell^{-2}$ *for some* $\kappa < c_T$*. Then for all* $\xi \in H^{1/2}(\mathbb{R}^3) \otimes H^{1/2}_{\text{as}}(\mathbb{R}^{3(N-1)})$ *we have*

$$T^{\text{per},\mu,N}_{\text{off}}(\xi^{\text{per}}) \geq -\frac{\tilde{\Lambda}(m,\kappa)}{1-\kappa/c_T}\left(\frac{2\pi}{\ell}\right)^{3N}\sum_{\vec{q}\in\mathbb{L}^N} L_{\mu,N}(\vec{q})|\hat{\xi}^{\text{per}}(\vec{q})|^2 \tag{3.4.47}$$

where

$$\tilde{\Lambda}(m,\kappa) := \inf_{\delta>0}\sup_{\substack{\tilde{s},K\in\mathbb{R}^3\\ Q_\mu^2>(c_T-\kappa)N^{5/3}\ell^{-2}}}\left(\frac{2\pi}{\ell}\right)^3\sum_{\tilde{t}\in\mathbb{L}+AK}\lambda_{\tilde{s},Q_\mu,K,m,\delta}(\tilde{t}) \tag{3.4.48}$$

with

$$\begin{aligned}\lambda_{\tilde{s},Q_\mu,K,m,\delta}(\tilde{t}) := {}& \frac{(\tilde{s}-AK)^2+2Q_\mu^2+N\delta\ell^{-2}}{\pi^2(1+m)}\left(\frac{m(m+2)}{(m+1)^2}\tilde{s}^2+\frac{m}{m+1}(2Q_\mu^2+AK^2)\right)^{-1/4}\\ &\times\frac{1}{(\tilde{t}-AK)^2+\delta\ell^{-2}}\left(\frac{m(m+2)}{(m+1)^2}\tilde{t}^2+\frac{m}{m+1}(2Q_\mu^2+AK^2)\right)^{-1/4}\\ &\times\frac{\left|\tilde{s}\cdot\tilde{t}\right|}{\left[\tilde{s}^2+\tilde{t}^2+\frac{m}{1+m}(2Q_\mu^2+AK^2)\right]^2-\left[\frac{2}{(1+m)}\tilde{s}\cdot\tilde{t}\right]^2}\,.\end{aligned} \tag{3.4.49}$$

Proof. The proof works in almost the exact same way as in [50], hence we will not spell out the details. The main difference is that we now have to write sums instead of integrals, and in particular this implies that we have to choose the weight function $h(s,\hat{q}_1)$ (see [50, Eq. (4.12)]) differently, namely as

$$h(s,\hat{q}_1) = (s^2+\delta\ell^{-2})\prod_{i=2}^{N}(q_i^2+\delta\ell^{-2})\,. \tag{3.4.50}$$

For comparison $\delta = 0$ was used in [50]. Following the proof in [50, Sect. 4] this choice gives a lower bound to the off-diagonal term of the form

$$T^{\text{per},\mu,N}_{\text{off}}(\xi^{\text{per}}) \geq -\tilde{\Lambda}_{\delta,\mu}(m)\left(\frac{2\pi}{\ell}\right)^{3N}\sum_{\vec{q}\in\mathbb{L}^N} L_{\mu,N}(\vec{q})|\hat{\xi}^{\text{per}}(\vec{q})|^2 \tag{3.4.51}$$

with a prefactor $\tilde{\Lambda}_{\delta,\mu}(m)$ equal to

$$\begin{aligned}&\sup_{\tilde{s},K\in\mathbb{R}^3,Q^2>c_TN^{5/3}\ell^{-2}}\frac{(\tilde{s}-AK)^2+2Q^2+N\delta\ell^{-2}}{\pi^2(1+m)}\left(\frac{m(m+2)}{(m+1)^2}\tilde{s}^2+\frac{m}{m+1}(2Q^2+AK^2)+\frac{2m}{m+1}\mu\right)^{-1/4}\\ &\times\left(\frac{2\pi}{\ell}\right)^3\sum_{\tilde{t}\in\mathbb{L}+AK}\frac{1}{(\tilde{t}-AK)^2+\delta\ell^{-2}}\left(\frac{m(m+2)}{(m+1)^2}\tilde{t}^2+\frac{m}{m+1}(2Q^2+AK^2)+\frac{2m}{m+1}\mu\right)^{-1/4}\\ &\times\frac{\left|\tilde{s}\cdot\tilde{t}\right|}{\left[\tilde{s}^2+\tilde{t}^2+\frac{m}{1+m}(2Q^2+AK^2)+\frac{2m}{m+1}\mu\right]^2-\left[\frac{2}{(1+m)}\tilde{s}\cdot\tilde{t}\right]^2}\,.\end{aligned} \tag{3.4.52}$$

Since (3.4.45) holds under our assumption on μ, we see that $\inf_{\delta>0}\tilde{\Lambda}_{\delta,\mu}(m) \leq (1-\kappa/c_T)^{-1}\tilde{\Lambda}(m,\kappa)$, which yields the desired result. □

3.4.4 A bound on $\tilde{\Lambda}(m, \kappa)$

We will not evaluate $\tilde{\Lambda}(m, \kappa)$ directly but we will compare it with $\Lambda(m)$, which is defined in [50, Eq. (2.8)] and which was already referred to in (3.2.2) above. The expression $\Lambda(m)$ can be written as

$$\Lambda(m) := \sup_{\substack{\tilde{s}, K \in \mathbb{R}^3 \\ Q_\mu^2 > 0}} \int_{\mathbb{R}^3} \lambda_{\tilde{s}, Q_\mu, K, m, 0}(\tilde{t}) \, d\tilde{t} = \sup_{\substack{\tilde{s}, K \in \mathbb{R}^3 \\ Q_\mu^2 > (c_T - \kappa) N^{5/3} \ell^{-2}}} \int_{\mathbb{R}^3} \lambda_{\tilde{s}, Q_\mu, K, m, 0}(\tilde{t}) \, d\tilde{t}. \tag{3.4.53}$$

The additional constraint on Q_μ in the latter supremum has no effect because of the scaling properties of $\lambda_{\tilde{s}, Q_\mu, K, m, 0}$, specifically $\lambda_{\nu\tilde{s}, \nu Q_\mu, \nu K, m, 0}(\nu\tilde{t}) = \nu^{-3} \lambda_{\tilde{s}, Q_\mu, K, m, 0}(\tilde{t})$ for any $\nu > 0$, which allows to fix one of the parameters when taking the supremum. The expression (3.4.48) differs from (3.4.53) by the non-zero value of δ, as well as the sum instead of an integral. In the following lemmas we will compare the two.

The next Lemma gives a pointwise bound on $\lambda_{\tilde{s}, Q_\mu, K, m, \delta}$. For its statement it will be convenient to define $C_\ell(s)$ as the cube with side length $2\pi/\ell$ centered at $s \in \mathbb{R}^3$, i.e.,

$$C_\ell(s) = \left[-\frac{\pi}{\ell}, \frac{\pi}{\ell} \right]^3 + s. \tag{3.4.54}$$

Lemma 3.4.6. *For $m \gtrsim 1$ we have*

$$\lambda_{\tilde{s}, Q_\mu, K, m, \delta}(\tilde{t}) \lesssim \frac{1}{m} \frac{1}{t^{5/2}} \frac{s^2 + 2Q_\mu^2 + N\delta\ell^{-2}}{(s^2 + 2Q_\mu^2)^{1/4}} \frac{1}{s^2 + t^2 + 2Q_\mu^2} \tag{3.4.55}$$

where $\tilde{s} = s + AK$ and $\tilde{t} = t + AK$ for $t \in \mathbb{L} \setminus \{0\}$. Moreover,

$$\ell^{-3} \sum_{\tilde{t} \in \mathbb{L} + AK} \max_{\tau \in C_\ell(\tilde{t})} \lambda_{\tilde{s}, Q_\mu, K, m, \delta}(\tau) \lesssim \frac{1}{m} \left(1 + \frac{N\delta}{\ell^2 Q_\mu^2} + \frac{1}{\delta \ell Q_\mu} + \frac{N}{\ell^3 Q_\mu^3} \right). \tag{3.4.56}$$

Proof. For the pointwise bound (3.4.55) we will proceed similarly to [50, Sect. 6]. Using the Cauchy-Schwarz inequality we have

$$|\tilde{t} \cdot \tilde{s}| \le \frac{1}{2} \left[\tilde{s}^2 + \tilde{t}^2 + \frac{m}{1+m} (2Q_\mu^2 + AK^2) \right] \tag{3.4.57}$$

and also

$$\left[\tilde{s}^2 + \tilde{t}^2 + \frac{m}{1+m} (2Q_\mu^2 + AK^2) \right]^2 - \left[\frac{2}{(1+m)} \tilde{s} \cdot \tilde{t} \right]^2 \ge \frac{m(m+2)}{(1+m)^2} \left[\tilde{s}^2 + \tilde{t}^2 + \frac{m}{1+m} (2Q_\mu^2 + AK^2) \right]^2. \tag{3.4.58}$$

By minimizing over K we find that

$$\tilde{s}^2 + \tilde{t}^2 + \frac{m}{1+m} (2Q_\mu^2 + AK^2) \ge \frac{m(2+m)}{2 + 4m + m^2} \left[s^2 + t^2 + 2Q_\mu^2 \right] \tag{3.4.59}$$

and

$$\frac{m(m+2)}{(m+1)^2} \tilde{s}^2 + \frac{m}{m+1} (2Q_\mu^2 + AK^2) \ge \frac{m}{m+1} \left(s^2 + 2Q_\mu^2 \right). \tag{3.4.60}$$

By combining these bounds we get for (3.4.49) the pointwise bound

$$\lambda_{\tilde{s},Q_\mu,K,m,\delta}(\tilde{t}) \leq \left(\frac{m+1}{m}\right)^{3/2} \frac{m^2+4m+2}{2\pi^2 m(m+2)^2} \left(s^2 + 2Q_\mu^2 + N\delta\ell^{-2}\right) \times \left(s^2+2Q_\mu^2\right)^{-1/4} \frac{1}{t^2+\delta\ell^{-2}} \left(t^2+2Q_\mu^2\right)^{-1/4} \frac{1}{s^2+t^2+2Q_\mu^2} \tag{3.4.61}$$

from which (3.4.55) readily follows.

We denote the right side of (3.4.55) by $\lambda^>(t) = \lambda^>_{s,Q_\mu,K,m,\delta}(t)$ and we will write $\lambda(\tilde{t}) = \lambda_{\tilde{s},Q_\mu,K,m,\delta}(\tilde{t})$ in the following. That is, (3.4.55) reads $\lambda(\tilde{t}) \lesssim \lambda^>(t)$. First we treat the term $\tilde{t} = AK$ in (3.4.56). Using (3.4.61) we can bound

$$\ell^{-3}\lambda(\tilde{t}) \lesssim \frac{1}{m\delta\ell Q_\mu}\frac{s^2+2Q_\mu^2+N\delta\ell^{-2}}{s^2+t^2+2Q_\mu^2} \lesssim \frac{1}{m}\left(\frac{1}{\delta\ell Q_\mu}+\frac{N}{\ell^3 Q_\mu^3}\right) \tag{3.4.62}$$

for any $\tilde{t}$ and hence, in particular, for $\tilde{t} \in C_\ell(AK)$. For the case $0 \neq t \in \mathbb{L}$, we note that for $\tau_1, \tau_2 \in C_\ell(t)$ the bound $|\tau_1| \leq \sqrt{11}|\tau_2|$ holds, and hence

$$\lambda^>(\tau_1) \leq 11^{9/4}\lambda^>(\tau_2)\,. \tag{3.4.63}$$

In particular, the maximal value of $\lambda^>$ in $C_\ell(\tau)$ is dominated by the average value, and therefore

$$\begin{aligned}\ell^{-3}\sum_{\tilde{t}\in\mathbb{L}+AK}\max_{\tau\in C_\ell(\tilde{t})}\lambda(\tau) &\lesssim \ell^{-3}\sum_{\substack{t\in\mathbb{L}\\ t\neq 0}}\lambda^>(t) + \frac{1}{m}\left(\frac{1}{\delta\ell Q_\mu}+\frac{N}{\ell^3Q_\mu^3}\right)\\ &\lesssim \sum_{\substack{t\in\mathbb{L}\\ t\neq 0}}\int_{C_\ell(t)}\lambda^>(t)\,\mathrm{d}t + \frac{1}{m}\left(\frac{1}{\delta\ell Q_\mu}+\frac{N}{\ell^3Q_\mu^3}\right)\\ &\lesssim \int_{\mathbb{R}^3}\lambda^>(t)\,\mathrm{d}t + \frac{1}{m}\left(\frac{1}{\delta\ell Q_\mu}+\frac{N}{\ell^3Q_\mu^3}\right). \end{aligned} \tag{3.4.64}$$

As a last step we explicitly evaluate the integral, which results in the bound

$$\int_{\mathbb{R}^3}\lambda^>(t)\,\mathrm{d}t \lesssim \frac{1}{m}\left(1+\frac{N\delta}{\ell^2Q_\mu^2}\right). \tag{3.4.65}$$

This completes the proof of the lemma. □

Lemma 3.4.7. *For $m \gtrsim 1$ we have*

$$\left|\int_{\mathbb{R}^3}\lambda_{\tilde{s},Q_\mu,K,m,\delta}(\tilde{t})\,\mathrm{d}\tilde{t} - \left(\frac{2\pi}{\ell}\right)^3\sum_{\tilde{t}\in\mathbb{L}+AK}\lambda_{\tilde{s},Q_\mu,K,m,\delta}(\tilde{t})\right| \lesssim \frac{1}{m}\left(\frac{1}{\ell Q_\mu}+\frac{1}{\delta^{1/2}}\right)\left(1+\frac{N\delta}{\ell^2Q_\mu^2}+\frac{1}{\delta\ell Q_\mu}+\frac{N}{\ell^3Q_\mu^3}\right). \tag{3.4.66}$$

Proof. As in the proof of the previous Lemma, we denote $\lambda(\tilde{t}) = \lambda_{\tilde{s},Q_\mu,K,m,\delta}(\tilde{t})$, and write it as

$$\lambda(\tilde{t}) = c_5((\tilde{s}-AK)^2+2Q_\mu^2+N\delta\ell^{-2})(c_1\tilde{s}^2+c_2Q_\mu^2+c_3K^2)^{-1/4} \times \frac{1}{(\tilde{t}-AK)^2+\delta\ell^{-2}}(c_1\tilde{t}^2+c_2Q_\mu^2+c_3K^2)^{-1/4}\frac{|\tilde{s}\cdot\tilde{t}|}{(\tilde{s}^2+\tilde{t}^2+c_2Q_\mu^2+c_3K^2)^2-(c_4\tilde{s}\cdot\tilde{t})^2} \tag{3.4.67}$$

with appropriate coefficients c_1, c_2, c_3, c_4, c_5 depending on m. Its gradient equals

$$\nabla\lambda(\tilde{t}) = \underbrace{-2\frac{\tilde{t}-AK}{(\tilde{t}-AK)^2+\delta\ell^{-2}}\lambda(\tilde{t})}_{\text{I}} \underbrace{-\frac{1}{2}\frac{c_1\tilde{t}}{c_1\tilde{t}^2+c_2Q_\mu^2+c_3K^2}\lambda(\tilde{t})}_{\text{II}}$$
$$\underbrace{-\frac{4\tilde{t}(\tilde{s}^2+\tilde{t}^2+c_2Q_\mu^2+c_3K^2)-2c_4^2\tilde{s}(\tilde{s}\cdot\tilde{t})}{(\tilde{s}^2+\tilde{t}^2+c_2Q_\mu^2+c_3K^2)^2-(c_4\tilde{s}\cdot\tilde{t})^2}\lambda(\tilde{t})}_{\text{III}} + \underbrace{\frac{\tilde{s}}{\tilde{t}\cdot\tilde{s}}\lambda(\tilde{t})}_{\text{IV}}\,. \tag{3.4.68}$$

We can quantify the difference between the Riemann sum and the integral by

$$\left|\int_{\mathbb{R}^3}\lambda(\tilde{t})\,\mathrm{d}\tilde{t} - \left(\frac{2\pi}{\ell}\right)^3\sum_{\tilde{t}\in\mathbb{L}+AK}\lambda(\tilde{t})\right| \lesssim \ell^{-4}\sum_{\tilde{t}\in\mathbb{L}+AK}\max_{\tau\in C_\ell(\tilde{t})}|\nabla\lambda(\tau)|\,. \tag{3.4.69}$$

With the aid of the triangle inequality we can treat the terms I – IV separately.

We can bound I as

$$|\text{I}| \leq \frac{2}{\sqrt{(\tilde{t}-AK)^2+\delta\ell^{-2}}}\lambda(\tilde{t}) \leq \frac{2\ell}{\delta^{1/2}}\lambda(\tilde{t})\,. \tag{3.4.70}$$

For the second term we obtain

$$|\text{II}| \leq \frac{1}{2}\sqrt{\frac{c_1}{c_2}}\frac{1}{Q_\mu}\lambda(\tilde{t}) = \frac{1}{2^{3/2}}\sqrt{\frac{m+2}{m+1}}\frac{1}{Q_\mu}\lambda(\tilde{t}) \lesssim \frac{1}{Q_\mu}\lambda(\tilde{t})\,. \tag{3.4.71}$$

For III, we use similar estimates as in Lemma 3.4.6 to get

$$|\text{III}| \lesssim \frac{|\tilde{t}|+|\tilde{s}|}{\tilde{s}^2+\tilde{t}^2+c_2Q_\mu^2+c_3K^2}\lambda(\tilde{t}) \lesssim \frac{1}{Q_\mu}\lambda(\tilde{t})\,. \tag{3.4.72}$$

Finally, for IV we have to proceed slightly differently. If we use

$$|\tilde{s}| \leq \frac{1}{2\sqrt{c_2}Q_\mu}(\tilde{s}^2+\tilde{t}^2+c_2Q_\mu^2+c_3K^2) \tag{3.4.73}$$

instead of (3.4.57), we see that we can bound |III| from above by Q_μ^{-1} times the right side of (3.4.61). Using Lemma 3.4.6 we conclude that

$$\begin{aligned}(3.4.69) &\leq \ell^{-4}\sum_{\tilde{t}\in\mathbb{L}+AK}\max_{\tau\in C_\ell(\tilde{t})}(|\text{I}|+|\text{II}|+|\text{III}|+|\text{IV}|)\\ &\lesssim \frac{1}{m}\left(\frac{1}{\ell Q_\mu}+\frac{1}{\delta^{1/2}}\right)\left(1+\frac{N\delta}{\ell^2Q_\mu^2}+\frac{1}{\delta\ell Q_\mu}+\frac{N}{\ell^3Q_\mu^3}\right).\end{aligned} \tag{3.4.74}$$

Here we have used that the bound (3.4.56) holds also with $\lambda_{\tilde{s},Q_\mu,K,m,\delta}$ replaced by the right side of (3.4.61), as shown in the proof of Lemma 3.4.6. This completes the proof. □

Lemma 3.4.8. *There exists a* $c_\Lambda > 0$ *such that*

$$\tilde{\Lambda}(m,\kappa) \leq \Lambda(m) + \frac{1}{m}\frac{c_\Lambda}{(1-\kappa/c_T)^2}N^{-2/9} \tag{3.4.75}$$

whenever $\kappa < c_T$ *and* $\Lambda(m) \leq 1$, *where* c_T *is defined in* (3.4.44).

Proof. We first note that $\Lambda(m) \leq 1$ implies $m \gtrsim 1$. Moreover, from the definition (3.4.49) we have

$$\lambda_{\tilde{s},Q_\mu,K,m,\delta}(\tilde{t}) \leq \left(1 + \frac{N\delta}{2\ell^2 Q_\mu^2}\right)\lambda_{\tilde{s},Q_\mu,K,m,0}(\tilde{t})\,. \tag{3.4.76}$$

Combining this with Lemma 3.4.7 and taking the supremum over $\tilde{s}$, K and $Q_\mu^2 \geq (c_T - \kappa)N^{5/3}\ell^{-2}$, we obtain

$$\tilde{\Lambda}(m,\kappa) - \Lambda(m) \lesssim \frac{1}{m}\inf_{\delta>0}\sup_{Q_\mu^2 \geq (c_T-\kappa)N^{5/3}\ell^{-2}}\left[\frac{N\delta}{\ell^2 Q_\mu^2} + \left(\frac{1}{\ell Q_\mu} + \frac{1}{\delta^{1/2}}\right)\left(1 + \frac{N\delta}{\ell^2 Q_\mu^2} + \frac{1}{\delta \ell Q_\mu} + \frac{N}{\ell^3 Q_\mu^3}\right)\right] \tag{3.4.77}$$

where we also used that $\Lambda(m) \lesssim m^{-1}$ for $m \gtrsim 1$. The supremum over Q_μ is clearly achieved for $Q_\mu^2 = (c_T - \kappa)N^{5/3}\ell^{-2}$. For an upper bound, we shall choose $\delta \sim N^{4/9}$, which yields the desired bound

$$\tilde{\Lambda}(m,\kappa) - \Lambda(m) \lesssim \frac{1}{m}(c_T - \kappa)^{-2}N^{-2/9}\,. \tag{3.4.78}$$

□

3.4.5 Proof of Theorem 3.4.1

Using Prop. 3, Eq. (3.4.46) and Lemma 3.4.8, we get the lower bound

$$\begin{aligned} N^{-1}T^{\text{per}}_{\alpha,\mu,N}(\xi^{\text{per}}) \geq{}& \left(\frac{2m\alpha}{m+1} - \frac{1}{N^{5/3}\ell}\frac{c_L'}{c_T - \kappa}\right)\|\xi^{\text{per}}\|^2 \\ &+ \frac{1}{1-\kappa/c_T}\left(1 - \kappa/c_T - \Lambda(m) - \frac{c_\Lambda N^{-2/9}}{m(1-\kappa/c_T)^2}\right)\left(\frac{2\pi}{\ell}\right)^{3N}\sum_{\vec{q}\in\mathbb{L}^N} L_{\mu,N}(\vec{q})|\xi^{\text{per}}(\vec{q})|^2 \end{aligned} \tag{3.4.79}$$

for any $0 < \kappa < c_T$ and $\mu \geq -\kappa N^{5/3}/\ell^2$. Note that the coefficient in front of the last sum is positive for all $N > N_0(\kappa, m)$, defined in (3.4.2). If α is large enough such that also the first term on the right side of (3.4.79) is non-negative, we conclude that $T^{\text{per}}_{\alpha,\mu,N}(\xi^{\text{per}}) \geq 0$.

