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PhD thesis

One-dimensional Dilute Quantum Gases and Their Ground State Energies

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Abstract

In this thesis, we study the ground state energy of one-dimensional dilute quantum systems with repulsive pair potentials. We review part of the general theory of many-body quantum mechanics. We then prove results describing conditions under which, we can associate a unique self-adjoint many-body Hamiltonian to certain repulsive pair-potential.
The point-interacting solvable models in one dimension, i.e. the Lieb-Liniger and Yang-Gaudin models, are reviewed and certain results related to their ground state energy in the dilute limit are proved.
We proceed by proving a ground state energy expansion for the Bose gas. This is done by proving first an upper bound and next a matching lower bound. The ground state energy is found, up to next-to-leading order, to depend on the potential only through the scattering length. Thus the system exhibits universality similar to that observed for higher dimensional systems. Our result covers the well known results on the ground state energy of the Lieb-Liniger model in the Tonks-Girardeau (dilute) limit. However, our result allows for a very general class of potentials, including potential that differ significantly from the point interacting δ-potentials for example by having positive scattering length. As corollaries, we find similar result for spin polarized Fermi gases and gases with intermediate particle statistics, i.e. anyons.
Finally we study the spin–1/2 Fermi gas. Here we conjecture a ground state energy expansion based on the solvable models at hand. The upper bound from the bosonic case is generalized by realizing the spins, in a given trial state, to be described by an effective antiferromagnetic Heisenberg chain. Thereby, we prove an upper bound matching our conjecture. As corollaries, we find similar results for spin-1/2 bosons and for fermions and particles with spatial symmetry with spin-dependent potentials. Furthermore, we generalize parts of the lower bound proof from the bosonic case, and prove in this case for spin–1/2 fermions a lower bound related to the Lieb-Liniger-Heisenberg ground state energy. We notice that for spin-dependent potentials in certain regimes identified with a ferromagnetic phase, the lower bound is reduced to that of the Lieb-Liniger model. Thus a lower bound, matching the previous upper bound, is proved in the ferromagnetic phase for spin-dependent potentials.

Resumé

I denne afhandling studerer vi grundtilstandsenergien af endimensionelle kvantegasser med frastødende parpotentialer ved lav tæthed. Vi opsummerer dele af den generelle teori omkring mangelegemekvantemekanik. Derefter beviser vi under hvilket betingelser en unik selvadjungeret mangelegeme Hamilton-operator kan associeres til et givet parpotentiale. De punktinteragerende løsbare modeller i én dimension, dvs. Lieb-Liniger og Yang-Gaudin modellerne, opsummeres og visse resultater relateret til deres grundtilstandsenergi i lavtæthedsgrænsen bevises.
Vi forsætter ved at bevise en udvikling af grundtilstandsenergien for Bose-gassen. Dette gøres ved at vise først en øvre begrænsning og derefter en matchende nedre begrænsning. Det vises at grundtilstandsenergien, til næstledende orden, kun afhænger af potentialet igennem spredningslængden. Dermed udviser systemet universalitet, som ligner den observeret i tilsvarende højeredimensionelle systemer. Vores resultat dækker det velkendte resultat vedrørende grundtilstandenergien af Lieb-Liniger modellen i Tonks-Girardeau grænsen, altså den lavtæthedsgrænsen. Dog holder vores resultat for mere generelle parpotentialer, inklusiv potentialer der afviger markant fra δ-potentialer ekspemelvis ved at have positiv spredningslængde. Som korollarer finder vi lignende resultater for den spin-polariserede Fermi-gas og gasser med mellemliggende partikelstatistikker, altså anyoner.
Endeligt studederer vi spin–1/2 Fermi-gassen. Her præsenterer vi, som en formodning, en udvikling af grundtilstandsenergien baseret på kendte løsbare modeller. Den øvre begrænsning fra det bosoniske tilfælde generaliseres ved at indse, at partiklernes spin, i en givet variationsbølgefunktion, kan beskrives ved en effektiv antiferromagnetisk Heisenberg-kæde. Dermed beviser vi en øvre begrænsning, der tilsvarer den fremsatte formodning. Som korollarer finder vi lignende resultater for spin–1/2 bosoner og for fermioner og partikler med rumlig symmetri med spin-afhængige potentialer. Ydermere generaliserer vi dele af beviset for den nedre begrænsning fra det bosoniske tilfælde, og vi beviser i dette tilfælde en nedre begrænsning for spin–1/2 fermioner, der relaterer grundtilstandsenergien til dén fra Lieb-Liniger-Heisenberg modellen. Vi bemærker, at for spin-afhængige potentialer i visse regimer, som vi identificerer med en ferromagnetisk fase, reducerer den nedre begrænsing til dén af Lieb-Liniger modellen. Dermed bevises en nedre begrænsning, der matcher den førviste øvre begrænsning i netop den ferromagnetiske fase for spin-afhængige potentialer.

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Contents

Preprint Included as Part of This Thesis

[ARS22] Ground state energy of dilute Bose gases in 1D,
Johannes Agerskov, Robin Reuvers, and Jan Philip Solovej,
ArXiv, arXiv:2203.17183
This preprint was revised before being included in this thesis.

Chapter 1

Introduction

Since the seminal work of Lee, Huang, and Yang in 1957 [LHY57, LY57, HY57], there has been a tremendous interest in dilute quantum gases and their ground state energy expansions. Finding good approximations for the bosonic ground state energy, at least in two and three dimensions, is intimately related to understanding the formation of Bose-Einstein condensates. Furthermore, such ground state energy expansions often exhibit universality. More specifically, the ground state energy of dilute systems tends to depend on the interaction potential only through the scattering length. This interest has in the mathematical physics literature grown during the last decades culminating in the recent completion of a rigorous proof of the Lee-Huang-Yang formula in 2019 [YY09, FS20][1]. With the problem essentially solved for the three dimensional Bose gas, it is natural to seek similar ground state energy expansions in other dimensions or with different particle statistics. Recently, the two dimensional bosonic ground state energy expansion was proven to analogous precision in [FGJ$^+$22], and previously the fermionic ground state energy expansions have been studied in both two and three dimensions [LSS05].