In case $2m\alpha < (m+1)c_L'(c_T - \kappa)^{-1}N^{-5/3}\ell^{-1}$, on the other hand, we need to dominate the first term on the right side of (3.4.79) by the second. We use (3.4.44) to obtain the lower bound

$$L_{\mu,N}(\vec{q}) \geq 2\pi^2\left(\frac{2m}{m+1}\right)^{3/2} Q_\mu \geq 2\pi^2\left(\frac{2m}{m+1}\right)^{3/2}\sqrt{\mu + \kappa N^{5/3}\ell^{-2}}\,. \tag{3.4.80}$$

In particular, if we choose

$$\mu = -\kappa N^{5/3}\ell^{-2} + \frac{1}{4\pi^4}\frac{m+1}{2m}\frac{(1-\kappa/c_T)^2[\alpha - (2m)^{-1}(m+1)c_L'(c_T-\kappa)^{-1}N^{-5/3}\ell^{-1}]_-^2}{(1 - \kappa/c_T - \Lambda(m) - c_\Lambda m^{-1}(1-\kappa/c_T)^{-2}N^{-2/9})^2} \tag{3.4.81}$$

we again conclude that $T^{\text{per}}_{\alpha,\mu,N}(\xi^{\text{per}}) \geq 0$.

Note that for our choice of μ, satisfying in particular $\mu \geq -c_T N^{5/3}\ell^{-2}$, we have

$$\int_{B^{N+1}}\left(|\tilde{\nabla}\phi_\mu^{\text{per}}|^2 + \mu|\phi_\mu^{\text{per}}|^2\right) \geq 0 \tag{3.4.82}$$

for all $\phi_\mu^{\rm per} \in H^1_{\rm per}(B^{N+1})$ that are antisymmetric in the last N variables. Hence the positivity of $T^{\rm per}_{\alpha,\mu,N}(\xi^{\rm per})$ implies that $F^{\rm per}_{\alpha,N}(\psi^{\rm per}) \geq -\mu\|\psi^{\rm per}\|^2$. In combination with Lemmas 3.4.3 and 3.4.4, this completes the proof of Theorem 3.4.1. To simplify its statement, we have additionally used that

$$(1-\kappa/c_T)^2[\alpha - (2m)^{-1}(m+1)c_L'(c_T-\kappa)^{-1}N^{-5/3}\ell^{-1}]_-^2 \leq [\alpha - (2m)^{-1}(m+1)c_L' c_T^{-1}\ell^{-1}]_-^2 \quad (3.4.83)$$

for $N \geq 1$, and defined

$$c_L := \frac{m^{**}+1}{2m^{**}}\frac{c_L'}{c_T} \quad (3.4.84)$$

in Eq. (3.4.3), where $m^{**} \approx 0.36$ is chosen such that $m \geq m^{**}$ for $\Lambda(m) \leq 1$. □

3.5 Proof of Theorem 3.2.1

In this section we will give the proof of our main result, Theorem 3.2.1.

Let $B = (0,L)^3$ and $\bar{B} = \bigcup_i^M \bar{B}_i$ a disjoint decomposition into cubes $B_i = (0,\ell)^3 + z_i$ with $z_i \in \mathbb{R}^3$. We will choose ℓ such that $L/\ell \in \mathbb{N}$ in which case $M = (L/\ell)^3$. Let $1/4 > \varepsilon > 0$ and let $\eta \in C_0^\infty(B_\varepsilon(0))$ be non-negative, where we denote by $B_\varepsilon(0)$ the centered ball of radius ε. In the following we will assume that ε is a fixed constant independent of all parameters (for example $\varepsilon = 1/8$ works). For $x \in B$, define

$$J_i(x) = \left(\frac{\int_{B_i}\eta(\ell^{-1}(x-y))\,\mathrm{d}y}{\int_B \eta(\ell^{-1}(x-y))\,\mathrm{d}y}\right)^{1/2}. \quad (3.5.1)$$

Then $\operatorname{supp} J_i \subseteq B_i + B_{\ell\varepsilon}(0)$ and $J_i(x) = 1$ for $x \in \ell(\varepsilon, 1-\varepsilon)^3 + z_i$. Moreover, $\sum_{i=1}^M J_i^2(x) = 1$ for $x \in B$ by construction. The derivative of J_i can be bounded uniformly in i and M by a constant c_η depending only on η (and hence ε) as

$$|\nabla J_i|^2 \leq \frac{c_\eta}{\ell^2}. \quad (3.5.2)$$

Let $\psi \in D(F_{\alpha,N})$ be such that $\operatorname{supp}\psi \subseteq B^{N+1}$ and $\|\psi\|_2 = 1$. We use the IMS formula, Prop. 2, for the quadratic form $F_{\alpha,N}$ to localize the impurity particle (with coordinate x_0). With $J_i\psi$ denoting the function $(J_i\psi)(x_0,\vec{x}) = J_i(x_0)\psi(x_0,\vec{x})$ we obtain

$$F_{\alpha,N}(\psi) = \sum_{i=1}^M F_{\alpha,N}(J_i\psi) - \frac{1}{2m}\sum_{i=1}^M \int |\nabla J_i(x_0)|^2 |\psi(x_0,\vec{x})|^2\,\mathrm{d}x_0\,\mathrm{d}\vec{x}. \quad (3.5.3)$$

We note that the last term is bounded by

$$\sum_{i=1}^M \int |\nabla J_i(x_0)|^2|\psi(x_0,\vec{x})|^2 \leq \frac{c_\eta}{\ell^2}\sum_{i=1}^M \int_{\partial J_i} |\psi(x_0,\vec{x})|^2\,\mathrm{d}x_0\,\mathrm{d}\vec{x} \leq \frac{8c_\eta}{\ell^2} \quad (3.5.4)$$

since $\varepsilon < 1/2$, where $\partial J_i = \operatorname{supp}|\nabla J_i|$. Recall the definition of the mean density, $\rho = NL^{-3}$. We will choose $\ell \sim \rho^{-1/3}$ which means that (3.5.3) is of the order $\rho^{2/3}$.

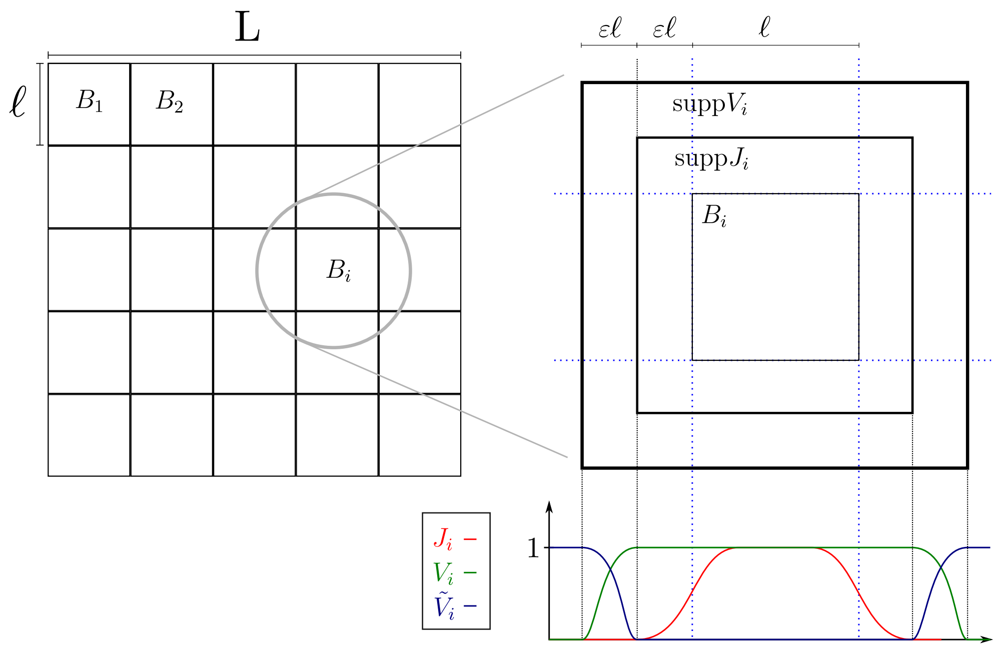

Figure 3.1: A sketch of the setup, the partitions J_i, V_i, $\tilde{V}_i$ and their boxes of support.

In the next step we want to localize the other particles, to be able to distinguish whether they are close to the impurity or far from it. Because we violate the antisymmetry constraint by doing so, we will work with the extended quadratic form $\tilde{F}_{\alpha,N}$ defined in (3.3.4). Let $V \in C_0^\infty(\mathbb{R}^3)$ satisfy $0 \le V \le 1$, with $\operatorname{supp} V \subseteq [-2\varepsilon, 1+2\varepsilon]^3$ and $V(x) = 1$ for $x \in [-\varepsilon, 1+\varepsilon]^3$. We define $V_i(x) = V((x - z_i)/\ell)$ and $\tilde{V}_i(x) := \sqrt{1 - V_i(x)^2}$. Figure 3.1 visualizes this setup.

We localize all the remaining particles using the IMS formula in Prop. 2, with the localization functions

$$(x_1, \dots, x_N) \mapsto \prod_{j\in A} V_i(x_j) \prod_{k\in A^c} \tilde{V}_i(x_k) \tag{3.5.5}$$

for $A \subseteq \{1, \dots, N\}$, where $A^c = \{1, \dots, N\} \setminus A$. For short we define

$$\varphi_{i,A}(x_0, \vec{x}) := J_i(x_0) \prod_{k\in A} V_i(x_k) \prod_{j\in A^c} \tilde{V}_i(x_j)\psi(x_0, \vec{x})\,. \tag{3.5.6}$$

A straightforward calculation using Prop. 2 and the fact that $V_i^2 + \tilde{V}_i^2 = 1$ shows that

$$F_{\alpha,N}(J_i\psi) = \sum_{A\subseteq\{1,\dots,N\}} \left(\tilde{F}_{\alpha,N}\left(\varphi_{i,A}\right) - \frac{1}{2} \sum_{j=1}^{N} \int \left(|\nabla V_i(x_j)|^2 + |\nabla \tilde{V}_i(x_j)|^2 \right) \left|\varphi_{i,A}(x_0, \vec{x})\right|^2 \mathrm{d}x_0 \, \mathrm{d}\vec{x} \right). \tag{3.5.7}$$

Here it is necessary to introduce the extended quadratic form $\tilde{F}_{\alpha,N}$ since the functions $\varphi_{i,A}$ are not antisymmetric in all N variables $(x_1, \dots, x_N)$. They are still separately antisymmetric in the coordinates in A and in the ones in A^c, however.

In the next lemma we will show that the energy $\tilde{F}_{\alpha,N}(\varphi_{i,A})$ splits up into a non-interacting energy for the particles in A^c that are localized away from the impurity, and in a point interacting quadratic form for particles in A.

Lemma 3.5.1. *We define the functions* $\varphi_{i,A}^{\vec{p}_{A^c}} \in L^2(\mathbb{R}^{3(|A|+1)})$ *and* $\varphi_{i,A}^{p_0,\vec{p}_A} \in L^2(\mathbb{R}^{3|A^c|})$ *via their Fourier transforms as*

$$\hat{\varphi}_{i,A}^{\vec{p}_{A^c}}(p_0,\vec{p}_A) = \hat{\varphi}_{i,A}(p_0,\vec{p}) = \hat{\varphi}_{i,A}^{p_0,\vec{p}_A}(\vec{p}_{A^c}) \,. \tag{3.5.8}$$

Then

$$\tilde{F}_{\alpha,N}(\varphi_{i,A}) = \int F_{\alpha,|A|}(\varphi_{i,A}^{\vec{p}_{A^c}})\, \mathrm{d}\vec{p}_{A^c} + \int \left\langle \varphi_{i,A}^{p_0,\vec{p}_A} \middle| -\tfrac{1}{2}\textstyle\sum_{i\in A^c}\Delta_i \middle| \varphi_{i,A}^{p_0,\vec{p}_A} \right\rangle \mathrm{d}\vec{p}_A\, \mathrm{d}p_0 \,. \tag{3.5.9}$$

Proof. We define ξ_j and ϕ_μ for some $\mu > 0$ using the unique decomposition $\varphi_{i,A} = \phi_\mu + \sum_{j=1}^N G_\mu \xi_j$. Corollary 3.3.2 implies that $\xi_j = 0$ for $j \in A^c$. Hence

$$\begin{aligned}\tilde{F}_{\alpha,N}(\varphi_{i,A}) = \int \mathrm{d}\vec{p}_{A^c}\Bigg[&\int |\hat{\phi}_\mu(p_0,\vec{p})|^2 \left(\frac{1}{2m}p_0^2 + \frac{1}{2}\vec{p}^2 + \mu\right) \mathrm{d}\vec{p}_A\, \mathrm{d}p_0 - \mu \int |\hat{\varphi}_{i,A}(p_0,\vec{p})|^2\, \mathrm{d}\vec{p}_A\, \mathrm{d}p_0 \\ &+ \frac{2m}{m+1}\alpha \sum_{i\in A} \int |\hat{\xi}_i(p_i,\hat{p}_i)|^2\, \mathrm{d}\vec{p}_A + \sum_{i\in A}\int L_{\mu,N}(p_i,\hat{p}_i)|\hat{\xi}_i(p_i,\hat{p}_i)|^2\, \mathrm{d}\vec{p}_A \\ &- \sum_{\substack{i,j\in A\\ i\neq j}} \int \frac{\hat{\xi}_i^*(p_0+p_i,\hat{p}_i)\hat{\xi}_j(p_0+p_j,\hat{p}_j)}{\frac{1}{2m}p_0^2 + \frac{1}{2}\vec{p}^2 + \mu}\, \mathrm{d}\vec{p}_A\, \mathrm{d}p_0\Bigg]. \end{aligned} \tag{3.5.10}$$

Following the argumentation in the proof of Lemma 3.4.4 we see that the expression inside the integral over $\vec{p}_{A^c}$ is independent of μ. In particular this allows us to shift $\mu \to \mu - \vec{p}_{A^c}^2/2$ for fixed $\vec{p}_{A^c}$, which gives

$$\begin{aligned}\tilde{F}_{\alpha,N}(\varphi_{i,A}) = \int \mathrm{d}\vec{p}_{A^c}\Bigg[&\int |\hat{\phi}_{\mu-\vec{p}_{A_c}^2/2}(p_0,\vec{p})|^2 \left(\frac{1}{2m}p_0^2 + \frac{1}{2}\vec{p}_A^2 + \mu\right) \mathrm{d}\vec{p}_A\, \mathrm{d}p_0 \\ &- \left(\mu - \frac{\vec{p}_{A^c}^2}{2}\right)\int |\hat{\varphi}_{i,A}(p_0,\vec{p})|^2\, \mathrm{d}\vec{p}_A\, \mathrm{d}p_0 \\ &+ \frac{2m}{m+1}\alpha \sum_{i\in A} \int |\hat{\xi}_i(p_i,\hat{p}_i)|^2\, \mathrm{d}\vec{p}_A + \sum_{i\in A}\int L_{\mu,|A|}(p_i,\vec{p}_{A\setminus\{i\}})|\hat{\xi}_i(p_i,\hat{p}_i)|^2\, \mathrm{d}\vec{p}_A \\ &- \sum_{\substack{i,j\in A\\ i\neq j}} \int \frac{\hat{\xi}_i^*(p_0+p_i,\hat{p}_i)\hat{\xi}_j(p_0+p_j,\hat{p}_j)}{\frac{1}{2m}p_0^2 + \frac{1}{2}\vec{p}_A^2 + \mu}\, \mathrm{d}\vec{p}_A\, \mathrm{d}p_0\Bigg] \end{aligned} \tag{3.5.11}$$

where we used the fact that $L_{\mu-\vec{p}_{A^c}^2/2,N}(p_i,\hat{p}_i) = L_{\mu,|A|}(p_i,\vec{p}_{A\setminus\{i\}})$. The result then follows by noting that the Fourier transform of the regular part of $\varphi_{i,A}^{\vec{p}_{A^c}}$ for fixed $\vec{p}_{A^c}$ is equal to $\hat{\phi}_{\mu-\vec{p}_{A^c}^2}(\,\cdot\,,\vec{p}_{A^c})$, and using the the antisymmetry of $\varphi_{i,A}^{\vec{p}_{A^c}}$. □

We can apply a similar decomposition also to the second term in (3.5.7). For simplicity, let

$$W_i(x) = \frac{1}{2}\left(|\nabla V_i(x)|^2 + |\nabla \tilde{V}_i(x)|^2\right). \tag{3.5.12}$$

Then (3.5.7) and (3.5.9) imply that we can write

$$F_{\alpha,N}(J_i\psi) = \sum_{A\subseteq\{1,\dots,N\}} \|\varphi_{i,A}\|^2 \left[\mathfrak{A}_{i,A} + \mathfrak{B}_{i,A}\right] \tag{3.5.13}$$

where

$$\mathfrak{A}_{i,A} = \|\varphi_{i,A}\|^{-2} \int \left(F_{\alpha,|A|}(\varphi_{i,A}^{\vec{p}_{A^c}}) - \left\langle \varphi_{i,A}^{\vec{p}_{A^c}} \middle| \sum\nolimits_{j\in A} W_i(x_j) \middle| \varphi_{i,A}^{\vec{p}_{A^c}} \right\rangle \right) \mathrm{d}\vec{p}_{A^c} \tag{3.5.14}$$

and

$$\mathfrak{B}_{i,A} = \|\varphi_{i,A}\|^{-2} \int \left\langle \varphi_{i,A}^{p_0,\vec{p}_A} \middle| \sum\nolimits_{j\in A^c} \left(-\tfrac{1}{2}\Delta_j + W_i(x_j)\right) \middle| \varphi_{i,A}^{p_0,\vec{p}_A} \right\rangle \mathrm{d}\vec{p}_A \, \mathrm{d}p_0 \,. \tag{3.5.15}$$

To obtain a lower bound on $\mathfrak{A}_{i,A}$ we can use Theorem 3.4.1, and for the non-interacting part $\mathfrak{B}_{i,A}$ we use the following proposition. We recall that the energy E_n^D on the box $B = (0, L)^3$ was defined in the beginning of Section 3.2 as the ground state energy of the non-interacting Hamiltonian H_0^n with Dirichlet boundary conditions.

Proposition 4. *For $n \in \mathbb{N}$, let $\phi \in H^1_{\mathrm{as}}(\mathbb{R}^{3n})$ be supported in $(0, L)^{3n}$, with $\|\phi\|_2 = 1$, and let $1 \leq i \leq M$. Then*

$$\sum_{j=1}^{n} \int \left(\tfrac{1}{2}|\nabla_j \phi|^2 - W_i(x_j)|\phi|^2\right) \geq E_n^D - const \left(\frac{n^{1/3}}{\ell L} + \ell^{-2} + \frac{n\ell}{L^3}\right). \tag{3.5.16}$$

Proof. The result follows in a straightforward way from Corollary 3.A.4, which is an adaptation of the Lieb-Thirring inequality at positive density derived in [24]. We use that $|\operatorname{supp}(W_i)| \lesssim \ell^3$ and $\|W_i\|_\infty \lesssim \ell^{-2}$. This allows us to bound the right side of (3.A.54) as

$$\int_B \left(\frac{n^{1/3}}{L}|W|^2 + |W|^{5/2} + \frac{n}{L^3}|W| \right) \lesssim \frac{n^{1/3}}{\ell L} + \ell^{-2} + \frac{n\ell}{L^3} \tag{3.5.17}$$

from which the statement readily follows. □

Since $\varphi_{i,A}^{p_0,\vec{p}_A}$ is an antisymmetric function supported in $B^{|A^c|}$, Prop. 4 implies that

$$\left\langle \varphi_{i,A}^{p_0,\vec{p}_A} \middle| \sum\nolimits_{j\in A^c} \left(-\tfrac{1}{2}\Delta_j + W_i(x_j)\right) \middle| \varphi_{i,A}^{p_0,\vec{p}_A} \right\rangle \geq \left(E^D_{|A^c|} - \mathrm{const}\left(\bar{\rho}^{1/3}\ell^{-1} + \ell^{-2} + \bar{\rho}\ell\right)\right) \|\varphi_{i,A}^{p_0,\vec{p}_A}\|^2 \tag{3.5.18}$$

where we used $|A^c| \leq N$ in the error term. To minimize the error we choose $\ell \sim \rho^{-1/3}$. The factor on the right side of (3.5.16) then equals $E^D_{N-|A|} - \mathrm{const}\,\rho^{2/3}$. Because of the condition that $L/\ell \in \mathbb{N}$ we cannot choose ℓ without restriction but it is always possible to choose a value such that $\ell \sim \rho^{-1/3}$. We define e_N to be the N-th eigenvalue of the one-particle Dirichlet Laplacian on $B = (0, L)^3$. Then $E^D_{N-|A|} \geq E^D_N - |A|e_N$. Moreover, we can bound $e_N \lesssim \rho^{2/3}$. In particular,

$$\mathfrak{B}_{i,A} \geq E^D_N - \mathrm{const}\,(|A| + 1)\,\rho^{2/3} \,. \tag{3.5.19}$$

We proceed with a lower bound on $\mathfrak{A}_{i,A}$. Theorem 3.4.1 can be used for a lower bound on $F_{\alpha,|A|}$ only if $|A| > N_0$, with N_0 defined in (3.4.2). In case that $|A| \leq 2N_0$ we use the bound (3.2.2) originating form [50] instead, which implies that

$$F_{\alpha,|A|}(\varphi_{i,A}^{\vec{p}_{A^c}}) \gtrsim -\frac{\alpha_-^2}{(1 - \Lambda(m))^2} \left\| \varphi_{i,A}^{\vec{p}_{A^c}} \right\|^2 \tag{3.5.20}$$

using $m \gtrsim 1$. In combination with $\|W_i\|_\infty \lesssim \bar{\rho}^{2/3}$ this gives the lower bound

$$\mathfrak{A}_{i,A} \gtrsim -\frac{\alpha_-^2}{(1 - \Lambda(m))^2} - |A|\bar{\rho}^{2/3} \tag{3.5.21}$$

and hence

$$\mathfrak{A}_{i,A} + \mathfrak{B}_{i,A} \geq E_N^D - \text{const}\left(\frac{\alpha_-^2}{(1-\Lambda(m))^2} + (N_0+1)\bar{\rho}^{2/3}\right) \tag{3.5.22}$$

in case $|A| \leq 2N_0$.

For $|A| \geq 2N_0$, we use the bound in Theorem 3.4.1 on $F_{\alpha,|A|}(\varphi_{i,A}^{\vec{p}_{A^c}})$. Since $\varphi_{i,A}^{\vec{p}_{A^c}}$ is an $|A|+1$-particle wavefunction supported in a cube of side length $\ell(1+2\varepsilon)$, Theorem 3.4.1 implies that

$$F_{\alpha,|A|}(\varphi_{i,A}^{\vec{p}_{A^c}}) \geq \left(\kappa\frac{|A|^{5/3}}{\ell^2(1+2\varepsilon)^2} - U\right)\|\varphi_{i,A}^{\vec{p}_{A^c}}\|^2 \tag{3.5.23}$$

with

$$U = \frac{1}{4\pi^4}\frac{m+1}{2m}\frac{[\alpha - c_L\ell^{-1}]_-^2}{(1-\kappa/c_T - \Lambda(m))^2(1-2^{-2/9})^2}\,. \tag{3.5.24}$$

In combination with (3.5.19) and $\|W_i\|_\infty \lesssim \bar{\rho}^{2/3}$ this yields the bound

$$\begin{aligned}\mathfrak{A}_{i,A} + \mathfrak{B}_{i,A} &\geq E_N^D + \kappa\frac{|A|^{5/3}}{\ell^2(1+2\varepsilon)^2} - \text{const}\,(|A|+1)\,\rho^{2/3} - U \\ &\geq E_N^D - U - \text{const}\,\kappa^{-3/2}\bar{\rho}^{2/3}\end{aligned} \tag{3.5.25}$$

where we have minimized over $|A|$ in the last step, and used that $\varepsilon \lesssim 1$ and $\ell \sim \bar{\rho}^{-1/3}$.

We are still free to choose κ in such a way as to minimize the error terms. We shall choose $\kappa = c_T\nu(1-\Lambda(m))$ for some $0 < \nu < 1$ (e.g., $\nu = 1/2$). Then $N_0 \lesssim (1-\Lambda(m))^{-9/2}$, and hence (3.5.22) and (3.5.25) together yield the bound

$$\begin{aligned}\mathfrak{A}_{i,A} + \mathfrak{B}_{i,A} &\geq E_N^D - \text{const}\left(\frac{[\alpha - c_L\ell^{-1}]_-^2}{(1-\Lambda(m))^2} + \frac{\rho^{2/3}}{(1-\Lambda(m))^{9/2}}\right) \\ &\geq E_N^D - \text{const}\left(\frac{\alpha_-^2}{(1-\Lambda(m))^2} + \frac{\rho^{2/3}}{(1-\Lambda(m))^{9/2}}\right)\end{aligned} \tag{3.5.26}$$

which is valid for all $A \subset \{1,\ldots,N\}$. In combination with (3.5.3), (3.5.4) and (3.5.13), this completes the proof of Theorem 3.2.1. □

Appendices

3.A Lieb-Thirring inequality in a box

In this appendix we will follow the analysis of [24] to show a positive density Lieb-Thirring inequality for a system of non-interacting fermions in a box with Dirichlet boundary conditions. When reformulated via a Legendre transformation as a bound on the difference between the ground state energies with and without an external potential, we will see that this inequality in particular implies Prop. 4.

Let $C_L = [-L/2, L/2]^3$ be the cube in $\mathbb{R}^3$ and let $\Pi^-_{L,\mu} := \mathbb{1}(-\Delta_L \leq \mu)$, where Δ_L denotes the Dirichlet Laplacian on C_L. For short we will just write Π^- for $\Pi^-_{L,\mu}$, and $\Pi^+ = 1 - \Pi^-$. For a density matrix γ we denote the corresponding density by ρ_γ. Of particular relevance for us is the density corresponding to Π^-, which we denote by ρ_0. Differently to the case of periodic boundary conditions (discussed in [24]), ρ_0 is not a constant and is given by

$$\rho_0(x) = \sum_{\substack{p \in \pi\mathbb{N}^3/L \\ p^2 \leq \mu}} |\phi_p(x)|^2 \tag{3.A.1}$$

where ϕ_p are the eigenvectors of $-\Delta_L$ to the eigenvalues p^2, i.e.,

$$\phi_p(x) = \left(\frac{2}{L}\right)^{3/2} \prod_{j=1}^{3} \cos(p_j x_j) \tag{3.A.2}$$

for $x = (x_1, x_2, x_3) \in \mathbb{R}^3$. Since the absolute value of each eigenvector is pointwise bounded by $(2/L)^{3/2}$ we have

$$\rho_0(x) \leq \left(\frac{2}{L}\right)^3 \sum_{\substack{p \in \pi\mathbb{N}^3/L \\ p^2 \leq \mu}} 1 \leq \left(\frac{2}{L}\right)^3 \frac{4\pi}{3} \frac{\mu^{3/2} L^3}{\pi^3} = \frac{2^5 \mu^{3/2}}{3\pi^2}\,. \tag{3.A.3}$$

Remark. *Since the lowest eigenvalue of $-\Delta_L$ equals $3\pi^2 L^{-2}$, the problem simplifies for $\mu < 3\pi^2 L^{-2}$ since the projections $\Pi^\pm_{L,\mu}$ become trivial. In this case we can simply apply the original Lieb-Thirring inequality [31] to obtain the desired bound. For our application we shall need $\mu \gg L^{-2}$, however, hence we shall restrict our attention to $\mu \geq 3\pi^2 L^{-2}$ in the following theorem.*

For a real number t we denote its positive part by t_+ and its negative part by t_-. In particular, $t = t_+ - t_-$.

Theorem 3.A.1. *Let $\mu \geq 3\pi^2 L^{-2}$. Let Q be a self-adjoint operator of finite rank satisfying $-\Pi^-_{L,\mu} \leq Q \leq 1 - \Pi^-_{L,\mu}$, with density ρ_Q. There exist positive constants $\tilde{K}$ and η independent of μ, L and Q such that*

$$\operatorname{tr}(-\Delta_L - \mu)Q \geq \tilde{K} \int_{C_L} S\left((|\rho_Q(x)| - \eta L^{-1}\mu)_+\right) \mathrm{d}x \tag{3.A.4}$$

with

$$S(\rho) := (\mu^{3/2} + \rho)^{5/3} - \mu^{5/2} - \frac{5}{3}\mu\rho\,. \tag{3.A.5}$$

Remark. *In [24] a similar result was proven for the Laplacian with periodic boundary conditions and we mostly follow that proof.*

Remark. *The crucial properties of the function S are its positivity and the fact that $S(\rho)$ behaves like $\mu^{-1/2}\rho^2$ for small ρ and like $\rho^{5/3}$ for large ρ. For technical reasons it will also be convenient that S is convex.*

Essential for the proof will be to separate a given Q into $Q = (\Pi^+ + \Pi^-)Q(\Pi^+ + \Pi^-) =: Q^{++} + Q^{+-} + Q^{-+} + Q^{--}$. The densities associated to $Q^{\pm\pm}$ will be denoted by $\rho^{\pm\pm}$. Before we proceed with the proof of the theorem we show the following Lemma.

Lemma 3.A.2. *Assume $\Pi^- \leq Q \leq 1 - \Pi^-$. Then*

$$\operatorname{tr}\left(| - \Delta_L - \mu|Q^2\right) \leq \operatorname{tr}(-\Delta_L - \mu)Q\,. \tag{3.A.6}$$

Proof. We claim that $Q^2 \leq Q^{++} - Q^{--}$, which follows from the condition on Q. In fact,

$$-\Pi^- \leq Q \leq 1 - \Pi^- \;\Rightarrow\; 0 \leq Q + \Pi^- \leq 1 \;\Rightarrow\; (Q + \Pi^-)^2 \leq Q + \Pi^-\,. \tag{3.A.7}$$

Expanding the last inequality proves the claim. Hence

$$\begin{aligned} \operatorname{tr}(|\Delta_L + \mu|Q^2) &\leq \operatorname{tr}(|\Delta_L + \mu|Q^{++}) - \operatorname{tr}(|\Delta_L + \mu|Q^{--}) \\ &= \operatorname{tr}((-\Delta_L - \mu)Q^{++}) + \operatorname{tr}((-\Delta_L - \mu)Q^{--}) = \operatorname{tr}((-\Delta_L - \mu)Q)\,. \end{aligned} \tag{3.A.8}$$

□

Proof of Theorem 3.A.1. We shall treat $Q^{\pm\pm}$ separately and combine the various terms at the end using the convexity of S.

Part 1. Q^{++}, Q^{--}

We shall follow the method introduced by Rumin in [58]. With the aid of the spectral projections $P_e := \mathbb{1}(|\Delta_L + \mu| \geq e)$ we have the layer cake representation

$$|\Delta_L + \mu| = \int_0^\infty P_e \,\mathrm{d}e\,. \tag{3.A.9}$$

Let us assume that γ is a smooth enough finite rank operator with $0 \leq \gamma \leq 1$. Then

$$\operatorname{tr}|\Delta_L + \mu|\gamma = \int_0^\infty \mathrm{d}e\; \operatorname{tr}(P_e\gamma P_e) = \int_0^\infty \mathrm{d}e \int_{C_L} \rho_e(x)\,\mathrm{d}x \tag{3.A.10}$$

where ρ_e denotes the density of the finite rank operator $P_e\gamma P_e$. For a bounded measurable set A we estimate

$$\begin{aligned}\int_A \rho_e(x)\,\mathrm{d}x &= \operatorname{tr}(\mathbb{1}_A P_e\gamma P_e) = \left\|\mathbb{1}_A P_e \gamma^{1/2}\right\|_{\mathfrak{S}_2}^2 \\ &\geq \left(\left\|\mathbb{1}_A\gamma^{1/2}\right\|_{\mathfrak{S}_2} - \left\|\mathbb{1}_A P_e^\perp \gamma^{1/2}\right\|_{\mathfrak{S}_2}\right)_+^2 \\ &= \left(\left(\int_A \rho_\gamma\right)^{1/2} - \left\|\mathbb{1}_A P_e^\perp\gamma^{1/2}\right\|_{\mathfrak{S}_2}\right)_+^2 \end{aligned} \tag{3.A.11}$$

where ρ_γ denotes the density of γ and we used the triangle inequality for the Hilbert-Schmidt norm $\|\cdot\|_{\mathfrak{S}_2}$. Because $\|\gamma\| \leq 1$ we further get

$$\left\|\mathbb{1}_A P_e^\perp \gamma^{1/2}\right\|_{\mathfrak{S}_2}^2 = \operatorname{tr}(\mathbb{1}_A P_e^\perp \gamma P_e^\perp \mathbb{1}_A) \leq \left\|\mathbb{1}_A P_e^\perp\right\|_{\mathfrak{S}_2}^2 \|\gamma\| \leq |A| f(e) \tag{3.A.12}$$

with

$$\begin{aligned} f(e) &:= \left(\frac{2}{L}\right)^3 \sum_{\substack{p\in\pi\mathbb{N}^3/L \\ |p^2-\mu|<e}} 1 = \left(\frac{2}{L}\right)^3 \sum_{\substack{n\in\mathbb{N}^3/2 \\ |\frac{4\pi^2}{L^2}n^2-\mu|<e}} 1 \\ &= \left(\frac{2}{L}\right)^3 \left[\left|\mathbb{N}^3/2 \cap B\left(\frac{L}{2\pi}(\mu+e)^{1/2}\right)\right| - \left|\mathbb{N}^3/2\cap \bar{B}\left(\frac{L}{2\pi}(\mu-e)_+^{1/2}\right)\right|\right] \end{aligned} \tag{3.A.13}$$

where $B(R)$ denotes the centered open ball with radius R and $\bar{B}(R)$ its closure. Here we used

$$\left\|\mathbb{1}_A P_e^\perp\right\|_{\mathfrak{S}_2}^2 = \sum_{\substack{p\in\pi\mathbb{N}^3/L \\ |p^2-\mu|<e}} \int_A |\phi_p(x)|^2\,\mathrm{d}x \leq |A| \sum_{\substack{p\in\pi\mathbb{N}^3/L \\ |p^2-\mu|<e}} \sup_{x\in A} |\phi_p(x)|^2 \leq |A| f(e) \tag{3.A.14}$$

where we bounded the eigenfunction ϕ_p of $-\Delta_L$ to the eigenvalue p^2 by $|\phi_p(x)| \leq (2/L)^{3/2}$. Taking $A = B(R) + x$ with $R \to 0$ we obtain the pointwise bound

$$\rho_e(x) \geq (\sqrt{\rho_\gamma(x)} - \sqrt{f(e)})_+^2\,. \tag{3.A.15}$$

Hence we get

$$\operatorname{tr}|\Delta_L + \mu|\gamma \geq \int_{C_L} \mathrm{d}x \int_0^\infty \mathrm{d}e(\sqrt{\rho_\gamma(x)} - \sqrt{f(e)})_+^2 = \int_{C_L} R(\rho_\gamma(x))\,\mathrm{d}x \tag{3.A.16}$$

with

$$R(\rho) := \int_0^\infty \left(\sqrt{\rho} - \sqrt{f(e)}\right)_+^2 \mathrm{d}e\,. \tag{3.A.17}$$

To obtain the desired result we have to analyze $R(\rho)$ in more detail. In the following we will use C to denote a generic constant, whose value can change throughout the computation. Obviously

$$\left|\left|\mathbb{N}^3/2 \cap B(R)\right| - \frac{4\pi}{3}R^3\right| \lesssim \max(1, R^2) \tag{3.A.18}$$

and the same statement holds if one takes the closure $\bar{B}(R)$ instead of $B(R)$. For $0 < x < 1$ and $M > 0$, (3.A.18) allows us to bound

$$\begin{aligned}&|\mathbb{N}^3/2 \cap B(M(1+x)^{1/2})| - |\mathbb{N}^3/2 \cap \bar{B}(M(1-x)^{1/2})| \\ &\leq \frac{4\pi M^3}{3}\left((1+x)^{3/2} - (1-x)_+^{3/2}\right) + C\max(1, M^2) \\ &\lesssim M^3 x + \max(1, M^2)\,, \end{aligned} \tag{3.A.19}$$

where we used $(1+x)^{3/2} - (1-x)_+^{3/2} \lesssim x$. Applying (3.A.19) to $f(e)$ for $e/\mu < 1$ we get

$$f(e) \lesssim \mu^{1/2} e + \frac{\mu}{L} \tag{3.A.20}$$

using that $\mu \gtrsim L^{-2}$ by assumption. For $e \geq \mu$ we get

$$f(e) = \left(\frac{2}{L}\right)^3 \left|\mathbb{N}^3/2 \cap B\left(\frac{L}{2\pi}(\mu+e)^{1/2}\right)\right| \leq \frac{C}{L^3}\left(L^3(\mu+e)^{3/2}\right) \leq Ce^{3/2}\,. \tag{3.A.21}$$

Combining both statements we have thus shown that

$$f(e) \leq C\left(\frac{\mu}{L} + \mu^{1/2} e \mathbb{1}(e \leq \mu) + e^{3/2}\mathbb{1}(e > \mu)\right) = u + g(e) \tag{3.A.22}$$

with

$$g(e) := Ce\max(\mu^{1/2}, e^{1/2})\,, \quad u := C\frac{\mu}{L}\,. \tag{3.A.23}$$

Using the explicit form of g, one readily checks that

$$R(\rho) = \int_0^\infty \left(\sqrt{\rho} - \sqrt{f(e)}\right)_+^2 \mathrm{d}e \geq \int_0^\infty \left(\sqrt{\rho} - \sqrt{u} - \sqrt{g(e)}\right)_+^2 \mathrm{d}e \gtrsim S((\rho - 2u)_+)\,, \tag{3.A.24}$$

where we have also used that $(\sqrt{\rho} - \sqrt{u})_+^2 \geq \frac{1}{2}(\rho - 2u)_+$. In combination with (3.A.16), this shows that

$$\operatorname{tr}|-\Delta_L - \mu|\gamma \gtrsim \int_{C_L} S((\rho_\gamma(x) - CL^{-1}\mu)_+)\,\mathrm{d}x\,. \tag{3.A.25}$$

We apply this for $\gamma = Q^{++}$ and $\gamma = -Q^{--}$ and obtain

$$\operatorname{tr}(-\Delta_L - \mu)Q^{\pm\pm} \gtrsim \int_{C_L} S\left((|\rho^{\pm\pm}(x)| - CL^{-1}\mu)_+\right)\mathrm{d}x\,. \tag{3.A.26}$$

Part 2. Q^{+-}, Q^{-+}

In the next step we want to prove bounds for Q^{+-} and Q^{-+}. We introduce

$$\begin{aligned}\Pi_0^+ &= \mathbb{1}(\mu < -\Delta_L < \mu + \sqrt{\mu}/L) & \Pi_0^- &= \mathbb{1}(\mu - \sqrt{\mu}/L \leq -\Delta_L \leq \mu) \\ \Pi_1^+ &= \mathbb{1}(\mu + \sqrt{\mu}/L \leq -\Delta_L) & \Pi_1^- &= \mathbb{1}(-\Delta_L < \mu - \sqrt{\mu}/L)\end{aligned} \tag{3.A.27}$$

and split $Q^{+-} = (\Pi_0^+ + \Pi_1^+)Q(\Pi_0^- + \Pi_1^-) = Q_{00}^{+-} + Q_{10}^{+-} + Q_{01}^{+-} + Q_{11}^{+-}$. The following three parts of the proof will treat these terms. We start with $Q_{00}^{\pm}$.

Part 3. Q_{00}^{+-}

The density of Q_{00}^{+-} is equal to

$$\rho_{00}^{+-}(x) = \sum_{\substack{k\in(\pi\mathbb{N}/L)^3 \\ \mu<k^2<\mu+\sqrt{\mu}/L}} \sum_{\substack{j\in(\pi\mathbb{N}/L)^3 \\ \mu-\sqrt{\mu}/L\le j^2\le\mu}} \langle\phi_k|Q\phi_j\rangle\phi_k(x)\phi_j(x)\,. \tag{3.A.28}$$

Using $\|Q\| \le 1$, we can bound this as

$$\begin{aligned} |\rho_{00}^{+-}(x)| &\le \Big(\sum_{\substack{k\in(\pi\mathbb{N}/L)^3 \\ \mu<k^2<\mu+\sqrt{\mu}/L}} |\phi_k(x)|^2\Big)^{1/2} \Big(\sum_{\substack{j\in(\pi\mathbb{N}/L)^3 \\ \mu-\sqrt{\mu}/L\le j^2\le\mu}} |\phi_j(x)|^2\Big)^{1/2} \\ &\le \left(\frac{2}{L}\right)^3 \sqrt{|\{\mu \le k^2 \le \mu + \sqrt{\mu}/L\}|}\sqrt{|\{\mu - \sqrt{\mu}/L \le j^2 \le \mu\}|} \le C\frac{\mu}{L} \end{aligned} \tag{3.A.29}$$

where we applied (3.A.19) in the last step.

Part 4. Q_{10}^{+-}, Q_{01}^{+-}

Next we will bound ρ_{10}^{+-}. For a general function W (viewed as a multiplication operator), we have

$$\begin{aligned} |\operatorname{tr}(WQ_{10}^{+-})| &= \left|\operatorname{tr}\left(\Pi_0^- W \frac{\Pi_1^+}{|-\Delta_L-\mu|^{1/2}}|-\Delta_L-\mu|^{1/2}Q\right)\right| \\ &\le \sqrt{\operatorname{tr}|-\Delta_L-\mu|Q^2}\left\|\Pi_0^- W\frac{\Pi_1^+}{|-\Delta_L-\mu|^{1/2}}\right\|_{\mathfrak{S}^2}\,. \end{aligned} \tag{3.A.30}$$

To bound the first factor, we can used Lemma 3.A.2. For the second term we need to use the specific form of the eigenfunctions for the Dirichlet Laplacian. Using (3.A.2) we get

$$|\langle\phi_p|W\phi_q\rangle|^2 = \left(\frac{1}{2L}\right)^6 \left|\sum_{A,B\in\{1,-1\}^3} \hat{W}((A_jp_j)_j - (B_jq_j)_j)\right|^2 \lesssim L^{-6}\sum_{A,B\in\{1,-1\}^3} |\hat{W}((A_jp_j)_j-(B_jq_j)_j)|^2 \tag{3.A.31}$$

where $(A_jp_j)_j$ and $(B_jq_j)_j$ denote the vectors obtained by component-wise multiplication. Hence

$$\begin{aligned} \left\|\Pi_0^- W\frac{\Pi_1^+}{|-\Delta_L-\mu|^{1/2}}\right\|_{\mathfrak{S}^2}^2 &= \sum_{\substack{p,q\in(\pi\mathbb{N}/L)^3 \\ \mu-\sqrt{\mu}/L\le p^2\le\mu \\ q^2>\mu+\sqrt{\mu}/L}} \frac{|\langle\phi_p|W\phi_q\rangle|^2}{q^2-\mu} \le \frac{L}{\sqrt{\mu}} \sum_{\substack{p,q\in(\pi\mathbb{N}/L)^3 \\ \mu-\sqrt{\mu}/L\le p^2\le\mu \\ q^2>\mu+\sqrt{\mu}/L}} |\langle\phi_p|W\phi_q\rangle|^2 \\ &\lesssim \frac{1}{L^6}\frac{L}{\sqrt{\mu}} \sum_{\substack{p,q\in(\pi(\mathbb{Z}\setminus\{0\})/L)^3 \\ \mu-\sqrt{\mu}/L\le p^2\le\mu \\ q^2>\mu+\sqrt{\mu}/L}} |\hat{W}(p-q)|^2 \\ &\lesssim \frac{1}{L^6}\frac{L}{\sqrt{\mu}} \sum_{q\in(\pi(\mathbb{Z}\setminus\{0\})/L)^3} |\hat{W}(q)|^2 \sum_{\mu-\sqrt{\mu}/L\le p^2\le\mu} 1 \lesssim \sqrt{\mu}\,\|W\|_2^2\,. \end{aligned} \tag{3.A.32}$$

The sum of (3.A.31) is included in the second line of the previous calculation by extending the sum over $p, q \in \mathbb{N}^3$ to $p, q \in (\mathbb{Z} \setminus \{0\})^3$, and we have again used (3.A.19) in the last step.