The general one-dimensional dilute Bose gas, or quantum gas in general, has been surprisingly little studied both in the physics and mathematics literature. This may be partly due to the presence of solvable models in one dimension. In 1963 Lieb and Liniger showed that the one-dimensional Bose gas with point (delta-function) interactions is solvable by Bethe ansatz [LL63]. In practice, this means that one may obtain algebraic equations for the ground

[1] While the lower bound was made fully general in terms of assumptions on the interaction potential in 2021 [FS21], weakening the assumptions under which the upper bound can be proven is still an active field of research.

state and excited energies, by realizing the eigenstates to be superpositions of plane waves with suitable scattering boundary conditions. Similarly, in 1967, the one-dimensional spin–1/2 Fermi gas with point interactions was shown, in the physics literature, to be solvable by means of a generalized Bethe ansatz [Yan67]. This argument was one year later further generalized to accommodate any symmetry of the domain and hence any spin [Sut68]. Some effort has since then gone into arguing that various confined three dimensional systems may be well approximated by such point interacting systems in one dimension, leaving the analysis of the spectrum already complete [Ols98, PSW00, DLO01, LSY03, LSY04, SY08]. In [LSY03, LSY04, SY08] it was shown that such an approximation indeed is valid in certain confinement regimes. We call this regime the *weak confinement regime*, and it is described by having the trapping length scale, in the transverse direction much longer than the three dimensional scattering length scale. This means that transverse excitations cannot be neglected. On the other hand, one may instead consider the *strong confinement regime*, described by having the transverse trapping length scale much shorter than the scattering length scale. In this regime, the spectrum will presumably be well described by a purely one-dimensional system, with the three dimensional potential simply restricted to a line. A crucial difference in this case, is that the one-dimensional scattering length arising from such confinements may be positive, as opposed to the effective Lieb-Liniger model in which the one-dimensional scattering length always is negative.

In this thesis, we analyze ground state energies of general one-dimensional dilute gasses. This covers the strongly point interacting models but further extends the result to models with positive scattering lengths. The ground state energy expansion for one-dimensional dilute bosons and spin polarized fermions was recently obtained in [ARS22], which appears, in a revised edition, as Chapter 3 of this thesis. The expansion obtained will exhibit similar universality to the three and two dimensional cases. However, one major difference is apparent in the analysis and phenomenology of the one-dimensional gas: There is no Bose-Einstein condensation. This fact may be traced back to the celebrated theorem of Hohenberg, Mermin, and Wagner [Hoh67, MW66], which excludes longe-range order for one-dimensional interacting systems. Thus the formation of a condensate is broken by the interaction in one dimension. This famous result is in agreement with the results found in this thesis, where we

explicitly verify that the ground state energy shows greater similarity to energies arising from Slater determinant states than to energies arising from a condensate.
The proof of a ground state energy expansion for the one-dimensional dilute Bose gas and spin polarized Fermi gas leaves the question of whether there is a similar expansion for the total ground state of the spin–1/2 fermionic system. Such an expansion is conjectured in Chapter 3 ([ARS22]), based on the solvable models at hand for such a system. We present in Chapter 4 a proof of an upper bound matching this conjecture. In the proof, we define a trial state in which the spin part is determined variationally. Interestingly, the variational problem determining the spin part is that of the one-dimensional Heisenberg chain. In the case of the usual spin–1/2 fermions, we get the antiferromagnetic Heisenberg chain. However, we will show that for models of a different symmetry or with spin-dependent potentials, the spin chain may be both ferro- or antiferromagnetic. Furthermore, we will present an idea of how to prove a corresponding lower bound. We do this by proving results that are analogous to findings of Chapter 3 ([ARS22]). However, it will be apparent that certain results do not generalize for the spin–1/2 Fermi system straightforwardly. We then present a conjecture which, if proven true, allows us to complete the generalization of the Chapter 3 results. We give heuristic arguments for the validity of this conjecture, but also highlight where these arguments are lacking in mathematical rigor. Finally, we notice that the result of Chapter 3 do generalize for spin–1/2 systems with other symmetries or spin-dependent potentials exactly when the system is in a ferromagnetic phase.

We summarize here overall the structure of this thesis: In Chapter 2, we review relevant concepts in many-body quantum mechanics. Furthermore, since we will allow for quite general interactions in the later analysis, we review under which conditions on the interaction potential the dynamics of quantum systems can be defined in terms of a lower bounded self-adjoint Hamiltonian. We prove a result stating that in one dimension this is possible for any interaction potential that is the sum of a σ-finite measure and an absolutely continuous measure. After this we review the concept of diluteness and known results about dilute quantum gases. Finally, we both review and prove certain result about two solvable models in one dimension. In Chapter 3, we find and prove ground state energy expansions for both the one-dimensional

Bose and spin polarized Fermi gas. In Chapter 4, we generalize some results from Chapter 3 in order to prove an upper bound on the ground state energy of the one-dimensional dilute spin–1/2 Fermi gas. Furthermore, we generalize certain results related to the lower bound in Chapter 3. Finally, we notice that completing the proof of a lower bound for the spin–1/2 Fermi gas, is possible by proving a conjecture on the ground state energy of a model known as the Lieb-Liniger-Heisenberg model in its antiferromagnetic phase. We also note, in the ferromagnetic phase, that a tight lower bound on the Lieb-Liniger-Heisenberg model is trivially valid. Thus for certain other symmetries or spin-dependent potential, we find a tight lower bound exactly when they are in a ferromagnetic phase in this sense. In Chapter 5, we give a final summary of our findings and discuss open problems.