Choosing for $W = (\rho_{10}^{+-})^*$ we thus get from (3.A.30)

$$\int_{C_L} |\rho_{10}^{+-}|^2 \leq C\mu^{1/2} \operatorname{tr}(-\Delta_L - \mu)Q\,. \tag{3.A.33}$$

In a similar way we can treat ρ_{01}^{+-} with the result that also

$$\int_{C_L} |\rho_{01}^{+-}|^2 \leq C\mu^{1/2} \operatorname{tr}(-\Delta_L - \mu)Q\,. \tag{3.A.34}$$

Part 5. Q_{11}^{+-}

Similarly to above we again introduce a multiplication operator W, and estimate

$$\left|\operatorname{tr}(W\Pi_1^+ Q\Pi_1^-)\right| \leq \left\| \frac{\Pi_1^+}{|\Delta_L + \mu|^{1/4}} W \frac{\Pi_1^-}{|\Delta_L + \mu|^{1/4}} \right\|_{\mathfrak{S}^2} \left\| |\Delta_L + \mu|^{1/4} Q |\Delta_L + \mu|^{1/4} \right\|_{\mathfrak{S}^2}\,. \tag{3.A.35}$$

The second factor we bound by

$$\left\| |\Delta_L + \mu|^{1/4} Q |\Delta_L + \mu|^{1/4} \right\|_{\mathfrak{S}^2} \leq \left\| |\Delta_L + \mu|^{1/2} Q \right\|_{\mathfrak{S}^2} = \operatorname{tr}(|\Delta_L + \mu| Q^2)^{1/2} \tag{3.A.36}$$

and Lemma 3.A.2. For the first one, we have

$$\begin{aligned} \left\| \frac{\Pi_1^+}{|\Delta_L + \mu|^{1/4}} W \frac{\Pi_1^-}{|\Delta_L + \mu|^{1/4}} \right\|_{\mathfrak{S}^2}^2 &= \sum_{\substack{p,q \in (\pi\mathbb{N}^3/L) \\ p^2 > \mu + \sqrt{\mu}/L \\ q^2 < \mu - \sqrt{\mu}/L}} \frac{|\langle \phi_p | W \phi_q \rangle|^2}{(\mu - q^2)^{1/2}(p^2 - \mu)^{1/2}} \\ \leq \frac{C}{L^6} \sum_{\substack{p,q \in (\pi\mathbb{Z}^3/L) \\ p^2 > \mu + \sqrt{\mu}/L \\ q^2 < \mu - \sqrt{\mu}/L}} \frac{|\hat{W}(q-p)|^2}{(\mu - q^2)^{1/2}(p^2 - \mu)^{1/2}} &= \frac{C}{L^3} \sum_{k \in (\pi\mathbb{Z}^3/L)} \Phi(k) |\hat{W}(k)|^2 \leq C \sup_k \Phi(k) \, \|W\|_2^2 \end{aligned} \tag{3.A.37}$$

with

$$\Phi(k) = \frac{1}{L^3} \sum_{\substack{q \in (\pi\mathbb{Z}^3/L) \\ (q-k)^2 > \mu + \sqrt{\mu}/L \\ q^2 < \mu - \sqrt{\mu}/L}} \frac{1}{(\mu - q^2)^{1/2}((q-k)^2 - \mu)^{1/2}}\,. \tag{3.A.38}$$

In [24, Proof of Thm. 5.1] it was shown that $\sup_k \Phi(k) \lesssim \mu^{1/2}$ for $\mu \gtrsim L^{-2}$. Hence the choice $W = (\rho_{11}^{+-})^*$ yields

$$\int_{C_L} |\rho_{11}^{+-}|^2 \lesssim \mu^{1/2} \operatorname{tr}((-\Delta_L - \mu)Q)\,. \tag{3.A.39}$$

Part 6. *Combining the above estimates*

By combining (3.A.34) and (3.A.39) we obtain

$$\mu^{-1/2} \int_{C_L} |\rho^{+-} - \rho_{00}^{+-}|^2 \leq C \operatorname{tr}(-\Delta_L - \mu)Q\,. \tag{3.A.40}$$

Using that $|\rho_{00}^{+-}| \leq C\mu/L$, as shown in (3.A.29), this further implies that

$$\mu^{-1/2} \int_{C_L} (|\rho^{+-}| - C\mu/L)_+^2 \leq C \operatorname{tr}(-\Delta_L - \mu)Q\,. \tag{3.A.41}$$

The integrand in the left side is bounded from below by $CS((|\rho^{+-}|-C\mu/L)_+)$, hence

$$\int_{C_L} S\left((|\rho^{+-}|-C\mu/L)_+\right) \le C\,\mathrm{tr}(-\Delta_L-\mu)Q\,. \tag{3.A.42}$$

Since $|\rho^{+-}| = |\rho^{-+}|$, the same bound holds for ρ^{-+} as well. Combining (3.A.26) and (3.A.42) and using the convexity of S we get

$$\begin{aligned}\mathrm{tr}(-\Delta_L-\mu)Q &\gtrsim \int_{C_L} S\left(\frac{(|\rho^{++}|+|\rho^{--}|+|\rho^{+-}|+|\rho^{-+}|-C\mu/L)_+}{4}\right)\\ &\ge \int_{C_L} S\left(\frac{(|\rho_Q|-C\mu/L)_+}{4}\right) \gtrsim \int_{C_L} S\left((|\rho_Q|-C\mu/L)_+\right). \end{aligned}\tag{3.A.43}$$

This completes the proof of Theorem 3.A.1. □

By taking a Legendre transform, the result above implies that following potential version of the Lieb-Thirring inequality.

Theorem 3.A.3. *Assume that V is a real-valued function in $L^{5/2}([-L/2,-L/2]^3)$, and $\mu \ge 3\pi^2L^{-2}$. Then we have*

$$\begin{aligned}0 &\ge -\mathrm{tr}(-\Delta_L+V-\mu)_- + \mathrm{tr}(-\Delta_L-\mu)_- - \int_{C_L}\rho_0 V\\ &\ge -K\int_{C_L}\left(\mu^{1/2}|V|^2+|V|^{5/2}+L^{-1}\mu|V|\right)\end{aligned}\tag{3.A.44}$$

with $K>0$ independent of L,μ and V.

Remark. *In case that $\mu < 3\pi^2L^{-2}$ we have $-\Delta_L-\mu>0$, and therefore* $\mathrm{tr}(-\Delta_L-\mu)_- = 0$ *and also $\rho_0 = 0$. One can thus obtain a lower bound using the standard Lieb-Thirring inequality [31] applied to a potential $V-\mu$ in this case.*

Proof. We start with the identity

$$-\mathrm{tr}(A+B)_- = \inf_{0\le\gamma\le1}\mathrm{tr}(A+B)\gamma \tag{3.A.45}$$

for hermitian matrices A and B, where an optimizer is clearly $\mathbb{1}(A+B\le0)$. With $P^- = \mathbb{1}(A\le0)$ and $Q=\gamma-P^-$, (3.A.45) reads

$$-\mathrm{tr}(A+B)_- = \inf_{-P^-\le Q\le 1-P^-}\mathrm{tr}(A+B)Q+\mathrm{tr}(A+B)P^-\,. \tag{3.A.46}$$

Defining $P_B^- = \mathbb{1}(A+B\le0)$ we equivalently get

$$\mathrm{tr}(A+B)(P_B^- - P^-) = \inf_{-P^-\le Q\le1-P^-}\mathrm{tr}(A+B)Q\,. \tag{3.A.47}$$

This equality can be extended to allow $A=-\Delta-\mu$ and $B=V$ (see [24, Thm 4.1]). Using this and applying Theorem 3.A.1 we get

$$\begin{aligned}\mathrm{tr}(-\Delta_L-\mu)_- - \mathrm{tr}(-\Delta_L+V-\mu)_- - \int_{C_L}\rho_0V &\ge \inf_\rho\left(\tilde K\int_{C_L}S((|\rho|-\eta L^{-1}\mu)_+)+\int_{C_L}V\rho\right)\\ &\ge \inf_{\rho\ge0}\left(\tilde K\int_{C_L}S((\rho-\eta L^{-1}\mu)_+)-\int_{C_L}|V|\rho\right)\end{aligned}\tag{3.A.48}$$

where the infimum in the first line is over functions $\rho : \mathbb{R}^3 \to \mathbb{R}$, while in the second we can restrict to non-negative functions ρ. We can pull the infimum inside the integral for a lower bound. Clearly we can assume that $\rho \geq \eta L^{-1}\mu$. Introducing $\gamma = \rho - \eta L^{-1}\mu$ we have

$$\inf_{\gamma\geq 0}\left(\tilde{K}S(\gamma) - |V|\gamma - \eta L^{-1}\mu|V|\right) = \tilde{K}\left(\frac{2}{3}\mu^{5/2} + \tilde{K}^{-1}|V|\mu^{3/2} - \frac{2}{3}\left(\mu + \tilde{K}^{-1}\frac{3|V|}{5}\right)^{5/2}\right) - \eta L^{-1}\mu|V| . \tag{3.A.49}$$

Using that

$$x^{5/2} + \frac{5}{2}x^{3/2}y - (x+y)^{5/2} \geq -\frac{15\sqrt{x}y^2}{8} - y^{5/2} \tag{3.A.50}$$

for $x = \mu$ and $y = 3\tilde{K}^{-1}|V|/5$ gives the bound

$$(3.A.49) \gtrsim -\mu^{1/2}|V|^2 - |V|^{5/2} - L^{-1}\mu|V| . \tag{3.A.51}$$

Plugging this into (3.A.48) proves the Theorem. □

We apply the above theorem for a potential $V \in L^{5/2}(C_L)$ with $V \leq 0$, choosing μ as e_N, the Nth eigenvalue of the Dirichlet Laplacian $-\Delta_L$. In particular, $\mu \geq e_1 = 3\pi^2 L^{-2}$ which allows us to use Theorem 3.A.3. The ground state energy E_N^D for N non-interacting particles confined to C_L was defined in the beginning of Section 3.2 and can be written as $E_N^D = \sum_{i=1}^N e_i$.

We denote by e_k^V the kth eigenvalue of $-\Delta_L + V$, and by $E_N^{V,D}$ the sum of the lowest N eigenvalues of $-\Delta_L + V$, i.e., $E_N^{V,D} = \sum_{i=1}^N e_i^V$. Theorem 3.A.3 implies that

$$\mathrm{tr}(-\Delta_L - \mu)_- = -E_N^D + Ne_N \geq \mathrm{tr}(-\Delta_L + V - e_N)_- - R \geq -E_N^{V,D} + Ne_N - R \tag{3.A.52}$$

with

$$R = \mathrm{const}\int_{C_L}\left(\mu^{1/2}|V|^2 + |V|^{5/2} + L^{-1}\mu|V|\right) - \int_{C_L}\rho_0 V . \tag{3.A.53}$$

We used that since $V \leq 0$ the operator $-\Delta_L + V - e_N$ has at least N non-positive eigenvalues, and therefore we can get a lower bound on the trace of its negative part by summing only the first N of them.

From the above calculation, together with $\rho_0 \lesssim \mu^{3/2}$ and $\mu = e_N \lesssim N^{2/3}/L^2$, we deduce the following corollary.

Corollary 3.A.4. *Let $V \in L^{5/2}(C_L)$ with $V \leq 0$ and let E_N^D denote the ground state energy of N non-interacting fermions confined to C_L. With $E_N^{V,D}$ we denote the ground state energy of the corresponding Hamiltonian with external potential V. Then*

$$E_N^D - E_N^{V,D} \lesssim \int_{C_L}\left(\frac{N^{1/3}}{L}|V|^2 + |V|^{5/2} + \frac{N}{L^3}|V|\right) . \tag{3.A.54}$$

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CHAPTER 4

Stability of the $2+2$ fermionic system with point interactions

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Abstract

We give a lower bound on the ground state energy of a system of two fermions of one species interacting with two fermions of another species via point interactions. We show that there is a critical mass ratio $m_2 \approx 0.58$ such that the system is stable, i.e., the energy is bounded from below, for $m \in [m_2, m_2^{-1}]$. So far it was not known whether this $2+2$ system exhibits a stable region at all or whether the formation of four-body bound states causes an unbounded spectrum for all mass ratios, similar to the Thomas effect. Our result gives further evidence for the stability of the more general $N+M$ system.

4.1 Introduction

Systems of particles interacting via point interactions are frequently used in physics to model short range forces. In these models the shape of the interaction potential enters only via the scattering length. Originally point interactions were introduced in the 1930s to model nuclear interactions [5, 6, 19, 68, 72], and later they were also successfully applied to other areas of physics like polarons (see [40] and references there) or cold atomic gases [74].

Given $N \geq 1$ fermions of one type with mass $1/2$ and $M \geq 1$ fermions of another type with mass $m/2 > 0$, point interaction models give a meaning to the formal expression

$$-\sum_{i=1}^{N} \Delta_{x_i} - \frac{1}{m} \sum_{j=1}^{M} \Delta_{y_j} + \gamma \sum_{i=1}^{N} \sum_{j=1}^{M} \delta(x_i - y_j) \tag{4.1.1}$$

for $\gamma \in \mathbb{R}$. Because of the existence of discontinuous functions in $H^1(\mathbb{R}^n)$ for $n \geq 2$, this expression is ill-defined in dimensions larger than one. In the following we restrict our attention to the three-dimensional case but we note that the system also exhibits interesting behavior in two dimensions [15, 16, 28].

A mathematically precise version of (4.1.1) in three dimensions was constructed in [15, 20] and we will work here with the model introduced there. We note that even though these models are mathematically well-defined it is not established whether they can be obtained as a limit of genuine Schrödinger operators with interaction potentials of shrinking support. (See, however, [1] for the case $N = M = 1$, and [3] for models in one dimension.)

It was already known to Thomas [68] that systems with point interactions are inherently unstable for bosons, in the sense that the energy is not bounded from below, if there are at least three particles involved. It turns out that in the case that the particles are fermions the question of stability is more delicate as it depends on the mass ratio of the two species, in general.

The case $N = M = 1$ is completely understood as it reduces to a one particle problem [1]. In this case there exists a one-parameter family of Hamiltonians describing point interactions parameterized by the inverse scattering length, and they are bounded from below for all masses.

Beside this trivial case also the $2 + 1$ case (i.e., $N = 2$ and $M = 1$), where the two particles of the same species are fermions, is well understood [4, 11–13, 15, 45–48, 59]. There is a critical mass ratio $m^* \approx 0.0735$ such that the system is unstable for $m < m^*$ and stable otherwise. It is remarkable that this critical mass ratio does not depend on the strength of the interaction, i.e., the scattering length. Recently in [4] the spectrum of the $2 + 1$ system was discussed in more detail. Moreover, it was shown in [12, 47] that in a certain mass range other models describing point interactions can be constructed.

For larger systems of fermions even the question of stability is generally open. In [50] the stability result for the $2 + 1$ case was recently extended to the general $N + 1$ problem ($N \geq 2$ and $M = 1$). In particular it was shown that there exists a critical mass $m_1 \approx 0.36$ such that the system's energy is bounded from below, uniformly in N, for $m \geq m_1$. As a consequence of the $2 + 1$ case this $N + 1$ system is unstable for $m < m^*$, but the behavior for $m \in [m^*, m_1)$ is unknown.

By separating particles one can obtain an upper bound on the ground state energy of the general $N + M$ problem using the bounds for the $N + 1$ or the $1 + M$ problem. We note that the latter is, up to an overall factor, equivalent to the $M + 1$ problem with m replaced by its inverse. Hence the fact that $m_1 < 1$ gives hope that there exists a mass region where the general $N + M$ system is stable for all N and M. The simplest problem of this kind is the $2 + 2$ case. So far there are only numerical results on its stability available [18, 42]. In particular, the analysis in [18] suggests that the critical mass for the $2 + 2$ case should be equal to m^*, i.e., the one for the $2 + 1$ case.

In this paper we give a rigorous proof of stability for the $2+2$ system in a certain window of mass ratios. We find a critical mass $m_2 \approx 0.58$ such that the system is stable if $m \in [m_2, m_2^{-1}] \approx [0.58, 1.73]$. We note that the critical mass m_2 is not optimal and we cannot make any further statements about the mass range $[m^*, m_2] \cup [m_2^{-1}, m^{*-1}]$. The behavior for these masses, and in particular the question whether $m_2 = m^*$, still represents an open problem.

4.2 The model

For $p_1, p_2, k_1, k_2 \in \mathbb{R}^3$ and $m > 0$, let

$$h_0(p_1, p_2, k_1, k_2) = p_1^2 + p_2^2 + \frac{1}{m}\left(k_1^2 + k_2^2\right) . \tag{4.2.1}$$

We will work with the quadratic form F_α introduced in [20] for $2+2$ particles. Its form domain is given by

$$D(F_\alpha) = \{\psi = \varphi + G_\mu\xi \mid \varphi \in H^1_{\mathrm{as}}(\mathbb{R}^6) \otimes H^1_{\mathrm{as}}(\mathbb{R}^6), \xi \in H^{1/2}(\mathbb{R}^9)\} \tag{4.2.2}$$

where, for some (arbitrary) $\mu > 0$, $G_\mu\xi$ is the function with Fourier transform

$$\widehat{G_\mu\xi}(p_1, p_2, k_1, k_2) = \sum_{i,j\in\{1,2\}} (-1)^{i+j}(h_0(p_1, p_2, k_1, k_2) + \mu)^{-1}\hat{\xi}(p_i + k_j, \hat{p}_i, \hat{k}_j) \tag{4.2.3}$$

and we used the notation that $\hat{p}_1 = p_2, \hat{p}_2 = p_1$ and analogously for k. The space $H^1_{\mathrm{as}}(\mathbb{R}^6)$ denotes antisymmetric functions in $H^1(\mathbb{R}^3) \otimes H^1(\mathbb{R}^3)$. Note that because of the requirement $\varphi \in H^1(\mathbb{R}^{12})$ the decomposition $\psi = \varphi + G_\mu\xi$ is unique. Note also that the Hilbert space under consideration consists of functions that are antisymmetric in the first two and last two variables, i.e., under both the exchange $p_1 \leftrightarrow p_2$ and $k_1 \leftrightarrow k_2$.

For $\alpha \in \mathbb{R}$, the quadratic form we consider is given by

$$F_\alpha(\psi) = H(\varphi) - \mu \|\psi\|_2^2 + 4T_\mu(\xi) + 4\alpha \|\xi\|_2^2 , \tag{4.2.4}$$

where

$$H(\varphi) = \int_{\mathbb{R}^{12}} (h_0(p_1, p_2, k_1, k_2) + \mu) |\hat{\varphi}(p_1, p_2, k_1, k_2)|^2 \, dp_1\, dp_2\, dk_1\, dk_2 \tag{4.2.5}$$

and $T_\mu(\xi) = \sum_{i=0}^3 \phi_i(\xi)$, with the ϕ_i of the form

$$\phi_0(\xi) = 2\pi^2 \left(\frac{m}{m+1}\right)^{3/2} \int |\hat{\xi}(P, p, k)|^2 \sqrt{\frac{P^2}{1+m} + p^2 + \frac{k^2}{m} + \mu}\, dP\, dp\, dk \tag{4.2.6}$$

$$\phi_1(\xi) = \int \frac{\hat{\xi}^*(p_1 + k_1, p_2, k_2)\hat{\xi}(p_2 + k_1, p_1, k_2)}{h_0(p_1, p_2, k_1, k_2) + \mu}\, dp_1\, dp_2\, dk_1\, dk_2 \tag{4.2.7}$$

$$\phi_2(\xi) = \int \frac{\hat{\xi}^*(p_1 + k_1, p_2, k_2)\hat{\xi}(p_1 + k_2, p_2, k_1)}{h_0(p_1, p_2, k_1, k_2) + \mu}\, dp_1\, dp_2\, dk_1\, dk_2 \tag{4.2.8}$$

$$\phi_3(\xi) = -\int \frac{\hat{\xi}^*(p_1 + k_1, p_2, k_2)\hat{\xi}(p_2 + k_2, p_1, k_1)}{h_0(p_1, p_2, k_1, k_2) + \mu}\, dp_1\, dp_2\, dk_1\, dk_2 . \tag{4.2.9}$$

We note that F_α is independent of the choice of $\mu > 0$. The parameter α corresponds to the inverse scattering length; more precisely, $\alpha = -2\pi^2/a$, with $a \in (-\infty, 0) \cup (0, \infty]$ the scattering length.