Chapter 2

Many-Body Quantum Mechanics

In this chapter, we give a brief introduction to many-body quantum mechanics. The chapter will serve to define relevant quantities, set up the mathematical framework, and state some preliminary results.

2.1 Many-body Wave Functions

In quantum mechanics, a system is described by a *state* or *wave function* in an underlying Hilbert space.

Definition 2.1. *A quantum system at a fixed time is a pair*

$$(\Psi, \mathcal{H}), \text{ with } \Psi \in \mathcal{H} \text{ and } \|\Psi\| = 1,$$

where $\mathcal{H}$ is a Hilbert space. Here Ψ is called the state or wave function of the system.

In this thesis, we are mostly interested in a quantum system consisting of N particles in a region $\Omega \subseteq \mathbb{R}^d$, possibly with spin degrees of freedom $\{S_i\}_{i\in 1,...,N}$. We will take Ω to be open, connected, and with a Lipschitz boundary, or the closure of such a set. We refer to d as the *dimension* of the system. Such a system is described by having

$$\mathcal{H} \subset L^2\left(\prod_{i=1}^{N}(\Omega \times \{-S_i, S_i+1, ..., S_i\})\right) = \otimes_{i=1}^{N} L^2\left(\Omega; \mathbb{C}^{2S_i+1}\right),$$

where S_i is the *spin* of the ith particle. Since we are more specifically interested in identical particles we will further restrict the structure of the underlying Hilbert space below.

Identical particles: Bosons and fermions

In the case when the particles in question are identical, i.e. indistinguishable, it turns out that one should restrict the underlying Hilbert space, to have certain symmetries. Considering N indistinguishable particles, we restrict to the physical configuration space $C_{p,N} = C_N/\mathrm{S}_N$, with $C_N := \{(x_1, \ldots, x_N) \in \Omega^N | x_i \neq x_j \text{ if } i \neq j\}$ on which the symmetric group, S_N, act freely. For $d \geq 2$, we then require the wave function of the system to take values in a unitary irreducible representation of the fundamental group $\pi_1(C_{p,N})$, where we noted that the physical configuration space is path-connected in order for $\pi_1(C_{p,N}, x)$ to be independent of $x \in C_{p,N}$.

Remark 2.2. *For $d \geq 3$ we have $\pi_1(C_{p,N}) = \mathrm{S}_N$, for $d = 2$ we have $\pi_1(C_{p,N}) = B_N$, where B_N is the braid group with N strands. For $d = 1$ we have $\pi_1(C_{p,N}) = \{1\}$. In the somewhat special case of $d = 1$, $C_{p,N} = \{x_1 < x_2 < \ldots < x_N\}$. In this configuration space, one can never interchange particles without crossing the singular excluded incidence (hyper)planes. Thus the allowed particle statistics are determined by the possible permutation invariant dynamics on this space. In Chapter 3 we will see examples of different particle statistics in one dimension.*

Remark 2.3. *Adding spin to the above considerations amounts to having*

$$C_N := \{(z_1, \ldots, z_N) \in (\Omega \times \{-S, \ldots, S\})^N \,|(z_i)_1 \neq (z_j)_1 \text{ if } i \neq j\},$$

and $C_{p,N} := C_N/S_N$. In this case, $C_{p,N}$ is not path connected, however, for each configuration of spins $\underline{s} = (s_1, \ldots, s_N) \in \{-S, \ldots, S\}^N$ the configuration spaces

$$C_{p,N,\underline{s}} = \{((x_1, s_1), \ldots, (x_N, s_N)) \in (\Omega \times \{-S, \ldots, S\})^N \,|x_i \neq x_j \text{ if } i \neq j\}/S_N$$

are path connected and their fundamental groups are isomorphic to the fundamental group in the spinless case independent of s.
Alternatively, one can view the wave function as a $(2S+1)^N$-dimensional vector bundle over the physical (spinless) configuration space.

In this thesis, we will mainly be interested in the two irreducible representations that are the symmetric representation and the anti-symmetric representation, in which we refer to the particles as *bosons* and *fermions* respectively. It is an empirical fact that bosons and fermions are the only types of elementary particles that are encountered in nature. Hence for bosons, we restrict to wave functions in the symmetric (or bosonic) subspace $L^2_s\left((\Omega \times \{-S, \ldots, S\})^N\right) \cong \vee_{i=1}^N L^2\left(\Omega; \mathbb{C}^{2S+1}\right)$ and for fermions, we restrict to wave-functions in the anti-symmetric (or fermionic) subspace $L^2_a\left((\Omega \times \{-S, \ldots, S\})^N\right) \cong \wedge_{i=1}^N L^2\left(\Omega; \mathbb{C}^{2S+1}\right)$.
To recap we list the following important definitions:

Definition 2.4. *A quantum system of N spin–S bosons in $\Omega \subseteq \mathbb{R}^d$ at fixed time is a pair*

$$(\Psi, \mathcal{H}), \text{ with } \Psi \in \mathcal{H} \text{ and } \|\Psi\| = 1,$$

where $\mathcal{H}$ is a closed subspace of $L^2_s\left((\Omega \times \{-S, \ldots, S\})^N\right) \cong \vee_{i=1}^N L^2\left(\Omega; \mathbb{C}^{2S+1}\right)$, and thus a Hilbert space.