It was shown in [20] that $T_\mu(\xi)$ is well-defined on $H^{1/2}(\mathbb{R}^9)$. To show stability, we need to prove that it is in fact positive. If, on the contrary, there exists a $\mu > 0$ and a $\xi \in H^{1/2}(\mathbb{R}^9)$ such that $T_\mu(\xi) < 0$, a simple scaling argument (choosing $\varphi = 0$ and using the scale invariance of F_0) can be used to deduce that F_α is unbounded from below for all $\alpha \in \mathbb{R}$.

The functionals ϕ_0 and ϕ_1 also appear in a similar form in the discussion of the 2 + 1 problem, and ϕ_2 can be seen as the analogous 1 + 2 term. The term ϕ_3 has no analogue in the 2 + 1 or 1 + 2 systems. Note that none of the ϕ_i for $1 \le i \le 3$ has a sign, and we expect that cancellations occur between them that are important for stability. In our proof below, we will first bound $\phi_0 + \phi_3$ from below by a positive quantity, which we then use to compensate separately the negative parts of ϕ_1 and ϕ_2. Since we shall neglect some positive terms, we cannot expect to obtain a sharp bound. In particular, whether $m_2 = m^*$, as suggested in [18], cannot be determined using this method.

4.3 Main result

For $a \in \mathbb{R}^3$, $b \geq 0$ and $m > 0$, let $O^m_{a,b}$ be the bounded operator on $L^2(\mathbb{R}^3)$ with integral kernel

$$O^m_{a,b}(p_1, p_2) = \left[(p_1 + a)^2 + b^2\right]^{-1/4} \left[(p_2 + a)^2 + b^2\right]^{-1/4} \times \frac{1}{p_1^2 + p_2^2 + \frac{2}{1+m} p_1 \cdot p_2 + \frac{2(2+m)}{(1+m)^2} a^2 + \frac{2m}{(1+m)^2} b^2} . \tag{4.3.1}$$

Let further

$$\Lambda(m) = -\frac{1}{2\pi^2} \frac{1+m}{\sqrt{m}} \inf_{a \in \mathbb{R}^3, b \geq 0} \inf \operatorname{spec} O^m_{a,b} . \tag{4.3.2}$$

Theorem 4.3.1. *For $m > 0$ such that $\Lambda(m) + \Lambda(1/m) \leq 1$, we have*

$$T_\mu(\xi) \geq (1 - \Lambda(m) - \Lambda(1/m)) \sqrt{2\mu}\, \pi^2 \left(\frac{m}{m+1}\right)^{3/2} \|\xi\|_2^2 \tag{4.3.3}$$

for any $\xi \in H^{1/2}(\mathbb{R}^9)$ and any $\mu > 0$.

This bound readily implies stability for F_α, as the following corollary shows.

Corollary 4.3.2. *For m such that $\Lambda(m) + \Lambda(1/m) < 1$, we have*

$$F_\alpha(\psi) \geq \begin{cases} 0 & \alpha \geq 0 \\ -\alpha^2 \left(\frac{m+1}{m}\right)^3 \frac{1}{2\pi^4 (1 - \Lambda(m) - \Lambda(1/m))^2} \|\psi\|_2^2 & \alpha < 0 \end{cases} \tag{4.3.4}$$

for any $\psi \in D(F_\alpha)$.

Proof. Without loss of generality we can assume that $\|\psi\|_2 = 1$. Using Theorem 4.3.1 and $H(\varphi) \geq 0$, we get

$$\begin{aligned} F_\alpha(\psi) + \mu &\geq 4T_\mu(\xi) + 4\alpha \|\xi\|_2^2 \\ &\geq 4\left[\alpha + (1 - \Lambda(m) - \Lambda(1/m)) \sqrt{2\mu}\, \pi^2 \left(\frac{m}{m+1}\right)^{3/2}\right] \|\xi\|_2^2 . \end{aligned}$$

In case $\alpha \geq 0$ we obtain $F_\alpha(\psi) \geq -\mu$, which shows the result as $\mu > 0$ was arbitrary. If $\alpha < 0$, we choose

$$\mu = \alpha^2 \left(\frac{m+1}{m}\right)^3 \frac{1}{2\pi^4 (1 - \Lambda(m) - \Lambda(1/m))^2} , \tag{4.3.5}$$

which yields the desired result. □

We thus proved stability as long as $\Lambda(m) + \Lambda(1/m) < 1$. To investigate the implication on m, let us first check what happens for $a = 0$ and $b = 0$. An explicit calculation following [11] shows that

$$\begin{aligned} \bar{\Lambda}(m) &:= -\frac{1}{2\pi^2} \frac{1+m}{\sqrt{m}} \inf \operatorname{spec} O^m_{0,0} \\ &= \frac{2}{\pi}(1+m)^2 \left(\frac{1}{\sqrt{m}} - \sqrt{2+m} \arcsin\left(\tfrac{1}{1+m}\right)\right) \end{aligned} \tag{4.3.6}$$

which satisfies $\bar{\Lambda}(m) + \bar{\Lambda}(1/m) < 1$ for $0.139 \lesssim m \lesssim 7.189$. This range of masses is the largest possible for which our approach can show stability.

While we do not know whether $\Lambda(m) = \bar{\Lambda}(m)$, we shall give in Section 4.5 a rough upper bound on $\Lambda(m)$ which shows that $\Lambda(m) + \Lambda(1/m) < 1$ for $0.58 \lesssim m \lesssim 1.73$.

4.4 Proof of Theorem 4.3.1

We shall split the proof into several steps.

4.4.1 Bound on ϕ_3

We shall rewrite ϕ_3 in (4.2.9) using center-of-mass and relative coordinates for each of the pairs (p_1, k_1) and (p_2, k_2). With $P_1 = p_1+k_1$, $q_1 = \frac{m}{1+m}p_1-\frac{1}{1+m}k_1$, $P_2 = p_2+k_2$ and $q_2 = \frac{m}{1+m}p_2-\frac{1}{1+m}k_2$, we have

$$\phi_3(\xi) = -\int dP_1\, dP_2\, dq_1\, dq_2 \times \frac{\hat{\xi}^*(P_1, \frac{P_2}{1+m} + q_2, \frac{mP_2}{1+m} - q_2)\hat{\xi}(P_2, \frac{P_1}{1+m} + q_1, \frac{mP_1}{1+m} - q_1)}{\frac{1}{1+m}\left(P_1^2 + P_2^2\right) + \frac{1+m}{m}\left(q_1^2 + q_2^2\right) + \mu}. \tag{4.4.1}$$

By completing the square, we can write, for any positive function w,

$$\phi_3(\xi) = \int \frac{dP_1\, dP_2\, dq_1\, dq_2}{w(q_2, P_1, P_2)w(q_1, P_2, P_1)} \times \frac{\frac{1}{2}\left|\chi_w(q_2, P_1, P_2) - \chi_w(q_1, P_2, P_1)\right|^2 - |\chi_w(q_2, P_1, P_2)|^2}{\frac{1}{1+m}\left(P_1^2 + P_2^2\right) + \frac{1+m}{m}\left(q_1^2 + q_2^2\right) + \mu} \tag{4.4.2}$$

where we denote $\chi_w(q, P_1, P_2) = \hat{\xi}(P_1, \frac{P_2}{1+m} + q, \frac{mP_2}{1+m} - q)w(q, P_1, P_2)$. We shall choose

$$w(q, P_1, P_2) = q^2 + \lambda^2\left(\tfrac{m}{(1+m)^2}\left(P_1^2 + P_2^2\right) + \tfrac{m}{1+m}\mu\right) \tag{4.4.3}$$

for some constant $\lambda \geq 0$. The first term in the numerator on the right side of (4.4.2) is manifestly positive. Performing the integration over q_1, the integral over the second term equals

$$\int dP_1\, dP_2\, dq_2 \left(-\frac{2\pi^2 m}{1+m}\right)\left|\hat{\xi}(P_1, \tfrac{1}{1+m}P_2 + q_2, \tfrac{m}{1+m}P_2 - q_2)\right|^2 \times \frac{q_2^2 + \lambda^2\left(\frac{m}{(1+m)^2}\left(P_1^2 + P_2^2\right) + \frac{m}{1+m}\mu\right)}{\lambda\sqrt{\frac{m}{(1+m)^2}\left(P_1^2 + P_2^2\right) + \frac{m}{1+m}\mu} + \sqrt{q_2^2 + \frac{m}{(1+m)^2}\left(P_1^2 + P_2^2\right) + \frac{m}{1+m}\mu}}. \tag{4.4.4}$$

Let us compare this latter expression with ϕ_0 in (4.2.6), which can be rewritten as

$$\phi_0(\xi) = \frac{2\pi^2 m}{m+1}\int |\hat{\xi}(P_1, \tfrac{1}{1+m}P_2 + q_2, \tfrac{m}{1+m}P_2 - q_2)|^2 \times \sqrt{q_2^2 + \frac{m}{(1+m)^2}\left(P_1^2 + P_2^2\right) + \frac{m}{1+m}\mu}\, dP_1\, dP_2\, dq_2\,. \tag{4.4.5}$$

For $0 \leq \lambda \leq 1$, one readily checks that

$$L_\lambda(P_1, P_2, q) := \sqrt{q^2 + \frac{m}{(1+m)^2}\left(P_1^2 + P_2^2\right) + \frac{m}{1+m}\mu} - \frac{q^2 + \lambda^2\left(\frac{m}{(1+m)^2}\left(P_1^2 + P_2^2\right) + \frac{m}{1+m}\mu\right)}{\lambda\sqrt{\frac{m}{(1+m)^2}\left(P_1^2 + P_2^2\right) + \frac{m}{1+m}\mu} + \sqrt{q^2 + \frac{m}{(1+m)^2}\left(P_1^2 + P_2^2\right) + \frac{m}{1+m}\mu}} \tag{4.4.6}$$

is non-negative. What we have shown here is that

$$\begin{aligned}&\phi_0(\xi) + \phi_3(\xi)\\ &\geq \frac{2\pi^2 m}{m+1}\int |\hat{\xi}(P_1, \tfrac{1}{1+m}P_2 + q, \tfrac{m}{1+m}P_2 - q)|^2 L_\lambda(P_1, P_2, q)\, dP_1\, dP_2\, dq\end{aligned} \tag{4.4.7}$$

for any $\lambda \geq 0$.

Note that for $\lambda^2 = 1/2$, L_λ takes the simple form

$$L_{1/\sqrt{2}}(P_1, P_2, q) = \frac{1}{\sqrt{2}}\sqrt{\tfrac{m}{(1+m)^2}\left(P_1^2 + P_2^2\right) + \tfrac{m}{1+m}\mu} \tag{4.4.8}$$

and is, in particular, independent of q.

4.4.2 Bound on ϕ_1

For the term ϕ_1 in (4.2.7), we shall switch to center-of-mass and relative coordinates for the particles (p_1, p_2, k_1). With $P = p_1 + p_2 + k_1$, $q_1 = \frac{1+m}{2+m}p_1 - \frac{1}{2+m}(p_2 + k_1)$ and $q_2 = \frac{1+m}{2+m}p_2 - \frac{1}{2+m}(p_1 + k_1)$, as well as $k = k_2$ for short, we have

$$\begin{aligned}\phi_1(\xi) = \frac{m}{1+m}\int & dP\, dq_1\, dq_2\, dk\\ &\times \frac{\hat{\xi}^*(\frac{1+m}{2+m}P - q_2, \frac{P}{2+m} + q_2, k)\hat{\xi}(\frac{1+m}{2+m}P - q_1, \frac{P}{2+m} + q_1, k)}{q_1^2 + q_2^2 + \frac{2}{1+m}q_1\cdot q_2 + \frac{m}{(1+m)(2+m)}P^2 + \frac{1}{1+m}k^2 + \frac{m}{1+m}\mu}\,.\end{aligned} \tag{4.4.9}$$

Defining

$$\ell_\lambda(q, P, k) = L_\lambda(\tfrac{1+m}{2+m}P - q, \tfrac{P}{2+m} + q + k, \tfrac{mq}{1+m} + \tfrac{mP}{(1+m)(2+m)} - \tfrac{k}{1+m}) \tag{4.4.10}$$

our aim is to obtain a lower bound on the operator on $L^2(\mathbb{R}^3)$ with integral kernel

$$\begin{aligned}&\ell_\lambda(q_1, P, k)^{-1/2}\ell_\lambda(q_2, P, k)^{-1/2}\\ &\times \frac{1}{q_1^2 + q_2^2 + \frac{2}{1+m}q_1\cdot q_2 + \frac{m}{(1+m)(2+m)}P^2 + \frac{1}{1+m}k^2 + \frac{m}{1+m}\mu}\end{aligned} \tag{4.4.11}$$

for suitable λ, uniformly in the fixed parameters P and k.

Let us take $\lambda^2 = 1/2$ for simplicity, in which case we have

$$\ell_{1/\sqrt{2}}(q, P, k) = \frac{\sqrt{m}}{1+m}\sqrt{\left(q + \tfrac{1}{2}k - \tfrac{m}{2(2+m)}P\right)^2 + \tfrac{1}{4}(P+k)^2 + \tfrac{1+m}{2}\mu}\,. \tag{4.4.12}$$

Note also that

$$\begin{aligned}&\frac{m}{(1+m)(2+m)}P^2 + \frac{1}{1+m}k^2\\ &= \frac{2m}{(1+m)^2}\left[\frac{2+m}{m}\left(\tfrac{1}{2}k - \tfrac{m}{2(2+m)}P\right)^2 + \frac{1}{4}(P+k)^2\right].\end{aligned} \tag{4.4.13}$$

With

$$a = \tfrac{1}{2}k - \tfrac{m}{2(2+m)}P \quad , \quad b^2 = \tfrac{1}{4}(P+k)^2 + \tfrac{1+m}{2}\mu \tag{4.4.14}$$

our task is thus to find a lower bound on the operator with integral kernel $\frac{1+m}{\sqrt{m}} O^m_{a,b}(q_1, q_2)$, defined in (4.3.1). The best lower bound equals $-2\pi^2\Lambda(m)$, by definition.

To summarize, what we have shown here is that

$$\phi_1(\xi) \geq -\Lambda(m)\frac{2\pi^2 m}{m+1}\int |\hat{\xi}(\tfrac{1+m}{2+m}P - q, \tfrac{P}{2+m} + q, k)|^2 \ell_{1/\sqrt{2}}(q, P, k)\, dP\, dq\, dk\,. \qquad (4.4.15)$$

Using (4.4.10), a simple change of variables shows that this is equivalent to

$$\begin{aligned}&\phi_1(\xi)\\ &\geq -\Lambda(m)\frac{2\pi^2 m}{m+1}\int |\hat{\xi}(P_1, \tfrac{P_2}{1+m} + q, \tfrac{mP_2}{1+m} - q)|^2 L_{1/\sqrt{2}}(P_1, P_2, q)\, dP_1\, dP_2\, dq\,. \end{aligned} \qquad (4.4.16)$$

4.4.3 Bound on ϕ_2

In exactly the same way we proceed with ϕ_2 in (4.2.8), which we rewrite as

$$\begin{aligned}&\phi_2(\xi)\\ &= \frac{m}{1+m}\int dP\, dq_1\, dq_2\, dp\\ &\qquad \times \frac{\hat{\xi}^*(\frac{1+m}{1+2m}P - q_2, p, q_2 + \frac{mP}{1+2m})\hat{\xi}(\frac{1+m}{1+2m}P - q_1, p, q_1 + \frac{mP}{1+2m})}{q_1^2 + q_2^2 + \frac{2m}{1+m}q_1\cdot q_2 + \frac{m}{(1+m)(1+2m)}P^2 + \frac{m}{1+m}p^2 + \frac{m}{1+m}\mu}\,. \end{aligned} \qquad (4.4.17)$$

If we now define

$$\tilde{\ell}_\lambda(q, P, p) = L_\lambda(\tfrac{1+m}{1+2m}P - q, p + q + \tfrac{mP}{1+2m}, \tfrac{mp}{1+m} - \tfrac{q}{1+m} - \tfrac{mP}{(1+m)(1+2m)}) \qquad (4.4.18)$$

we need a lower bound on the operator on $L^2(\mathbb{R}^3)$ with integral kernel

$$\begin{aligned}&\tilde{\ell}_\lambda(q_1, P, p)^{-1/2}\tilde{\ell}_\lambda(q_2, P, p)^{-1/2}\\ &\times \frac{1}{q_1^2 + q_2^2 + \frac{2m}{1+m}q_1\cdot q_2 + \frac{m}{(1+m)(1+2m)}P^2 + \frac{m}{1+m}p^2 + \frac{m}{1+m}\mu}\end{aligned} \qquad (4.4.19)$$

for fixed P and p. By proceeding as in the previous subsection, one readily checks that, for $\lambda^2 = 1/2$, its best lower bound is $-2\pi^2\Lambda(1/m)$, with Λ defined in (4.3.2). In particular, we have

$$\begin{aligned}&\phi_2(\xi)\\ &\geq -\Lambda(1/m)\frac{2\pi^2 m}{m+1}\int |\hat{\xi}(P_1, \tfrac{P_2}{1+m} + q, \tfrac{mP_2}{1+m} - q)|^2 L_{1/\sqrt{2}}(P_1, P_2, q)\, dP_1\, dP_2\, dq\,. \end{aligned} \qquad (4.4.20)$$

4.4.4 Combining above bounds

By combining the bounds (4.4.7), (4.4.16) and (4.4.20) from the previous three subsections, we obtain

$$\begin{aligned} T_\mu(\xi) &= \sum_{j=0}^{3} \phi_j(\xi) \\ &\geq (1 - \Lambda(m) - \Lambda(1/m)) \frac{2\pi^2 m}{m+1} \\ &\quad \times \int |\hat{\xi}(P_1, \tfrac{1}{1+m}P_2 + q, \tfrac{m}{1+m}P_2 - q)|^2 L_{1/\sqrt{2}}(P_1, P_2, q)\, dP_1\, dP_2\, dq \end{aligned} \tag{4.4.21}$$

with $L_{1/\sqrt{2}}$ defined in (4.4.8). In the case $\Lambda(m)+\Lambda(1/m) \leq 1$, we can further use $L_{1/\sqrt{2}}(P_1, P_2, q) \geq \sqrt{m\mu/(2(1+m))}$ for a lower bound. This completes the proof of Theorem 4.3.1.

4.5 Bound on $\Lambda(m)$

Note that $\Lambda(m) \geq \bar{\Lambda}(m)$. To obtain an upper bound, we use the Schur test. We first drop the positive part of the operator with integral kernel

$$k(p_1, p_2) = \left[p_1^2 + p_2^2 + \frac{2}{1+m} p_1 \cdot p_2 + \frac{2(2+m)}{(1+m)^2} a^2 + \frac{2m}{(1+m)^2} b^2 \right]^{-1} . \tag{4.5.1}$$

It follows from [50, Lemma 3] that the negative part of this operator has the integral kernel

$$\begin{aligned} k_-(p_1, p_2) &= \frac{-k(p_1, p_2) + k(p_1, -p_2)}{2} \\ &= \frac{2}{1+m} \frac{p_1 \cdot p_2}{\left[p_1^2 + p_2^2 + \frac{2(2+m)}{(1+m)^2} a^2 + \frac{2m}{(1+m)^2} b^2 \right]^2 - \frac{4(p_1 \cdot p_2)^2}{(1+m)^2}} . \end{aligned}$$

By applying the Cauchy-Schwarz inequality, we obtain, for any positive function h on $\mathbb{R}^3$ (possibly depending on a and b)

$$\begin{aligned} \Lambda(m) \leq \frac{1}{\pi^2 \sqrt{m}} \sup_{p_1, a, b} \int_{\mathbb{R}^3} \frac{h(p_1)}{h(p_2)} & \frac{|p_1 \cdot p_2|}{\left[p_1^2 + p_2^2 + \frac{2(2+m)}{(1+m)^2} a^2 + \frac{2m}{(1+m)^2} b^2 \right]^2 - \frac{4(p_1 \cdot p_2)^2}{(1+m)^2}} \\ & \times \left[(p_2 + a)^2 + b^2 \right]^{-1/2} dp_2 . \end{aligned} \tag{4.5.2}$$

By monotonicity, we can set $b = 0$, i.e,

$$\Lambda(m) \leq \frac{1}{\pi^2 \sqrt{m}} \sup_{p_1, a} \int_{\mathbb{R}^3} \frac{h(p_1)}{h(p_2)} \frac{|p_1 \cdot p_2|}{\left[p_1^2 + p_2^2 + \frac{2(2+m)}{(1+m)^2} a^2 \right]^2 - \frac{4(p_1 \cdot p_2)^2}{(1+m)^2}} |p_2 + a|^{-1} \, dp_2 . \tag{4.5.3}$$

We shall choose h to be even, i.e., $h(p) = h(-p)$, in which case we can symmetrize to get

$$\begin{aligned}\Lambda(m) \leq& \frac{1}{\pi^2 \sqrt{m}} \sup_{p_1,a} \int_{\mathbb{R}^3} \frac{h(p_1)}{h(p_2)} \frac{|p_1 \cdot p_2|}{\left[p_1^2 + p_2^2 + \frac{2(2+m)}{(1+m)^2} a^2\right]^2 - \frac{4(p_1 \cdot p_2)^2}{(1+m)^2}} \\ &\times \frac{1}{2}\left(\frac{1}{|p_2 + a|} + \frac{1}{|p_2 - a|}\right) dp_2 \\ \leq& \frac{1}{\pi^2 \sqrt{m}} \sup_{p_1,a} \int_{\mathbb{R}^3} \frac{h(p_1)}{h(p_2)} \frac{|p_1 \cdot p_2|}{\left[p_1^2 + p_2^2 + \frac{2(2+m)}{(1+m)^2} a^2\right]^2 - \frac{4(p_1 \cdot p_2)^2}{(1+m)^2}} \\ &\times \sqrt{\frac{p_2^2 + a^2}{\left(p_2^2 + a^2\right)^2 - 4(p_2 \cdot a)^2}} dp_2 \,. \end{aligned} \tag{4.5.4}$$

To maximize the right side, a wants to be parallel to p_1, i.e., $a = \kappa p_1$ for $\kappa \in \mathbb{R}$. This is a direct consequence of [50, Lemma 5]. We shall choose $h(p) = |p|$. By scale invariance we can set $|p_1| = 1$. We then obtain

$$\begin{aligned}\Lambda(m) \leq& \frac{4}{\pi \sqrt{m}} \sup_{\kappa \in \mathbb{R}} \int_0^1 dt \int_0^\infty dr \frac{r^2 t}{\left[1 + r^2 + \frac{2(2+m)}{(1+m)^2}\kappa^2\right]^2 - \frac{4r^2t^2}{(1+m)^2}} \\ &\times \sqrt{\frac{r^2 + \kappa^2}{(r^2 + \kappa^2)^2 - 4\kappa^2 r^2 t^2}} \,. \end{aligned} \tag{4.5.5}$$

We further bound $t \leq 1$ in the denominator of the first term in the integrand in (4.5.5), and use that

$$\left[1 + r^2 + \frac{2(2+m)}{(1+m)^2}\kappa^2\right]^2 - \frac{4r^2}{(1+m)^2} \geq \frac{m(m+2)}{(1+m)^2}\left[1 + r^2 + \frac{2\sqrt{2+m}}{(1+m)\sqrt{m}}\kappa^2\right]^2 . \tag{4.5.6}$$

Since

$$\int_0^1 dt\, t \sqrt{\frac{r^2 + \kappa^2}{(r^2 + \kappa^2)^2 - 4\kappa^2 r^2 t^2}} = \frac{1}{2r^2}\sqrt{r^2 + \kappa^2}\min\{1, r^2/\kappa^2\} \tag{4.5.7}$$

we therefore get

$$\Lambda(m) \leq \frac{2}{\pi} \frac{(1+m)^2}{m^{3/2}(m+2)} \sup_{\kappa \in \mathbb{R}} \int_0^\infty dr \frac{\sqrt{r^2 + \kappa^2}}{\left[1 + r^2 + \frac{2\sqrt{2+m}}{(1+m)\sqrt{m}}\kappa^2\right]^2} . \tag{4.5.8}$$

We define $c_m = 2\sqrt{2+m}/((1+m)\sqrt{m})$. After explicitly doing the integral, the bound (4.5.8) reads $\Lambda(m) \leq \lambda(m) := \sup_{\kappa > 0} \lambda(m, \kappa)$ with

$$\begin{aligned}\lambda(m,\kappa) :=& \frac{1}{\pi} \frac{(1+m)^2}{m^{3/2}(m+2)} \frac{1}{1 + c_m\kappa^2}\left(1 + \frac{\kappa^2}{\sqrt{1 + c_m\kappa^2}\sqrt{1 + \kappa^2(c_m - 1)}}\right. \\ &\left.\times \ln\left(\frac{\sqrt{1 + c_m\kappa^2} + \sqrt{1 + \kappa^2(c_m - 1)}}{\kappa}\right)\right). \end{aligned} \tag{4.5.9}$$

For our purpose it is important that $\lambda(1) \approx 0.427 < 1/2$ (see Fig. 4.1). By continuity, this implies that $\Lambda(m) + \Lambda(1/m) < 1$ for a window of mass ratios around 1. In fact, a numerical optimization over κ leads to the conclusion that $\Lambda(m) + \Lambda(1/m) < 1$ whenever $0.58 \approx m_2 < m < m_2^{-1} \approx 1.73$ (see Fig 4.2).

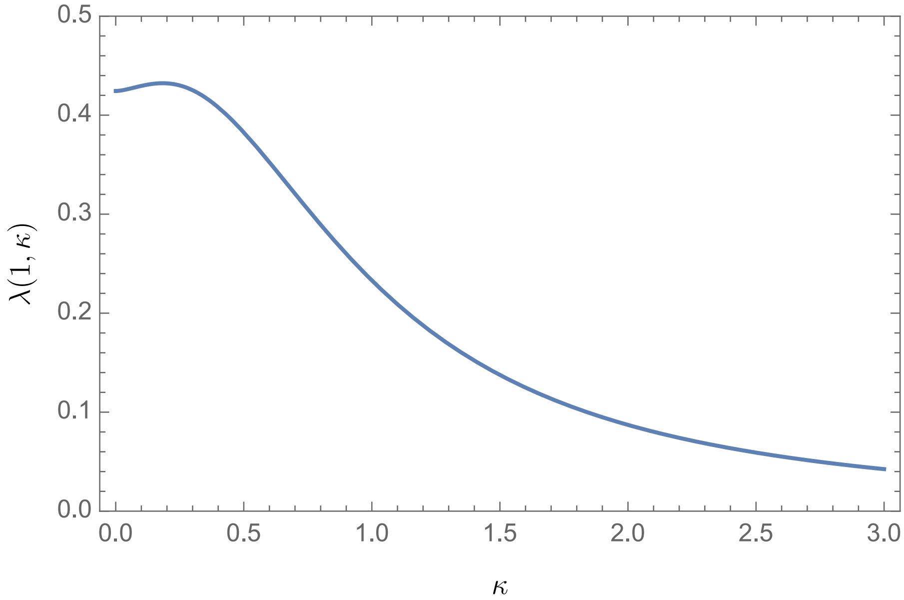

Figure 4.1: The function $\lambda(1, \kappa)$, with $\lambda(1) = \sup_\kappa \lambda(1, \kappa) \approx 0.427$

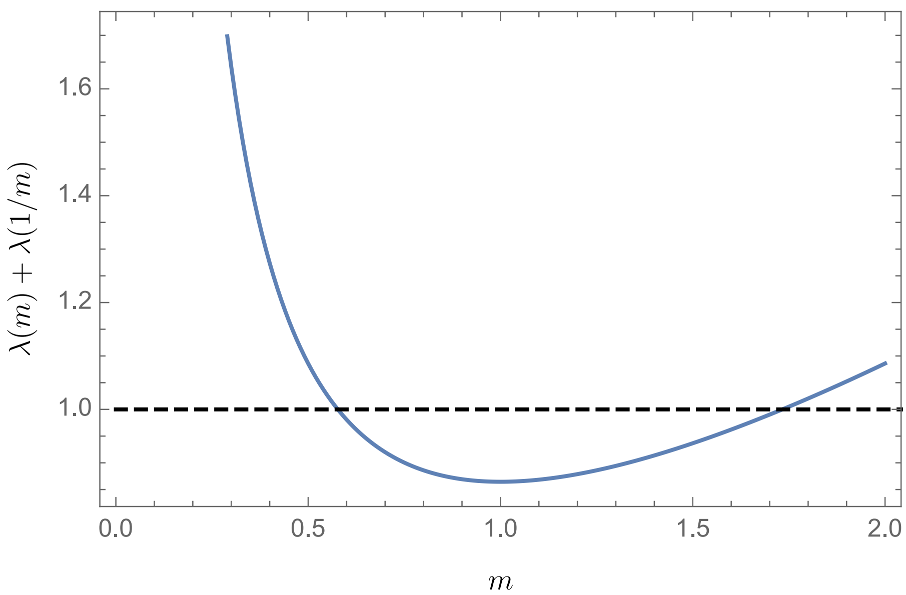

Figure 4.2: Our upper bound on $\Lambda(m) + \Lambda(1/m)$, given by $\lambda(m) + \lambda(1/m)$

CHAPTER 5

Triviality of a model of particles with point interactions in the thermodynamic limit

Thomas Moser, Robert Seiringer

Abstract

We consider a model of fermions interacting via point interactions, defined via a certain weighted Dirichlet form. While for two particles the interaction corresponds to infinite scattering length, the presence of further particles effectively decreases the interaction strength. We show that the model becomes trivial in the thermodynamic limit, in the sense that the free energy density at any given particle density and temperature agrees with the corresponding expression for non-interacting particles.

5.1 Introduction

Due to their relevance for cold-atom physics [74], quantum-mechanical models of particles with zero-range interactions have recently received a lot of attention. Of particular interest is the unitary limit of infinite scattering length, where one has scale invariance due to the lack of any intrinsic length scale (see, e.g., [8, 9, 26, 29, 70]). Despite some effort [11, 12, 15, 21, 50], it remains an open problem to establish the existence of a many-particle model with two-body point interactions. Such a model is known to be unstable in the case of bosons (a fact known as Thomas effect [8, 11, 68], closely related to the Efimov effect [17, 61, 73]) and hence can only exist for fermionic particles. In contrast, the two-body problem is completely understood and point interactions can be characterized via self-adjoint extensions of the Laplacian on $\mathbb{R}^3 \setminus \{0\}$ (see [1] for details). These self-adjoint extensions can be interpreted as corresponding to an attractive point interaction, parametrized by the scattering length a, with interaction strength increasing with $1/a$. For non-positive scattering length, $a \leq 0$, the attraction is too weak to support bound states, while there exists a negative energy bound state for $a > 0$.

In the case of non-positive scattering length, $a \leq 0$, corresponding to the absence of two-body bound states, point interactions can alternatively be defined via the quadratic form

$$\int_{\mathbb{R}^3} \left(\frac{1}{|x|} - \frac{1}{a} \right)^2 |\nabla f(x)|^2 \, \mathrm{d}x \qquad \text{on} \quad L^2(\mathbb{R}^3, (|x|^{-1} - a^{-1})^2 \mathrm{d}x) \tag{5.1.1}$$

The unitary limit corresponds to $a^{-1} = 0$. Recall that the scattering length is defined (see, e.g., [33, Appendix C]) via the asymptotic behavior of the solution to the zero-energy scattering equation, which in this case is simply equal to $|x|^{-1} - a^{-1}$, corresponding to $f \equiv 1$. To see that (5.1.1) corresponds to a point interactions at the origin, note that an integration by parts shows that

$$\int_{|x|\geq\varepsilon} \left(\frac{1}{|x|} - \frac{1}{a}\right)^2 |\nabla f(x)|^2 \, \mathrm{d}x = \int_{|x|\geq\varepsilon} \left|\nabla \left(\frac{1}{|x|} - \frac{1}{a}\right) f(x)\right|^2 \, \mathrm{d}x - \int_{|x|=\varepsilon} \left(\frac{1}{|x|} - \frac{1}{a}\right) \frac{1}{|x|^2} |f(x)|^2 \mathrm{d}\omega \tag{5.1.2}$$

for any $\varepsilon > 0$. The last term vanishes as $\varepsilon \to 0$ if f vanishes faster than $|x|^{1/2}$ at the origin.

We consider here a many-body generalization of (5.1.1), which was introduced in [2]. It has the advantage of being manifestly well-defined, via a non-negative Dirichlet form. As already noted above, in general it is notoriously hard to define many-body systems with point interactions, see [11, 12, 15, 21, 50], due to the inherent instability problems. The model under consideration here was studied in [25] were it was shown to satisfy a Lieb–Thirring inequality, i.e., the energy can be bounded from below by a semiclassical expression of the form $C \int \rho(x)^{5/3} \mathrm{d}x$, with ρ the particle density and C a positive constant. Up to the value of C, this is the same as the inequality for non-interacting fermions used by Lieb and Thirring [31, 34] in their proof of stability of matter. (For other recent work on Lieb-Thirring inequalities for interacting particles, see [36–39].)

The model considered here has the disadvantage that the interaction is not purely two-body, however. In fact, it is a full many-body interaction, its strength depends on the position of all the particles and is weakened due to their presence. We shall show here that the effects of the interaction actually disappear in the thermodynamic limit, and the thermodynamic free energy density agrees with the one for non-interacting fermions.

In the next section, we shall introduce the model and explain our main results. The rest of the paper is devoted to their proof.

5.2 Model and main results

For $N \geq 2$, $\vec{x} = (x_1, \dots, x_N) \in \mathbb{R}^{3N}$, let $g : \mathbb{R}^{3N} \to \mathbb{R}$ denote the function

$$g(\vec{x}) = \sum_{1\leq i<j\leq N} \frac{1}{|x_i - x_j|} \, . \tag{5.2.1}$$

We consider fermions with $q \geq 1$ internal (spin) states, described by wave functions in the subspace $\mathcal{A}_q^N \subset L^2((\mathbb{R}^3 \times \{1, \dots, q\})^N, g(\vec{x})^2 \mathrm{d}\vec{x})$ of functions that are totally antisymmetric with respect to permutations of the variables $y_i = (x_i, \sigma_i)$, where $x_i \in \mathbb{R}^3$ and $\sigma_i \in \{1, \dots, q\}$. For $\psi \in \mathcal{A}_q^N$, our model is defined via the quadratic form

$$\mathcal{E}_g(\psi) = \sum_{i=1}^N \int_{\mathbb{R}^{3N}} g(\vec{x})^2 |\nabla_i \psi(\vec{y})|^2 \mathrm{d}\vec{y} \tag{5.2.2}$$

where ∇_i stands for the gradient with respect to $x_i \in \mathbb{R}^3$, and we introduced the shorthand notation $\int \ldots \mathrm{d}\vec{y} = \sum_{\vec{\sigma}} \int \ldots \mathrm{d}\vec{x}$ with $\vec{\sigma} = (\sigma_1, \ldots, \sigma_N)$. Since g is a harmonic function away from the planes $\{x_i = x_j\}$ of particle intersection, an integration by parts as in (5.1.2) shows that (5.2.2) corresponds to a model of point interactions, as $\mathcal{E}_g(\psi) = \sum_{i=1}^N \int |\nabla_i g\psi|^2$ in case ψ has compact support away from these planes. More generally, $\mathcal{E}_g(\psi) = \sum_{i=1}^N \int |\nabla_i g\psi|^2$ holds if ψ vanishes faster than the square root of the distance to the planes of intersection, which is in particular the case for smooth and completely antisymmetric functions of the spatial variables. In other words, the model is trivial for $q = 1$.

For N particles in a cubic box $[0, L]^3 \subset \mathbb{R}^3$, the free energy at temperature $T = \beta^{-1} > 0$ is defined as usual as

$$F_g = -T \ln \operatorname{tr} e^{-\beta H_g} \tag{5.2.3}$$

where H_g denotes the operator defined by the quadratic form (5.2.2), restricted to functions in $\mathcal{A}_q^N \cap H^1(\mathbb{R}^{3N}; g(\vec{x})^2 \mathrm{d}\vec{x})$ with support in $([0, L]^3)^N$. The latter restriction corresponds to choosing Dirichlet boundary conditions on the boundary of the cube $[0, L]^3$. Alternatively, one can use the variational principle [32, Lemma 14.1] to write the free energy as

$$F_g(\beta, N, L) = -T \ln \sup_{\substack{\{\psi_k\} \\ \langle \psi_i | \psi_j \rangle_g = \delta_{ij}}} \sum_k e^{-\beta \mathcal{E}_g(\psi_k)} \tag{5.2.4}$$

where $\langle \cdot | \cdot \rangle_g$ denotes the inner product on $L^2((\mathbb{R}^3 \times \{1, \ldots, q\})^N, g(\vec{x})^2 \mathrm{d}\vec{x})$,

$$\langle \psi_i | \psi_j \rangle_g = \int_{\mathbb{R}^{3N}} g^2(\vec{x}) \overline{\psi_i(\vec{y})} \psi_j(\vec{y}) \mathrm{d}\vec{y}, \tag{5.2.5}$$

and the supremum is over all finite sets of orthonormal functions in $\mathcal{A}_q^N$ with support in $([0, L]^3)^N$. We are interested in the thermodynamic limit

$$f_g(\beta, \rho) = \lim_{N \to \infty} \frac{\rho}{N} F_g(\beta, N, (N/\rho)^{1/3}) \tag{5.2.6}$$

where $\rho > 0$ denotes the particle density.

In the non-interacting case corresponding to taking $g \equiv 1$, the free energy density can be evaluated explicitly, and is given by [67]

$$f(\beta, \rho) = \sup_{\mu \in \mathbb{R}} \left[\mu\rho - \frac{qT}{(2\pi)^3} \int_{\mathbb{R}^3} \ln\left(1 + e^{-\beta(p^2 - \mu)}\right) dp \right] \tag{5.2.7}$$

Our main result shows that the two functions, f_g and f, are actually identical.

Theorem 5.2.1. *For any $\beta > 0$ and $\rho > 0$, and any $q \geq 1$,*

$$f_g(\beta, \rho) = f(\beta, \rho) \tag{5.2.8}$$

We shall actually prove a stronger result below, namely a lower bound on $F_g(\beta, N, L)$ for finite N which agrees with the corresponding expression for non-interacting particles, $F(\beta, N, L)$, to leading order in N, with explicit bounds on the correction term. Note that the corresponding upper bound is trivial, since for functions $\phi \in C_0^\infty((\mathbb{R}^3 \times \{1,\ldots,q\})^N)$

$$\mathcal{E}_g(\phi/g) = \sum_{i=1}^{N} \int |\nabla_i \phi(\vec{y})|^2 \, d\vec{y} \tag{5.2.9}$$

and hence $F_g(\beta, N, L) \leq F(\beta, N, L)$. Moreover, as already noted above one has $F_g(\beta, N, L) = F(\beta, N, L)$ for $q = 1$, since functions in $\mathcal{A}_1^N$ vanish whenever $x_i = x_j$ for some $i \neq j$. Hence it suffices to consider the case $q \geq 2$.

Theorem 5.2.1 also holds true for the ground state energy, i.e., $\beta = \infty$, where $f(\infty, \rho) = \frac{3}{5}(6\pi^2/q)^{2/3}\rho^{5/3}$. The proof of the equality (5.2.8) in this case is actually substantially easier, as the analysis of the entropy in Section 5.6 is not needed.

Intuitively, the result in Theorem 5.2.1 can be explained via a comparison of (5.2.2) with (5.1.1). Effectively, the scattering process between two particles, i and j, say, corresponds to a non-zero scattering length of the form

$$-\frac{1}{a_{\text{eff}}} = \sum_{\{k,l\} \neq \{i,j\}} \frac{1}{|x_k - x_l|}. \tag{5.2.10}$$

In the limit of large particle number, the sum of these other terms diverges, corresponding to an effective scattering length zero, i.e., no interactions.

A minor modification of the proof shows that Theorem 5.2.1 also holds for a model where the function $1/|x|$ in (5.2.1) is replaced by $1/|x| - 1/a$ for $a \leq 0$, corresponding to a two-body interaction with negative scattering length a. This only increases the effective scattering length a_{eff}.

From Theorem 5.2.1 we conclude that the model (5.2.2) is not suitable to describe a gas of fermions with point interactions, as it becomes trivial in the thermodynamic limit. No non-trivial models that are proven to be stable for arbitrary particle number exist to this date, however. Such non-trivial models are not expected to be given by a Dirichlet form of the type (5.2.2), since such forms are naturally well-defined even in the bosonic case, where point-interaction models are known to become unstable due to the Thomas effect [8,11,17,61,68,73].

In the remainder of this paper, we shall give the proof of Theorem 5.2.1. We start with a short outline of the main steps in the next section.

5.3 Outline of the proof

In the first step in Section 5.4 we shall localize particles in small boxes. This part of the Dirichlet–Neumann bracketing technique is quite standard, but it does not directly allow us to reduce the problem to fewer particles, as the interactions depend on the location of all the particles, including the ones in different boxes. Still this step allows us to compare our model with the corresponding one for non-interacting fermions, by utilizing a suitable version of the Hardy inequality to quantify the effect of the deviation of the weight function g in (5.2.1) from being a constant. This analysis is done in Section 5.5. Note that the relevant constant to compare g with depends on the distribution of the particles in the various boxes, hence the importance of the first step. An important point in the analysis is a control on the particle number distribution, which is obtained in Prop. 5.

In Section 5.6 we shall give a rough bound on the entropy for large energy, which will allow us to conclude that that to compute the free energy (5.2.4), it suffices to consider only states with energy $E \lesssim N \ln N$. We do this by applying the localization technique to very small boxes, with side length decreasing with energy, in order to have to consider effectively only the ground states in each small box.

In the low energy sector, corresponding to energies $E \lesssim N \ln N$, our bounds in Section 5.5 allow to make a direct comparison of our model with non-interacting fermions. This comparison is detailed in Section 5.7. For this purpose, we shall choose much larger boxes than in the previous step, very slowly increasing to infinity with N in order for finite size effects to vanish in the thermodynamic limit. Finally, Section 5.8 collects all the results in the previous sections to give the proof of Theorem 5.2.1.

Throughout the proof, we shall use the letter c for universal constants independent of all parameters, even though c might have different values at different occurrences. Similarly, we use c_η for functions of $\eta = \beta\rho^{2/3}$ that are uniformly bounded for $\eta > \varepsilon$ for any $\varepsilon > 0$. Note that the free energy for noninteracting particles in (5.2.7) satisfies the scaling relation

$$f(\beta, \rho) = \rho^{5/3} f(\eta, 1)\,, \qquad \eta = \beta\rho^{2/3}\,, \tag{5.3.1}$$

and $\eta \to \infty$ corresponds to the zero-temperature limit.

5.4 Particle localization in small boxes

Given an integer $m \geq 2$, we shall divide the cube $[0, L]^3$ into $M = m^3$ disjoint cubes of side length $\ell = L/m$, denoted by $\{B_i\}_{i=1}^M$. In order to obtain a lower bound on $\mathcal{E}_g$, we introduce Neumann boundary conditions on the boundary of each box B_i.