Definition 2.5. *A quantum system of N spin–S fermions in $\Omega \subseteq \mathbb{R}^d$ at fixed time is a pair*

$$(\Psi, \mathcal{H}), \text{ with } \Psi \in \mathcal{H} \text{ and } \|\Psi\| = 1,$$

where $\mathcal{H}$ is a closed subspace of $L^2_a\left((\Omega \times \{-S, \ldots, S\})^N\right) \cong \wedge_{i=1}^N L^2\left(\Omega; \mathbb{C}^{2S+1}\right)$, and thus a Hilbert space.

2.2 Observables, Dynamics, and Energy

In general, we call any self-adjoint operator on $\mathcal{H}$ an *observable*. Physically, observables represent quantities that, in principle, can be measured in an experiment. It is a postulate of quantum mechanics that given an observable $\mathcal{O} = \int_{\sigma(\mathcal{O})} \lambda \, \mathrm{d}P_\lambda$, where $\{P_\lambda\}_{\lambda \in \sigma(\mathcal{O})}$ is the projection valued measure associated with $\mathcal{O}$ by the spectral theorem [RS81], the probability of measurement of $\mathcal{O}$ in the state $\Psi \in \mathcal{D}(\mathcal{O})$ having any outcome λ such that $\lambda \in M \subset \mathbb{R}$ is given by $P((\mathcal{O}, \Psi) \in M) = \int_{\lambda \in M} \langle \Psi, P_\lambda \Psi \rangle$. Furthermore, we define the expected value of an observable.

Definition 2.6. *The **expectation value** of an observable $\mathcal{O}$ in state $\Psi \in$*

$\mathcal{D}(\mathcal{O})$ *is*

$$\langle \mathcal{O} \rangle_\Psi := \int_{\lambda \in \sigma(\mathcal{O})} \lambda \langle \Psi, P_\lambda \Psi \rangle$$

where $\{P_\lambda\}_{\lambda \in \sigma(\mathcal{O})}$ *is the projection valued measure associated with* $\mathcal{O}$ *by the spectral theorem.*

In the previous section, we defined a quantum system at a fixed time. However, we are often interested in the dynamics of the system. In quantum mechanics, time evolution is modeled by the infinitesimal generator of time evolution, H, also known as the *Hamiltonian*. We will in this thesis take H to be a (time-independent) lower bounded self-adjoint operator on $\mathcal{H}$. A state evolves in time according to the Schrödinger equation

$$\Psi(t) = \exp\left(-iH(t - t_0)\right) \Psi(t_0),$$

where we have set $\hbar = 1$.

Remark 2.7. *By Stone's theorem [RS81], the existence of a self-adjoint Hamiltonian,* H*, is guaranteed for any time evolution described by* $\Psi(t) = U(t - t_0)\Psi(t_0)$*, when* $U(t)$ *is a strongly continuous one-parameter unitary group.*

Since the Hamiltonian, H, is self-adjoint, it represents an observable which we call *energy*. Furthermore, as H is lower bounded, there is a natural notion of the lowest energy of H.

Definition 2.8. *The* ***ground state energy*** *of* H *is defined by*

$$E_0(H) := \inf_{\Psi \in \mathcal{D}(\mathcal{H})} \frac{\langle \Psi, H\Psi \rangle}{\|\Psi\|^2}. \tag{2.2.1}$$

Furthermore, we define the notion of a *ground state* of H as

Definition 2.9. *We say that a (normalized) state* $\Psi \in \mathcal{D}(H) \subset \mathcal{H}$ *is a* ***ground state*** *of* H *if*

$$\langle H \rangle_\Psi = E_0(H).$$

Remark 2.10. *It follows from the spectral theorem (see [RS81]) that the ground state energy is given by*

$$E_0(H) = \inf(\sigma(H)),$$

where $\sigma(H)$ denotes the spectrum of H.

Remark 2.11. *It is straightforward to show that the quadratic form $\mathcal{D}(H) \ni \Psi \mapsto \langle \Psi, H\Psi \rangle$ is lower bounded and closable since H is lower bounded and self-adjoint.*

Definition 2.12. *Given a Hamiltonian, H, we define the **associated energy quadratic form**, $\mathcal{E}_H : \mathcal{D}(\mathcal{E}_H) \to \mathbb{R}$, as the closure of the quadratic form $\mathcal{D}(H) \ni \Psi \mapsto \langle \Psi, H\Psi \rangle$. When H is given from the context, we will often write $\mathcal{E}$ as short for $\mathcal{E}_H$.*

Remark 2.13. *From the definition of $\mathcal{E}_H$ and from Definition 2.8 it follows straightforwardly that we have*

$$E_0(H) = \inf_{\Psi \in \mathcal{D}(\mathcal{E}_H)} \frac{\mathcal{E}_H(\Psi)}{\|\Psi\|^2} = \inf_{\substack{\Psi \in \mathcal{D}(\mathcal{E}_H), \\ \|\Psi\|=1}} \mathcal{E}_H(\Psi), \tag{2.2.2}$$

as $\mathcal{D}(H)$ is form core for $\mathcal{E}_H$.

We refer to both (2.2.1) and (2.2.2) as *the variational principle*. We will often, in this thesis, take (2.2.2) as the very definition of the ground state energy. Furthermore, one can also define the dynamics of a quantum system by specifying an energy quadratic form in the following sense:

Remark 2.14 ([RS81] Theorem VIII.15)**.** *Given a densely defined, lower bounded, closable, quadratic form $\mathcal{E} : \mathcal{D}(\mathcal{E}) \to \mathbb{R}$ there exists a **unique** lower bounded, self-adjoint operator $H_\mathcal{E}$, such that $\mathcal{E}(\Psi) = \langle \Psi, H_\mathcal{E}\Psi \rangle$ for all $\Psi \in \mathcal{D}(H_\mathcal{E})$, and $\mathcal{D}(H_\mathcal{E})$ is form core for $\overline{\mathcal{E}}$, i.e. the form closure of $\langle \cdot, H_\mathcal{E} \cdot \rangle$ is equal to the form closure of $\mathcal{E}$.*

Thus we will frequently switch between the two equivalent formulations of the dynamics of a quantum system. Namely, the the operator, H, formulation and the quadratic form, $\mathcal{E}$, formulation.

Many-body Hamiltonians

Until this point, we have not specified the class of Hamiltonians that we will be interested in. We have stated that we will care mainly about Hamiltonians defined on the bosonic or fermionic subspace, however, no specification has been made about the dynamics on these subspaces. We are interested in

modeling N particles in some region $\Omega \subseteq \mathbb{R}^d$ that interact locally with each other. For the remainder of this subsection, we will ignore spin, remarking that including spin degrees of freedom is completely analogous. In practice, and for suitably mild interactions, this means that the Hamiltonian *formally* (meaning restricted to the fermionic or bosonic subspace of $C_0^\infty(\Omega^N)$) takes the form

$$H = \sum_{i=1}^{N} T_i + U(x_1, \ldots, x_N) \tag{2.2.3}$$

where T_i is the *kinetic energy operator* for particle i and the *potential* U is a multiplication operator which models the local interaction among the particles. The kinetic energy operator is taken to be[1]

$$T_i = -\frac{1}{2m_i}\Delta_i \qquad (\hbar = 1) \tag{2.2.4}$$

since we are interested in identical particles, we will from this point onward choose $m_i = 1/2$. As for the potential, V, we of course immediately restrict to permutation-invariant function, U, for identical particles. However, in the following, we will further restrict to a combination of having a trapping potential and radial pair potentials, which model pairwise interactions that only depend on the distances between particles. Such potentials take the form

$$U(x_1, \ldots, x_N) = \sum_{i<j} v(x_i - x_j) + \sum_{i=1}^{N} V(x_i) \tag{2.2.5}$$

where we take v to be a radial function and V is called the *trapping potential*. We will generally take v to be repulsive, meaning $v \geq 0$, with compact support. The trapping potential we will disregard i.e. $V = 0$. We will then in general take the true Hamiltonian to be a self-adjoint extension of the symmetric *formal* Hamiltonian. Now some models of stronger interactions, e.g. the hard core interaction, require a more delicate construction with respect to the initial definition of the formal Hamiltonian. However, the construction of the Hamiltonian can be done in a more unified manner when constructing the energy quadratic form.

Definition 2.15. *For a system of N bosons/fermions in region $\Omega \in \mathbb{R}^d$, we*

[1]This is usually justified by going through a canonical quantization procedure for the classical Hamiltonian function of the system we are interested in modeling.

define for $\sigma \in [0,\infty]$ ***the energy quadratic forms***

$$\mathcal{E}_{(v,\sigma)}(\Psi) = \int_{\Omega^N} \sum_{i=1}^{N} |\nabla_i \Psi|^2 + \sum_{i<j} v(x_i - x_j)\,|\Psi|^2 + \sigma \int_{\partial(\Omega^N)} |\Psi|^2\,, \qquad (2.2.6)$$

with domain $\mathcal{D}\left(\mathcal{E}_{(v,\sigma)}\right) = \{\Psi \in (C^\infty(\Omega^N))_{b/f} | \mathcal{E}_{(v,\sigma)}(\Psi) < \infty\}$. *With* $(C^\infty(\Omega^N))_{b/f}$ *meaning the bosonic/fermionic subspace of* $C^\infty(\Omega^N)$. $\sigma = \infty$ *is taken to mean Dirichlet boundary conditions.*

Of course $\mathcal{E}_{(v,\sigma)} \geq 0$ for any $\sigma \in [0,\infty]$ and $v \geq 0$. However, the closability of $\mathcal{E}_{(v,\sigma)}$ is not evident. In fact for general v, $\mathcal{E}_{(v,\sigma)}$ will be neither densely defined nor closable on $L^2_{s/a}(\Omega^N)$. However, it will be densely defined on a closed subspace $\mathcal{H}_{(v,\sigma)} := \overline{\mathcal{D}\left(\mathcal{E}_{(v,\sigma)}\right)}^{\|\cdot\|_2}$ of $L^2_{s/a}(\Omega^N)$, hence we take $\mathcal{H}_{(v,\sigma)}$ to be the Hilbert space of the system when this is the case. Closability of $\mathcal{E}_{(v,\sigma)}$ on $\mathcal{H}_{(v,\sigma)}$ is not necessarily satisfied. Thus we make the following definition

Definition 2.16. *We say a potential* $v \geq 0$ *is* ***allowed*** *in dimension* d, *if* $\mathcal{E}_{(v,\sigma)}$ *is closable on* $\mathcal{H}_{(v,\sigma)} := \overline{\mathcal{D}\left(\mathcal{E}_{(v,\sigma)}\right)}^{\|\cdot\|_2} \subset L^2_{s/a}(\Omega^N)$ *for any* $\sigma \in [0,\infty]$.

Remark 2.17. *There are plenty of allowed potentials, but the notion does depend on the dimension,* d. *For example,* $v = \delta_0$, *i.e. the delta function potential, is allowed in dimension* $d = 1$, *but not in dimension* $d \geq 2$. *This can be seen from the fact that for* $d = 1$ *the incidence planes are of co-dimension* 1, *and hence the trace theorem gives closability, but for* $d \geq 2$ *where the incidence planes are of co-dimension* ≥ 2 *it is known that the trace of* H^1 *is not contained in* L^2.