Specifically, given a vector $\vec{n} = \{n_1, \ldots, n_M\}$ of nonnegative integers with $\sum_{j=1}^M n_j = N$, let $\mathcal{B}_{\mathrm{sym}}(\vec{n})$ denote the subset of $[0, L]^{3N}$ where exactly n_j particles are in B_j, for all $1 \leq j \leq M$. More precisely, if

$$\mathcal{B}(\vec{n}) = B_1^{n_1} \times \cdots \times B_M^{n_M} \tag{5.4.1}$$

and, for general $A \subset \mathbb{R}^{3N}$ and $\pi \in S^N$ (the permutation group of N elements)

$$\pi(A) = \{\vec{x} : \pi^{-1}(\vec{x}) \in A\}\,, \qquad \pi(\vec{x}) := (x_{\pi(1)}, \ldots, x_{\pi(N)}) \tag{5.4.2}$$

we have

$$\mathcal{B}_{\mathrm{sym}}(\vec{n}) = \bigcup_{\pi \in S^N} \pi(\mathcal{B}(\vec{n})) \tag{5.4.3}$$

Then clearly

$$1 = \sum_{\vec{n}} \chi_{\mathcal{B}_{\mathrm{sym}}(\vec{n})}(\vec{x}) \tag{5.4.4}$$

for almost every $\vec{x} \in [0, L]^{3N}$. Correspondingly one can write for any $\psi \in \mathcal{A}_q^N$ supported in $[0, L]^{3N}$

$$\psi(\vec{y}) = \sum_{\vec{n}} \chi_{\mathcal{B}_{\mathrm{sym}}(\vec{n})}(\vec{x})\psi(\vec{y}) =: \sum_{\vec{n}} \psi^{\vec{n}}(\vec{y})\,. \tag{5.4.5}$$

Note that each $\psi^{\vec{n}}$ is a function in $\mathcal{A}_q^N$ with the property that it is non-zero only if exactly n_j particles are in B_j for any $1 \leq j \leq M$. In particular, the functions appearing in the decomposition on the right side of (5.4.5) all have disjoint support.

Conversely, given a set of functions $\psi^{\vec{n}} \in \mathcal{A}_q^N$ supported in $\mathcal{B}_{\mathrm{sym}}(\vec{n})$, we can define $\psi \in \mathcal{A}_q^N$ via (5.4.5). Hence there is a one-to-one correspondence between functions in $\mathcal{A}_q^N$ and sets of functions $\psi^{\vec{n}}$. We now redefine our energy functional $\mathcal{E}_g$ as

$$\mathcal{E}_g^\ell(\psi) = \sum_{\vec{n}} \sum_{i=1}^N \int_{\mathcal{B}_{\mathrm{sym}}(\vec{n})} g(\vec{x})^2 |\nabla_i \psi^{\vec{n}}(\vec{y})|^2 \mathrm{d}\vec{y} \tag{5.4.6}$$

This coincides with the definition (5.2.2) in case $\psi \in H^1((\mathbb{R}^3 \times \{1,\ldots,q\})^N, g(\vec{x})^2 \mathrm{d}\vec{x})$, but is more general since it allows for wave functions that are discontinuous at the boundaries of the B_j, effectively introducing Neumann boundary conditions there.

Note that with the definition (5.4.6) above, we have

$$\mathcal{E}_g^\ell(\psi) = \sum_{\vec{n}} \mathcal{E}_g^\ell(\psi^{\vec{n}}) \quad \text{for } \psi = \sum_{\vec{n}} \psi^{\vec{n}} \tag{5.4.7}$$

In particular, the corresponding operator is diagonal with respect to the direct sum decomposition of $\mathcal{A}_q^N$ into functions supported on $\mathcal{B}_{\mathrm{sym}}(\vec{n})$, and hence the min-max principle implies the bound

$$\sup_{\substack{\{\psi_k\} \\ \langle \psi_i | \psi_j \rangle_g = \delta_{ij}}} \sum_k e^{-\beta \mathcal{E}_g(\psi_k)} \leq \sum_{\vec{n}} \sup_{\substack{\{\psi_k^{\vec{n}}\} \\ \langle \psi_i^{\vec{n}} | \psi_j^{\vec{n}} \rangle_g = \delta_{ij}}} \sum_k e^{-\beta \mathcal{E}_g^\ell(\psi_k^{\vec{n}})} \tag{5.4.8}$$

where on the right side it is understood that each $\psi_j^{\vec{n}}$ is supported in $\mathcal{B}_{\mathrm{sym}}(\vec{n})$.

As a final step in this section we want to simplify the problem by getting rid of the antisymmetry requirement for particles localized in different boxes. There exists a simple isometry between functions $\psi^{\vec{n}}$ in $\mathcal{A}_q^N$ and functions whose support is on the smaller set $\mathcal{B}(\vec{n})$ in (5.4.1), where $x_1, \ldots, x_{n_1} \in B_1$, $x_{n_1+1}, \ldots, x_{n_1+n_2} \in B_2$, etc., and which are antisymmetric only with respect to permutations of the y_i corresponding to x_i in the same box. This isometry is simply

$$\psi^{\vec{n}} \mapsto \left(\frac{N!}{\prod_{j=1}^M n_j!} \right)^{1/2} \chi_{\mathcal{B}(\vec{n})} \psi^{\vec{n}} \tag{5.4.9}$$

Note that the normalization factor is chosen such that both sides have the same norm, and the left side can be obtained from the right by a suitable antisymmetrization over all variables y_i. Moreover, both functions yield the same value when plugged into $\mathcal{E}_g^\ell$. Let $\mathcal{A}_q^{N,\ell}(\vec{n})$ denote the set $\{\chi_{\mathcal{B}(\vec{n})}\psi \,:\, \psi \in \mathcal{A}_q^N\}$, i.e., functions supported in $\mathcal{B}(\vec{n})$ that are antisymmetric in the variables corresponding to the same box. The bound (5.4.8) and the above observation imply that

$$F_g(\beta, N, L) \geq -T \ln \sum_{\vec{n}} \sup_{\substack{\{\psi_k \in \mathcal{A}_q^{N,\ell}(\vec{n})\} \\ \langle \psi_i | \psi_j \rangle_g = \delta_{ij}}} \sum_k e^{-\beta \mathcal{E}_g^\ell(\psi_k)} \tag{5.4.10}$$

5.5 Energy and norm bounds

Our goal in this next step to derive a lower bound on $\mathcal{E}_g^\ell(\psi)$ for $\psi \in \mathcal{A}_q^{N,\ell}(\vec{n})$, i.e., functions supported in $\mathcal{B}(\vec{n})$, and to compare the norm of such a ψ with the standard, unweighted L^2

norm. For this purpose, we shall need a certain version of the Hardy inequality, which will be derived in the next subsection.

5.5.1 Hardy inequalities

Recall the usual Hardy inequality

$$\int_{\mathbb{R}^3} |\nabla f(x)|^2 \mathrm{d}x \geq \frac{1}{4} \int_{\mathbb{R}^3} \frac{|f(x)|^2}{|x|^2} \mathrm{d}x \tag{5.5.1}$$

for functions $f \in \dot{H}^1(\mathbb{R}^3)$. We shall need a local version of (5.5.1) on balls.

Lemma 5.5.1. *Let $B_\ell \subset \mathbb{R}^3$ denote the open centered ball with radius ℓ. For any $f \in H^1(B_\ell)$*

$$2\int_{B_\ell} |\nabla f(x)|^2 \mathrm{d}x + \frac{9}{2\ell^2} \int_{B_\ell} |f(x)|^2 \mathrm{d}x \geq \frac{1}{4} \int_{B_\ell} \frac{|f(x)|^2}{|x|^2} \mathrm{d}x \tag{5.5.2}$$

Proof. We apply the Hardy inequality (5.5.1) to the function $h(x) = f(x)[1 - |x|/\ell]_+$, where $[\,\cdot\,]_+$ denotes the positive part. For the right side of (5.5.1) we obtain

$$\begin{aligned} \frac{1}{4} \int_{B_\ell} \frac{|h(x)|^2}{|x|^2} \mathrm{d}x &= \frac{1}{4} \int_{B_\ell} \frac{|f(x)|^2}{|x|^2} \left(1 - \frac{2|x|}{\ell} + \frac{|x|^2}{\ell^2}\right) \mathrm{d}x \\ &\geq \frac{1-\varepsilon}{4} \int_{B_\ell} \frac{|f(x)|^2}{|x|^2} \mathrm{d}x - \frac{1-\varepsilon}{4\varepsilon\ell^2} \int_{B_\ell} |f(x)|^2 \mathrm{d}x \end{aligned} \tag{5.5.3}$$

for any $\varepsilon > 0$. For the left side of (5.5.1) a simple Schwarz inequality yields

$$\int_{B_\ell} |\nabla h(x)|^2 \mathrm{d}x \leq (1+\delta) \int_{B_\ell} |\nabla f(x)|^2 \mathrm{d}x + \frac{1+\delta}{\delta\ell^2} \int_{B_\ell} |f(x)|^2 \mathrm{d}x \tag{5.5.4}$$

for $\delta > 0$. In combination we obtain the desired inequality (5.5.2) by choosing $\varepsilon = 1/6$ and $\delta = 2/3$. □

For later use we need a version of Lemma 5.5.1 on cubes with arbitrary location relative to the singularity.

Lemma 5.5.2. *Let $C_\ell = [0, \ell]^3$. For any $y \in \mathbb{R}^3$ and any $f \in H^1(C_\ell)$,*

$$c_0 \int_{C_\ell} |\nabla f(x)|^2 \mathrm{d}x + \frac{c_1}{\ell^2} \int_{C_\ell} |f(x)|^2 \mathrm{d}x \geq \frac{1}{4} \int_{C_\ell} \frac{|f(x)|^2}{|x-y|^2} \mathrm{d}x \tag{5.5.5}$$

with $c_0 \leq 16$ and $c_1 \leq 144$.

The stated bounds on the constants c_0 and c_1 are presumably far from optimal, but suffice for our purpose.

Proof. If $y \notin C_\ell$, we can replace it by the point in C_ℓ closest to y. This can only increase the right side. Hence we may assume that $y \in C_\ell$. Let B denote the ball of radius $\ell/2$ around y. Then

$$\frac{1}{4}\int_{C_\ell \setminus B} \frac{|f(x)|^2}{|x-y|^2} \mathrm{d}x \le \frac{1}{\ell^2}\int_{C_\ell \setminus B} |f(x)|^2 \,\mathrm{d}x \tag{5.5.6}$$

Define a function $\tilde{f}$ by extending f to $[-\ell, 2\ell]^3$ as

$$\tilde{f}(x_1, x_2, x_3) = f(\tau(x_1), \tau(x_2), \tau(x_3)) \tag{5.5.7}$$

where

$$\tau(x) := \begin{cases} -x & x \in [-\ell, 0] \\ x & x \in [0, \ell] \\ 2\ell - x & x \in [\ell, 2\ell] \end{cases} \tag{5.5.8}$$

Then $\tilde{f} \in H^1([-\ell, 2\ell]^3)$. Since $B \subset [-\ell, 2\ell]^3$, we get with the aid of the Hardy inequality (5.5.2) on B (with $\ell/2$ in place of ℓ)

$$\begin{aligned} \frac{1}{4}\int_{C_\ell \cap B} \frac{|f(x)|^2}{|x-y|^2} \mathrm{d}x &\le \frac{1}{4}\int_B \frac{|\tilde{f}(x)|^2}{|x-y|^2} \mathrm{d}x \\ &\le 2\int_B |\nabla \tilde{f}(x)|^2 \mathrm{d}x + \frac{18}{\ell^2}\int_B |\tilde{f}(x)|^2 \mathrm{d}x \\ &\le 8\left(2\int_{C_\ell \cap B} |\nabla f(x)|^2 \mathrm{d}x + \frac{18}{\ell^2}\int_{C_\ell \cap B} |f(x)|^2 \mathrm{d}x\right) \end{aligned} \tag{5.5.9}$$

In the last step, we used that B intersects, besides C_ℓ, at most 7 other translates of C_ℓ, and that the intersection of B with these translates are, when reflected back to C_ℓ, contained in $C_\ell \cap B$ (see Fig. 5.1). In combination, (5.5.6) and (5.5.9) imply (5.5.5). □

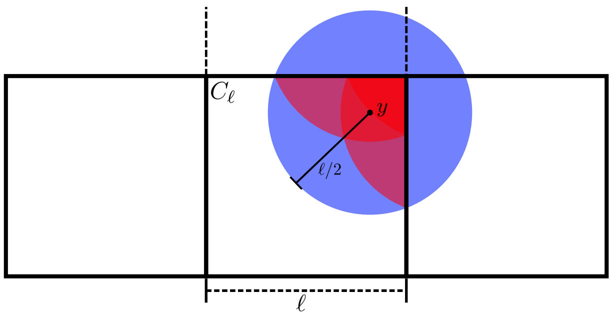

Figure 5.1: Two-dimensional illustration of the reflection technique used in the proof of Lemma 5.5.2. The box C_ℓ and two of its neighbor boxes are shown, as well as the ball B around $y \in C_\ell$. Using the extended function $\tilde{f}$ we can mirror $C_\ell \setminus B$ back into $C_\ell \cap B$. There are at most 8 reflected components in three dimensions, the worst case being if the ball B intersects with a corner of C_ℓ.

5.5.2 A lower bound on $\mathcal{E}_g^\ell$

Let ψ be an $L^2((\mathbb{R}^3 \times \{1,\dots,q\})^N, g(\vec{x})^2 \mathrm{d}\vec{y})$-normalized function in $\mathcal{A}_q^{N,\ell}(\vec{n})$, defined just above (5.4.10). Let d_{jk} denote the distance between boxes B_j and B_k. For $\vec{x} \in \mathcal{B}(\vec{n})$, we can bound

$$g(\vec{x}) \geq \sum_{1\leq j<k\leq M} \frac{n_j n_k}{d_{jk} + 2\sqrt{3}\ell} + \sum_{j=1}^{M} \frac{n_j(n_j-1)}{2\sqrt{3}\ell} \geq K_- + \frac{V}{4\sqrt{3}\ell} \tag{5.5.10}$$

where

$$K_- = \sum_{\substack{1\leq j<k\leq M \\ d_{jk}>0}} \frac{n_j n_k}{d_{jk} + 2\sqrt{3}\ell} \quad \text{and} \quad V = \sum_{j=1}^{M} n_j(n_j + m_j - 1) \tag{5.5.11}$$

Here m_k denotes the total number of particles in the 26 neighboring boxes of B_k. The bound (5.5.10) immediately leads to the lower bound

$$\mathcal{E}_g^\ell(\psi) \geq \left(K_- + \frac{V}{4\sqrt{3}\ell}\right)^2 \mathcal{E}^\ell(\psi) \tag{5.5.12}$$

for $\psi \in \mathcal{A}_q^{N,\ell}(\vec{n})$, where $\mathcal{E}^\ell$ on the right side stands for the energy functional for noninteracting particles, corresponding to $g \equiv 1$ in (5.4.6).

5.5.3 Bounds on norms

In the following, it will be necessary to compare the norm $\|\cdot\|_g = \langle\cdot|\cdot\rangle_g^{1/2}$ with the standard L^2 norm $\|\cdot\|$ without weight. For $\psi \in \mathcal{A}_q^{N,\ell}(\vec{n})$, the bound (5.5.10) immediately implies the lower bound

$$\|\psi\|_g \geq \left(K_- + \frac{V}{4\sqrt{3}\ell}\right)\|\psi\| \tag{5.5.13}$$

To obtain a corresponding upper bound, we proceed as follows. For given i, corresponding to $x_i \in B_k$ for some box B_k, let $\mathcal{N}[i]$ be the set of js with $j \neq i$ such that x_j is either in the same box B_k or in one of the 26 neighboring boxes touching B_k. With m_k as defined above, $|\mathcal{N}[i]| = n_k + m_k - 1$ for $x_i \in B_k$. Then

$$g(\vec{x}) \leq \frac{1}{2}\sum_{i=1}^{N}\sum_{j\in\mathcal{N}[i]} \frac{1}{|x_i - x_j|} + K_+ \quad \text{with} \quad K_+ = \sum_{\substack{1\leq j<k\leq M \\ d_{jk}>0}} \frac{n_j n_k}{d_{jk}} \tag{5.5.14}$$

for $\vec{x} \in \mathcal{B}(\vec{n})$. The Cauchy-Schwarz inequality implies

$$\|\psi\|_g^2 \leq (1+\varepsilon)K_+^2\|\psi\|^2 + \left(1+\varepsilon^{-1}\right)\frac{V}{4}\sum_{i=1}^{N}\sum_{j\in\mathcal{N}[i]} \int \frac{|\psi(\vec{y})|^2}{|x_i - x_j|^2}\mathrm{d}\vec{y} \tag{5.5.15}$$

for any $\varepsilon > 0$, where V is defined in (5.5.11). In the last term, we use the Hardy inequality (5.5.5) for the integration over x_i, and obtain

$$\begin{aligned}\|\psi\|_g^2 \leq &\left[(1+\varepsilon)K_+^2 + \frac{c_1}{\ell^2}\left(1+\varepsilon^{-1}\right)V^2\right]\|\psi\|^2 \\ &+ \left(1+\varepsilon^{-1}\right)c_0 V \sum_{i=1}^{N} |\mathcal{N}[i]| \int |\nabla_i \psi(\vec{y})|^2 \, \mathrm{d}\vec{y}\end{aligned} \tag{5.5.16}$$

If we reinsert $g(\vec{x})^2$ into the last integrand using (5.5.10), we thus obtain the following lemma.

Lemma 5.5.3. *For $\psi \in \mathcal{A}_q^{N,\ell}(\vec{n})$, we have the bounds*

$$\left(K_- + \frac{V}{4\sqrt{3}\ell}\right)^2 \|\psi\|^2 \le \|\psi\|_g^2 \le (1+\varepsilon)\left[K_+^2 + \frac{c_1}{\varepsilon\ell^2}V^2\right]\|\psi\|^2$$
$$+ \frac{(1+\varepsilon^{-1})c_0 V}{\left(K_- + \frac{V}{4\sqrt{3}\ell}\right)^2}\sum_{i=1}^N |\mathcal{N}[i]| \int |\nabla_i\psi(\vec{y})|^2 g(\vec{x})^2\,\mathrm{d}\vec{y} \tag{5.5.17}$$

for any $\varepsilon > 0$, where $K_\pm$ and V are defined in (5.5.11) *and* (5.5.14)*, respectively.*

5.5.4 A bound on the number of particles in a box

Let again ψ be a wavefunction in $\mathcal{A}_q^{N,\ell}(\vec{n})$ and let us assume it is normalized, i.e., $\|\psi\|_g = 1$. We have the following a priori bound.

Proposition 5. *There exists a constant $\kappa > 0$ such that for any normalized $\psi \in \mathcal{A}_q^{N,\ell}(\vec{n})$ and any $\ell > 0$ we have*

$$\mathcal{E}_g^\ell(\psi) \ge \frac{\kappa}{q^{2/3}}\sum_{j=1}^M \frac{\left[n_j - q\right]_+^{5/3}}{\ell^2} \tag{5.5.18}$$

Here $[\,\cdot\,]_+ = \max\{0, \cdot\}$ denotes the positive part. The bound (5.5.18) allows us to conclude that for all normalized $\psi \in \mathcal{A}_q^{N,\ell}(\vec{n})$ with $\mathcal{E}_g^\ell(\psi) < E$ we have $n_j \le q$ for all j if we choose ℓ such that $E\ell^2 q^{2/3} \le \kappa$. Furthermore, for large $E\ell^2$ we get the bound $\max_j n_j \lesssim q^{2/5}(E\ell^2)^{3/5}$.

Proof. We use Lemma 3 from [25] which states that for a subset $A \subseteq \{1,\dots,N\}$ corresponding to particles $x_k \in B_j$ for $k \in A$,

$$\sum_{i\in A}\int_{B_j^{|A|}} g(\vec{x})^2|\nabla_i\psi(\vec{y})|^2\mathrm{d}\vec{y}_A \ge \frac{\tilde{\kappa}}{\ell^2}\left[|A| - q\right]_+ \int_{B_j^{|A|}} g(\vec{x})^2|\psi(\vec{y})|^2\mathrm{d}y_A \tag{5.5.19}$$

for some $\tilde{\kappa} > 0$ independent of A, ℓ and ψ. Here $\vec{y}_A$ is short for $\{y_i\}_{i\in A}$. Integrating this over the $\{y_j\}_{j\notin A}$ and summing over j yields (5.5.18) with the exponent $5/3$ replaced by 1, and $\kappa = \tilde{\kappa}q^{2/3}$.

To raise the exponent from 1 to $5/3$, we partition B_j into μ^3 disjoint cubes $\{C_k\}_k$ of side length ℓ/μ for some integer $\mu \ge 1$. We use the identity

$$1 = \sum_{Q\subseteq A}\prod_{s\in Q}\chi_{C_k}(x_s)\prod_{t\in Q^c}\chi_{C_k^c}(x_t) \tag{5.5.20}$$

for $\vec{x}_A \in B_j^{|A|}$, where Q^c denotes $A\setminus Q$ and $C_k^c = B_j \setminus C_k$. By plugging (5.5.20) into (5.5.19) we obtain

$$\sum_{i\in A}\int_{B_j^{|A|}} g(\vec{x})^2|\nabla_i\psi(\vec{y})|^2\mathrm{d}\vec{y}_A = \sum_{i\in A}\sum_{k=1}^{\mu^3}\int_{B_j^{|A|}}\chi_{C_k}(x_i)g(\vec{x})^2|\nabla_i\psi(\vec{y})|^2\mathrm{d}\vec{y}_A$$
$$= \sum_{i\in A}\sum_{k=1}^{\mu^3}\sum_{Q\subseteq A}\int_{B_j^{|A|}}\prod_{s\in Q}\chi_{C_k}(x_s)\prod_{t\in Q^c}\chi_{C_k^c}(x_t)\chi_{C_k}(x_i)g(\vec{x})^2|\nabla_i\psi(\vec{x})|^2\mathrm{d}\vec{x}_A$$
$$= \sum_{k=1}^{\mu^3}\sum_{Q\subseteq A}\sum_{i\in Q}\int_{B_j^{|A|}}\prod_{s\in Q}\chi_{C_k}(x_s)\prod_{t\in Q^c}\chi_{C_k^c}(x_t)g(\vec{x})^2|\nabla_i\psi(\vec{x})|^2\mathrm{d}\vec{x}_A \tag{5.5.21}$$

For the integration over $\{y_s\}_{s\in Q}$ we can again use (5.5.19), with suitably rescaled variables to replace the integration over B_j with the one over C_k. (Note that g is homogeneous of order -1 and satisfies the simple scaling property $g(\lambda\vec{x}) = \lambda^{-1}g(\vec{x})$ for $\lambda > 0$.) This yields the bound

$$
\begin{aligned}
(5.5.21) &\geq \sum_{k=1}^{\mu^3} \sum_{Q\subseteq A} \frac{\mu^2\tilde{\kappa}}{\ell^2} (|Q| - q) \int_{C_k^{|Q|}} \mathrm{d}\vec{y}_Q \int_{C_k^{c(|A|-|Q|)}} \mathrm{d}\vec{y}_{Q^c}\, g(\vec{x})^2 |\psi(\vec{y})|^2 \\
&= \frac{\mu^2\tilde{\kappa}}{\ell^2}(|A| - \mu^3 q) \int_{B_j^{|A|}} g(\vec{x})^2|\psi(\vec{y})|^2 \mathrm{d}\vec{y}_A
\end{aligned}
\tag{5.5.22}
$$

In the last step, we used again the identity (5.5.20) as well as

$$
|A| = \sum_{k=1}^{\mu^3} \sum_{Q\subseteq A} |Q| \prod_{s\in Q} \chi_{C_k}(x_s) \prod_{t\in Q^c} \chi_{C_k^c}(x_t) \tag{5.5.23}
$$

Since the left side of (5.5.22) is obviously non-negative, we can replace $|A| - \mu^3 q$ by its positive part on the right side.