Remark 2.18. *For any radial measurable* $v : \mathbb{R} \to [0,\infty]$ *(note this implies that* $x \mapsto v(x_i - x_j)$ *is measurable since* $\mathbb{R}^{Nd} \ni x \mapsto x_i - x_j \in \mathbb{R}^d$ *is Lebesgue-Lebesgue measurable),* $\mathcal{E}_{(v,\sigma)}$ *is the quadratic form associated with a self-adjoint operator on some Hilbert space* $\mathcal{H}_{(v,\sigma)} \subset L^2_{s/a}(\Omega^N)$.
It is well known that $\mathcal{E}_{(0,\sigma)}$ *is closable on* $\mathcal{H}_{(0,\sigma)} \supseteq \mathcal{H}_{(v,\sigma)}$. *Hence* $\mathcal{E}_{(0,\sigma)}|_{\mathcal{D}\left(\mathcal{E}_{(v,\sigma)}\right)}$ *is closable on* $\mathcal{H}_{(v,\sigma)}$. *Thus closability of* $\mathcal{E}_{(v,\sigma)}$ *amounts to showing that* $\psi_n \xrightarrow{\|\cdot\|_2} 0$ *as* $n \to \infty$ *and* $(\psi_n)_{n\in\mathbb{N}} \subset L^2\left(\Omega^N, \underbrace{\sum_{i<j} v(x_i - x_j)\,\mathrm{d}\lambda^N}_{:=\mathrm{d}\mu_v}\right)$ *Cauchy,*

implies $\psi_n \xrightarrow{\|\cdot\|_{L^2(\Omega^N,\mathrm{d}\mu_v)}} 0$.
This is evident from the fact that $\psi_n \xrightarrow{\|\cdot\|_{L^2(\Omega^N,\mathrm{d}\mu_v)}} f$ *for some* $f \in L^2(\Omega^N, \mathrm{d}\mu_v)$ *by completeness. Now* ψ_n *has a subsequence that converges* λ^N*–almost everywhere to* 0*, and this subsequence further has a subsequence that converges* μ_v*–almost everywhere to* f*. Hence* $f = 0$ μ_v*–almost everywhere, as* $\mu_v \ll \lambda^N$*. Thus there is a corresponding self-adjoint operator* $H_{(v,\sigma)}$ *to* $\mathcal{E}_{(v,\sigma)}$ *on* $\mathcal{H}_{(v,\sigma)}$*, which we shall formally write as* $H_{(v,\sigma)} = -\sum_{i=1}^N \Delta_i + \sum_{1\le i<j\le N} v(x_i - x_j)$.

The argument from the previous remark may be generalized slightly in the case of $d = 1$, in order to show that any σ–finite symmetric measure $v(x_i - x_j)\,\mathrm{d}\lambda(x_i - x_j) := \mathrm{d}\mu_{v_{ij}}$ is an allowed potential. Notice that we slightly abuse notation and write $v(x_i - x_j)\,\mathrm{d}\lambda(x_i - x_j)$ even when v is a singular measure and thus has no density. However, we do think of v a being a one-dimensional measure in the sense that

$$v(x_i - x_j)\,\mathrm{d}\lambda^N := \mathrm{d}\mu_{v_{ij}} \times \mathrm{d}\lambda^{N-1}_{(x_i-x_j)=\text{ fixed}},$$

where we defined $\lambda^{N-1}_{(x_i-x_j)=\text{ fixed}}$ to be the measure such that $\mathrm{d}\lambda^N = \mathrm{d}(x_i - x_j) \times \mathrm{d}\lambda^{N-1}_{(x_i-x_j)=\text{ fixed}}$. The uniqueness of the product measure is guaranteed by σ-finiteness of v (μ_v). We will need the following essential lemma, where we use the notation $\lambda_k^{N-1} := \prod_{i\neq k} \lambda(x_i)$.

Lemma 2.19. *Let* $(f_n)_{n\in\mathbb{N}} \subset H^1(\Omega^N)$ *be a sequence such that* $\|f_n\|_{H^1} \to 0$ *as* $n \to \infty$*. Then defining* $f_n^k(t, \overline{x}^k) := f_n(x_1, \ldots, x_{k-1}, t, x_{k+1}, \ldots, x_N)$ *for any* $k = 1, \ldots, N$*, we have that* $(f_n^k)_{n\in\mathbb{N}}$ *has a subsequence that converges pointwise (in* t*) to* 0*,* λ_k^{N-1}*–a.e. for all* $k = 1, \ldots, N$.

Proof. We pass first to a subsequence, which we also denote f_n, such that f_n converges pointwise λ^N–a.e. to 0. Since $f_n \in H^1(\Omega^N)$, we know for any $k = 1, \ldots, N$ that $f_n^k(t, \overline{x}^k)$ are in $H^1(\Omega)$ (as functions of t) λ_k^{N-1}–a.e. [[EG91] Theorem 2 p. 164]. Now consider the $H^1(\Omega)$ norms $g_n^k(\overline{x}^k) := \left\|f_n^k(\cdot, \overline{x}^k)\right\|_{H^1(\Omega)}$. Clearly g_n^k constitute L^2 functions, with norms converging to 0 as $n \to \infty$. Hence there exists a subsequence that converges pointwise λ_k^{N-1}–almost everywhere to 0. So a subsequence $f_{n_i}^k$ exists, such that for λ_k^{N-1}–a.e. $\overline{x}^k$, $f_{n_i}^k(\cdot, \overline{x}^k)$ converges to 0 in $H^1(\Omega)$. But then $f_{n_i}^k(\cdot, \overline{x}^k)$ converges, by Morrey's inequality, pointwise to 0, for λ_k^{N-1}–a.e. $\overline{x}^k$. □

Using this lemma, we may prove the following Proposition

Proposition 2.20. *Let $d = 1$, then for any σ-finite measure, v, we have that $\mathcal{E}_{(v,\sigma)}$ is the quadratic form associated with a unique lower bounded self adjoint operator $H_{(v,\sigma)}$ on some Hilbert space $\mathcal{H}_{(v,\sigma)}$.*

Proof. As previously, we define $\mathcal{H}_{(v,\sigma)} := \overline{\mathcal{D}\left(\mathcal{E}_{(v,\sigma)}\right)}^{\|\cdot\|_2}$ and $\mathrm{d}\mu_v = \sum_{1\leq i<j\leq N} v(x_i - x_j)\,\mathrm{d}\lambda^N$. Clearly $\mathcal{E}_{(v,\sigma)}$ is lower bounded and densely defined in $\mathcal{H}_{(v,\sigma)}$. Closability amounts to showing that $\psi_n \xrightarrow{\|\cdot\|_{L^2(\Omega^N,\mathrm{d}\lambda^N)}} 0$ and $(\psi_n)_{n\in\mathbb{N}} \subset \mathcal{D}\left(\mathcal{E}_{(v,\sigma)}\right) \subset L^2\left(\Omega^N, \mathrm{d}\mu_v\right)$ Cauchy w.r.t the norm $\|\cdot\|_{\mathcal{E}_{(v,\sigma)}} = \sqrt{\mathcal{E}_{(v,\sigma)}(\cdot) + \|\cdot\|_2^2}$, implies $\psi_n \xrightarrow{\|\cdot\|_{L^2(\Omega^N,\mathrm{d}\mu_v)}} 0$. Now since $(\psi_n)_{n\in\mathbb{N}}$ is a Cauchy sequence in $L^2\left(\Omega^N, \mathrm{d}\mu_v\right)$, it has a subsequence that converges μ_v–almost everywhere to some function $f \in L^2\left(\Omega^N, \mathrm{d}\mu_v\right)$. Furthermore, this subsequence has a further subsequence that converges to 0, λ^N–almost everywhere. However, since $(\psi_n)_{n\in\mathbb{N}}$ converges to 0 in $H^1(\Omega^N, \mathrm{d}\lambda^N)$, by passing to a subsequence and after a linear coordinate transformation, Lemma 2.19 implies that for $(x_i - x_j)$ fixed $(\psi_n)_{n\in\mathbb{N}}$ converges $\lambda^{N-1}_{(x_i-x_j)=\text{ fixed}}$–a.e. to 0. But ψ_n also converges, by Tonelli's theorem, for $\mu_{v_{ij}}$–almost every $(x_i - x_j)$ to f, $\lambda^{N-1}_{(x_i-x_j)=\text{ fixed}}$–almost everywhere , and hence $f = 0$ $\mu_{v_{ij}}$–almost everywhere, $\lambda^{N-1}_{(x_i-x_j)=\text{ fixed}}$–almost everywhere. Thus we conclude, again by Tonelli's theorem, that $f = 0$ μ_v–almost everywhere. The proposition now follows from Remark 2.14. □

Remark 2.21. *By the very definition of the domain $\mathcal{D}\left(\mathcal{E}_{v,\sigma}\right)$, it is not hard to see that in one dimension, a potential of the form $v = \infty\delta_0$, i.e. an infinite point mass, is allowed. This potential creates a Dirichlet boundary condition on the incidence (hyper)planes in the domain.*

Remark 2.22. *It is clear that if v_1 and v_2 are allowed potentials, then v_1+v_2 is an allowed potential. Defining $\|\cdot\|_{\mathcal{E}_{(v,\sigma)}} := \sqrt{\mathcal{E}_{(v,\sigma)}(\cdot) + \|\cdot\|_2^2}$, this follows from the fact a Cauchy sequence w.r.t. the norm $\|\cdot\|_{\mathcal{E}_{(v_1+v_2,\sigma)}}$ is similarly Cauchy w.r.t. $\|\cdot\|_{\mathcal{E}_{(v_1,\sigma)}}$ and $\|\cdot\|_{\mathcal{E}_{(v_2,\sigma)}}$. In fact we have*

$$\max\left(\|\cdot\|_{\mathcal{E}_{(v_1,\sigma)}}, \|\cdot\|_{\mathcal{E}_{(v_2,\sigma)}}\right) \leq \|\cdot\|_{\mathcal{E}_{(v_1+v_2,\sigma)}} \leq \sqrt{\|\cdot\|^2_{\mathcal{E}_{(v_1,\sigma)}} + \|\cdot\|^2_{\mathcal{E}_{(v_2,\sigma)}}}.$$

Remark 2.23. *Combining Proposition 2.20, Remarks 2.18, 2.21, and 2.22 we conclude that potentials of the form $v = v_{\sigma\text{–finite}} + v_{meas.} + c\delta_0$, with $c \in \{0, \infty\}$, are allowed in one dimension, $d = 1$. Here $v_{\sigma\text{–finite}}$ is a σ–finite measure and $v_{meas.} : \mathbb{R} \to [0, \infty]$ is a measurable function. Of course $c\delta_0$ may be*

absorbed in the σ-finite measure when $c < \infty$, so only the $c = \infty$ case requires Remark 2.21. We will in Chapters 3 and 4 obtain results about the ground state energies of such systems.

Remark 2.24. *We emphasize that one can construct dynamics of a quantum system that are not given by a pair potential in the sense of the discussion above. It is, for example, possible to study point interactions in $d \geq 2$, however, they cannot be seen as arising from a potential (e.g. a δ-function potential). Instead, one studies in this case the self-adjoint extensions of the Laplacian on functions supported away from the incidence planes of the particles. [AGHKH12].*

2.3 The Scattering Length

When analyzing the dynamics of a quantum system, it is natural to define certain length scales, on which different processes take place. These length scales often play important roles in understanding the physics of the system, and thus often appear naturally in expressions for the energies of the system. One such length scale that will be of particular importance throughout this thesis is the *scattering length*. The intuition behind the name is that scattering occurs on this length scale. This intuition will be important throughout the thesis, especially when constructing low-energy trial states in order to estimate ground state energies by applying the variational principle. The scattering length has multiple equivalent definitions in the literature, but we shall here define it conveniently from a variational principle.