It remains to choose μ. If we ignore the restriction that $\mu \geq 1$ is an integer, we would choose $\mu = (2/5)(|A|/q)^{1/3}$ to obtain the desired coefficient $\propto |A|^{5/3}/q^{2/3}$. It is easy to see that

$$
\sup_{\mu\in\mathbb{N}} \mu^2 \left[|A| - \mu^3 q\right]_+ \geq \frac{c}{q^{2/3}} \left[|A| - q\right]_+^{5/3} \tag{5.5.24}
$$

for some universal constant $c > 0$. This proves the desired bound, with $\kappa = \tilde{\kappa}c$. □

5.6 A bound on the entropy

In this section we shall use the estimates above to give a rough bound on

$$
N_g(E) = \operatorname{tr} \chi_{H_g<E}\,, \tag{5.6.1}
$$

that is, the maximal number of orthonormal functions in $\mathcal{A}_q^N$ with $\mathcal{E}_g(\psi) < E$, for some (large) E. Its logarithm is, by definition, the entropy. Using the localization technique described in Section 5.4, the min-max principle implies that

$$
N_g(E) \leq \sum_{\vec{n}} N_g^{\vec{n}}(E) \tag{5.6.2}
$$

where $N_g^{\vec{n}}(E)$ is the maximal number of orthonormal functions in $\mathcal{A}_q^{N,\ell}(\vec{n})$ with $\mathcal{E}_g^{\ell}(\psi) < E$. Given E, we shall choose ℓ small enough such $E\ell^2 q^{2/3} \leq \kappa$, with κ the constant in Prop. 5. As remarked there, this implies that $n_j \leq q$ for all $1 \leq j \leq M$.

We will actually show that if $E\ell^2$ is small enough, then the spectral gap for an excitation is larger than E, and hence $N_g^{\vec{n}}(E)$ is simply equal to the dimension of the space of ground states.

Lemma 5.6.1. *There exists a universal constant $c > 0$ such that if we choose $E\ell^2 \leq c$, then*

$$
N_g^{\vec{n}}(E) = \prod_{j=1}^{M} \binom{q}{n_j} \tag{5.6.3}
$$

Proof. With the aid of (5.5.12) we have

$$\mathcal{E}_g^\ell(\psi) \geq \left(K_- + \frac{V}{4\sqrt{3}\ell}\right)^2 \mathcal{E}^\ell(\psi) \tag{5.6.4}$$

for $\psi \in \mathcal{A}_q^{N,\ell}(\vec{n})$. The ground states of the operator corresponding to the quadratic form $\mathcal{E}^\ell$ are all constant, i.e., they are simply products of anti-symmetric functions of the spin variables corresponding to each box, and have zero energy. The spectral gap above the ground state energy is given by $(\pi/\ell)^2$. With P_0 denoting the projection in $L^2(\mathcal{B}(\vec{n}), \mathrm{d}\vec{y})$ onto the ground state space, we thus have

$$\mathcal{E}^\ell(\psi) \geq \frac{\pi^2}{\ell^2} \|(1-P_0)\psi\|^2 \tag{5.6.5}$$

In order to bound the norm on the right side from below in terms of the weighted $\|\cdot\|_g$ norm, we shall use Lemma 5.5.3. In (5.5.17), we can simply bound

$$\sum_{i=1}^N |\mathcal{N}[i]| \int |\nabla_i\psi(\vec{y})|^2 g(\vec{x})^2\, \mathrm{d}\vec{y} < E\, \|\psi\|_g^2 \sum_{i=1}^N |\mathcal{N}[i]| = EV\, \|\psi\|_g^2 \tag{5.6.6}$$

to obtain

$$\|\psi\|_g^2 \leq \left[(1+\varepsilon)K_+^2 + \frac{c_1}{\ell^2}\left(1+\varepsilon^{-1}\right)V^2\right]\|\psi\|^2 + 48c_0\left(1+\varepsilon^{-1}\right)E\ell^2\|\psi\|_g^2 \tag{5.6.7}$$

for any $\varepsilon > 0$ and any $\psi \in \mathcal{A}_q^{N,\ell}(\vec{n})$ with $\mathcal{E}_g^\ell(\psi) < E\|\psi\|_g^2$. If $E\ell^2$ is small, we can take $\varepsilon = 1$ to conclude that

$$\|\psi\|_g^2 \leq c\left[K_+^2 + V^2\ell^{-2}\right]\|\psi\|^2 \tag{5.6.8}$$

Moreover, note that $K_+ \leq (1+2\sqrt{3})K_-$, since $d_{jk} > 0$ actually implies $d_{jk} \geq \ell$. We thus also have that

$$\|\psi\|_g^2 \leq c\left(K_- + \frac{V}{4\sqrt{3}\ell}\right)^2 \|\psi\|^2 \tag{5.6.9}$$

Applying this to $(1-P_0)\psi$ in (5.6.5) and inserting the resulting bound in (5.6.4) we obtain

$$\mathcal{E}_g^\ell(\psi) \geq c\ell^{-2}\, \|(1-P_0)\psi\|_g^2 \tag{5.6.10}$$

Finally, note that the ground states of $\mathcal{E}_g^\ell$ and $\mathcal{E}^\ell$ actually agree, up to a multiplicative normalization constant. Hence, if ψ is orthogonal to a ground state with respect to the inner product $\langle\cdot|\cdot\rangle_g$, then

$$\|(1-P_0)\psi\|_g^2 = \|\psi\|_g^2 + \|P_0\psi\|_g^2 \geq \|\psi\|_g^2 \tag{5.6.11}$$

This concludes the proof. □

In combination with (5.6.2), Lemma 5.6.1 yields the bound

$$N_g(E) \leq \sum_{\vec{n}} \prod_{j=1}^M \binom{q}{n_j} = \binom{qM}{N} \leq \left(\frac{qMe}{N}\right)^N \tag{5.6.12}$$

for $E\ell^2 \leq c$. We recall that the number of boxes is $M = (L/\ell)^3 = N/(\rho\ell^3)$, which is large for $E\ell^2 \sim 1$ and $E \gg L^{-2}$. Hence we get the upper bound

$$N_g(E) \leq \left(c\frac{qE^{3/2}}{\rho}\right)^N \tag{5.6.13}$$

for a suitable constant $c > 0$. This bound readily implies the following proposition.

Proposition 6. *Let $\{E_j\}_j$ denote the eigenvalues of the Hamiltonian H_g associated to the quadratic form $\mathcal{E}_g$ in* (5.2.2) *on $\mathcal{A}_q^N$. For given $\eta = \beta\rho^{2/3}$ there exists a $c_\eta > 0$ such that if $\bar{E} \geq c_\eta \beta^{-1} N \ln N$ then*

$$\sum_{E_j \geq \bar{E}} e^{-\beta E_j} \leq 2\, e^{-\frac{1}{2}\beta\bar{E}} \tag{5.6.14}$$

Proof. We have

$$\sum_{E_j \geq \bar{E}} e^{-\beta E_j} \leq \sum_{k\geq 0} N_g((k+2)\bar{E}) e^{-(k+1)\beta\bar{E}} \tag{5.6.15}$$

and thus the result follows if

$$N_g((k+2)\bar{E}) e^{-(k+\frac{1}{2})\beta\bar{E}} \leq \frac{1}{2^k} \tag{5.6.16}$$

for all $k \geq 0$. Using the bound (5.6.13) one easily checks that this is the case under the stated condition on $\bar{E}$ for suitable η. □

For evaluating the free energy, we can thus limit our attention to eigenvalues E_j satisfying $\beta E_j \leq c_\eta N \ln N$ for suitable $c_\eta > 0$. We shall show in the next section that in this low energy sector the eigenvalues are well approximated by the corresponding ones for non-interacting particles.

5.7 Comparison with non-interacting particles in the low-energy sector

We shall now investigate the bounds derived in Section 5.5 more closely and apply them to the low energy sector, where $\mathcal{E}_g(\psi) \leq E\|\psi\|_g^2$ for some $E \lesssim N \ln N$. We again localize the particles into boxes, this time with much larger ℓ, however. We start with the estimate on the ratio of the norm $\|\psi\|_g$ to the standard, non-weighted L^2 norm $\|\psi\|$.

Proposition 7. *Let $\psi \in \mathcal{A}_q^{N,\ell}(\vec{n})$ satisfy $\mathcal{E}_g^\ell(\psi) \leq E\|\psi\|_g^2$ for some E with $E\ell^2 \gtrsim 1$ for large N. Then*

$$1 \geq \left(K_- + \frac{V}{4\sqrt{3}\ell}\right)^2 \frac{\|\psi\|^2}{\|\psi\|_g^2} \geq 1 - \delta \tag{5.7.1}$$

with

$$\delta \leq c\left[q^{1/5}(E\ell^2)^{3/10} N^{-1/3}(\rho\ell^3)^{-1/6} + q^{2/5}(E\ell^2)^{11/10} N^{-7/6}(\rho\ell^3)^{-1/3}\right] \tag{5.7.2}$$

with K_- and V defined in (5.5.11).

We note that δ is small if

$$E\ell^2 \ll \min\{N^{10/9}(\rho\ell^3)^{5/9}, N^{35/33}(\rho\ell^3)^{10/33}\} \tag{5.7.3}$$

which gives us freedom to choose ℓ large while $E \lesssim N \ln N$. We will choose $\ell \sim N^\nu$ for rather small ν below, in which case the first term in (5.7.2) will be dominating.

Proof. The first bound in (5.7.1) follows immediately (5.5.17). For the lower bound, we use

$$\sum_{i=1}^{N} |\mathcal{N}[i]| \int |\nabla_i \psi(\vec{y})|^2 g(\vec{x})^2 \, d\vec{y} \leq 27\bar{n}E\|\psi\|_g^2 \tag{5.7.4}$$

in (5.5.17), where we denote $\bar{n} = \max_j n_j$. We can also bound $V \leq 27\bar{n}N$ and

$$K_- + \frac{V}{4\sqrt{3}\ell} \geq \frac{N(N-1)}{2\sqrt{3}L} \tag{5.7.5}$$

The second bound in (5.5.17) thus becomes

$$\left[1 - \left(1+\varepsilon^{-1}\right) c_0 \frac{12L^2(27\bar{n})^2}{N(N-1)^2} E\right] \|\psi\|_g^2 \leq \left[(1+\varepsilon)K_+^2 + \frac{c_1}{\ell^2}\left(1+\varepsilon^{-1}\right) V^2\right] \|\psi\|^2 \tag{5.7.6}$$

for arbitrary $\varepsilon > 0$. By assumption $E\ell^2$ is not small, hence we have $\bar{n} \leq cq^{2/5}(E\ell^2)^{3/5}$, as remarked after Proposition 5.

It remains to estimate the ratio K_-/K_+. We distinguish the contribution to the sum coming from $d_{jk} < r\sqrt{3}\ell$ and $d_{jk} \geq r\sqrt{3}\ell$, respectively, for some large integer r to be chosen below. We have

$$\begin{aligned}
K_+ - K_- &= \sum_{\substack{1\leq j<k\leq M \\ d_{jk}>0}} \frac{n_j n_k}{d_{jk}} \frac{2\sqrt{3}\ell}{d_{jk} + 2\sqrt{3}\ell} \\
&\leq \bar{n} \sum_{\substack{1\leq j<k\leq M \\ 0<d_{jk}<r\sqrt{3}\ell}} \frac{n_j}{d_{jk}} \frac{2\sqrt{3}\ell}{d_{jk}+2\sqrt{3}\ell} + \left(1+\frac{r}{2}\right)^{-1} \sum_{\substack{1\leq j<k\leq M \\ d_{jk}\geq r\sqrt{3}\ell}} \frac{n_j n_k}{d_{jk}} && (5.7.7) \\
&\leq c\frac{\bar{n}rN}{\ell} + \left(1+\frac{r}{2}\right)^{-1} K_+ && (5.7.8)
\end{aligned}$$

By optimizing over r as well as ε and using that $\bar{n} \leq cq^{2/5}(E\ell^2)^{3/5}$ we arrive at the desired result. □

In combination with (5.5.12), Proposition 7 yields the lower bound

$$\frac{\mathcal{E}_g^\ell(\psi)}{\|\psi\|_g^2} \geq \frac{\mathcal{E}^\ell(\psi)}{\|\psi\|^2}(1-\delta) \tag{5.7.9}$$

for $\psi \in \mathcal{A}_q^{N,\ell}(\vec{n})$ in the low energy sector $\mathcal{E}_g^\ell(\psi) < E$. This allows us to compare our model directly with non-interacting particles. Note that the eigenfunctions of the operator corresponding to the quadratic form on the right side are tensor products over different boxes and, in particular, the eigenvalues are simply sums over the corresponding eigenvalues of free fermions in each box. The bound (5.7.9) does not directly give us lower bounds on the eigenvalues of H_g, except for the lowest one, however. To complete the proof, we have to estimate the difference between the inner product $\langle \cdot | \cdot \rangle_g$ and the standard inner product on L^2, denoted by $\langle \cdot | \cdot \rangle$ in the following.

We define the multiplication operator

$$G = \left(K_- + \frac{V}{4\sqrt{3}\ell}\right)^{-1} g(\vec{x}) \tag{5.7.10}$$

which is larger or equal to 1 by (5.5.10). The bound (5.5.12) thus reads

$$\frac{\mathcal{E}_g^\ell(\psi)}{\|\psi\|_g^2} \geq \frac{\mathcal{E}^\ell(\psi)}{\|G\psi\|^2} = \frac{\langle\phi|G^{-1}HG^{-1}|\phi\rangle}{\|\phi\|^2} \tag{5.7.11}$$

where we introduced $\phi = G\psi$ and denoted by H the Hamiltonian for non-interacting particles, i.e., the Laplacian on $\mathcal{B}(\vec{n})$ with Neumann boundary conditions. Note that the orthogonality condition $\langle\psi_j|\psi_k\rangle_g = 0$ is equivalent to $\langle\phi_j|\phi_k\rangle = 0$. Given some $E_0 > 0$, we define the cut-off Hamiltonian

$$H_c = H\,\theta(E_0 - H)\,, \tag{5.7.12}$$

with θ denoting the Heaviside step function. This is clearly a bounded operator with $\|H_c\| \leq E_0$. Obviously

$$\langle\phi|G^{-1}HG^{-1}|\phi\rangle \geq \left\|H_c^{1/2}G^{-1}\phi\right\|^2 \tag{5.7.13}$$

which we further bound as

$$\begin{aligned}\left\|H_c^{1/2}G^{-1}\phi\right\|^2 &\geq \left(\left\|H_c^{1/2}\phi\right\| - \left\|H_c^{1/2}(1-G^{-1})\phi\right\|\right)^2\\ &\geq \left\|H_c^{1/2}\phi\right\|^2 - 2\left\|H_c^{1/2}\phi\right\|\left\|H_c^{1/2}\right\|\left\|(1-G^{-1})\phi\right\|\\ &\geq \left\|H_c^{1/2}\phi\right\|^2 - 2E_0\left\|(1-G^{-1})\phi\right\|\|\phi\|\end{aligned} \tag{5.7.14}$$

Now

$$\left\|(1-G^{-1})\phi\right\| \leq \left\|(1-G^{-2})^{1/2}\phi\right\| \leq \delta^{1/2}\,\|\phi\| \tag{5.7.15}$$

where we used $G \geq 1$ in the first and Proposition 7 in the second step. We conclude that

$$\frac{\mathcal{E}_g^\ell(\psi)}{\|\psi\|_g^2} \geq \frac{\langle\phi|H_c - 2E_0\delta^{1/2}|\phi\rangle}{\|\phi\|^2} \tag{5.7.16}$$

under the conditions stated in Proposition 7.

5.8 Convergence of the free energy

We now have all the necessary tools to complete the proof of Theorem 5.2.1. Proposition 6 implies that if we choose $\bar{E} = c_\eta\beta^{-1}N\ln N$ for a suitable constant $c_\eta > 0$, then

$$F_g(\beta, N, L) \geq -T\ln\left(2\,e^{-\frac{1}{2}\beta\bar{E}} + \sup_{\substack{\{\psi_k\in\mathcal{A}_q^N\}\\ \langle\psi_i|\psi_j\rangle_g=\delta_{ij}}} \sum_{k=1}^{N_g(\bar{E})} e^{-\beta\mathcal{E}_g(\psi_k)}\right) \tag{5.8.1}$$

Here $N_g(\bar{E})$ denotes the number of states with energy below $\bar{E}$, which was estimated in (5.6.13). We can write, alternatively,

$$\sup_{\substack{\{\psi_k\} \\ \langle\psi_i|\psi_j\rangle_g=\delta_{ij}}} \sum_{k=1}^{N_g(\bar{E})} e^{-\beta\mathcal{E}_g(\psi_k)} = \sup_{\substack{\{\psi_k\},\,\mathcal{E}_g(\psi_k)<\bar{E} \\ \langle\psi_i|\psi_j\rangle_g=\delta_{ij}}} \sum_k e^{-\beta\mathcal{E}_g(\psi_k)} \tag{5.8.2}$$

By localizing into small boxes of side length ℓ with Neumann boundary conditions, as detailed in Section 5.4, we further have by the min-max principle

$$(5.8.2) \leq \sum_{\vec{n}} \sup_{\substack{\{\psi\in\mathcal{A}_q^{N,\ell}(\vec{n})\},\,\mathcal{E}_g^\ell(\psi)\leq\bar{E} \\ \langle\psi_i|\psi_j\rangle_g=\delta_{ij}}} \sum_k e^{-\beta\mathcal{E}_g^\ell(\psi_k)} \tag{5.8.3}$$

If we choose $\bar{E}\ell^2 \gtrsim 1$, we can apply the bound (5.7.16) from the previous subsection. It implies

$$(5.8.3) \leq e^{2\beta E_0\delta^{1/2}} \sum_{\vec{n}} \sup_{\substack{\{\phi\in G\mathcal{A}_q^{N,\ell}(\vec{n})\},\,\langle\phi_k|H_c|\phi_k\rangle\leq\bar{E}+2E_0\delta^{1/2} \\ \langle\phi_i|\phi_j\rangle=\delta_{ij}}} \sum_k e^{-\beta\langle\phi_k|H_c|\phi_k\rangle} \tag{5.8.4}$$

with δ defined in Proposition 7. If we choose E_0 such that $\bar{E} + 2E_0\delta^{1/2} \leq E_0$, which is possible for $\delta < 1/4$, we can drop the cutoff in H_c and replace H_c by H, the Laplacian on $(\bigcup_j B_j)^N$ with Neumann boundary conditions. To obtain an upper bound on (5.8.4), we can then further neglect the bound on $\langle\phi_k|H|\phi_k\rangle$, and sum over all eigenvalues. We obtain

$$(5.8.4) \leq e^{2\beta E_0\delta^{1/2}} e^{-\beta F(\beta,N,L,\ell)} \tag{5.8.5}$$

where $F(\beta, N, L, \ell)$ denotes the free energy of non-interacting fermions in $\bigcup_j B_j$ (with Neumann boundary conditions on the boundaries of the B_j). In particular, in combination (5.8.1)–(5.8.5) imply

$$F_g(\beta, N, L) \geq F(\beta, N, L, \ell) - 2E_0\delta^{1/2} - T\ln\left(1 + 2\,e^{-\frac{1}{2}\beta\bar{E}} e^{-2\beta E_0\delta^{1/2}} e^{\beta F(\beta,N,L,\ell)}\right) \tag{5.8.6}$$

We will choose $\ell \gtrsim 1$, in which case $F(\beta, N, L, \ell) \sim N$ and hence the last term in (5.8.6) is, in fact, exponentially small in N, since $\bar{E} \sim N\ln N$. To complete the proof, it suffices to observe that

$$F(\beta, N, L, \ell) \geq F(\beta, N, L) - c_\eta \frac{N\rho^{1/3}}{\ell} \tag{5.8.7}$$

which is an easy exercise. To minimize the total error, we shall choose

$$\ell \sim \rho^{-1/3} N^{1/63} (\ln N)^{-23/21} \tag{5.8.8}$$

to obtain

$$F_g(\beta, N, L) \geq F(\beta, N, L) - c_\eta \rho^{2/3} N^{62/63} (\ln N)^{23/21} \tag{5.8.9}$$

This completes the proof of Theorem 5.2.1.

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