Consider the two-body problem in $\Omega = \mathbb{R}^d$ with a spherically symmetric positive potential of compact support $v \geq 0$. We allow for the potential, v, to be a measure when it makes sense, i.e. when it is *allowed*. Let $R_0 > 0$ be such that $\mathrm{supp}(v) \subset B_{R_0}$. Many assumptions on v can be weakened, but these conditions are sufficient for the scope of this thesis. The formal Hamiltonian can be written as

$$H_2 = -\frac{1}{2m_1}\Delta_1 - \frac{1}{2m_2}\Delta_2 + v(x_1 - x_2). \tag{2.3.1}$$

For now, we keep the masses, but we will be, for the most part, interested in the case $m_1 = m_2 = 1/2$. Defining the center of mass coordinate $X = (m_1x_1 + m_2x_2)/(m_1 + m_2)$ and the relative coordinate $y = x_1 - x_2$, we see

that the kinetic energy may be rewritten as

$$\begin{aligned}
-\frac{1}{2m_1}\Delta_1 - \frac{1}{2m_2}\Delta_2 &= -\sum_{i=1}^{d} \frac{1}{2m_1}\left(\frac{\partial y_i}{\partial (x_1)_i}\partial_{y_i} + \frac{\partial X_i}{\partial (x_1)_i}\partial_{X_i}\right)^2 \\
&\qquad + \frac{1}{2m_2}\left(\frac{\partial y_i}{\partial (x_2)_i}\partial_{y_i} + \frac{\partial X_i}{\partial (x_2)_i}\partial_{X_i}\right)^2 \\
&= -\sum_{i=1}^{d} \frac{1}{2m_1}\left(\partial_{y_i} + \frac{m_1}{m_1+m_2}\partial_{X_i}\right)^2 \\
&\qquad + \frac{1}{2m_2}\left(-\partial_{y_i} + \frac{m_2}{m_1+m_2}\partial_{X_i}\right)^2 \\
&= -\frac{1}{2\mu}\Delta_y - \frac{1}{2(m_1+m_2)}\Delta_X,
\end{aligned} \tag{2.3.2}$$

where $\mu \coloneqq \frac{m_1 m_2}{m_1+m_2}$. Thus we have separated the center of mass and relative motion and the Hamiltonian may be decomposed into

$$H = H_{\mathrm{CM}} + H_{\mathrm{rel}}, \tag{2.3.3}$$

with $H_{\mathrm{CM}} = -\frac{1}{2(m_1+m_2)}\Delta_X$ and $H_{\mathrm{rel}} = -\frac{1}{2\mu}\Delta_y + v(y)$. In scattering theory, we will generally be interested in the relative motion of particles. A natural question is whether we can locally minimize the relative energy of the two particles when they are near each other. The answer is affirmative, which can be seen by the following:
Consider the (R-local, relative) energy functional

$$\mathcal{E}_R(\psi) = \int_{B_R} \frac{1}{2\mu}\left|\nabla\psi\right|^2 + v\left|\psi\right|^2, \tag{2.3.4}$$

with $R > R_0$. Then we have

Theorem 2.25 (Theorem A.1 in [LY01])**.** *Let $R > R_0$, then in the class of functions*

$$\{\phi \in H^1(B_R) \mid \phi(x) = 1, \text{ for } x \in S_R\},$$

with S_R the sphere of radius R, there is a unique ϕ_0 that minimizes $\mathcal{E}_R$. This function is non-negative and spherically symmetric, $\phi_0(x) = f_0(|x|)$ for some $f \geq 0$, and it satisfies the equation

$$-\frac{1}{2\mu}\Delta\phi_0 + v\phi_0 = 0, \tag{2.3.5}$$

in the sense of distributions on B_R.

For $R_0 < r < R$ *we have*

$$f_0(r) = \begin{cases} (r-a)/(R-a) & \text{for } d = 1 \\ \ln(r/a)/\ln(R/a) & \text{for } d = 2 \\ (1-ar^{2-n})/(1-aR^{2-n}) & \text{for } d \geq 3 \end{cases} \tag{2.3.6}$$

for some length, a*, which we call* ***the (s-wave) scattering length****.*

The minimum value of $\mathcal{E}_R$ *is*

$$\mathcal{E}_R(\phi_0) = \begin{cases} 1/\mu(R-a) & \text{for } d = 1 \\ \pi/[\mu \ln(R/a)] & \text{for } d = 2 \\ \pi^{n/2}a/[\mu\Gamma(n/2)(1-aR^{2-n})] & \text{for } d \geq 3. \end{cases} \tag{2.3.7}$$

We note that in $d > 3$, the scattering length is not actually a length in the sense of units. This is purely an artifact of the conventions used in the definition.

Remark 2.26. *The scattering length is independent of* R*. This is seen by realizing that for a minimizer,* ϕ_0*, of* $\mathcal{E}_R$ *satisfying* $\phi_0(x) = 1$ *for* $x \in S_R$*, we have that* $\frac{1}{f_0(R')}\mathbb{1}_{\overline{B_{R'}}}\phi_0$ *with* $R_0 < R' < R$ *is a minimizer* $\mathcal{E}_{R'}$ *satisfying*

$$\left(\frac{1}{f_0(R')}\mathbb{1}_{\overline{B_{R'}}}\phi_0\right)(x) = 1, \text{ for } x \in S_{R'}.$$

The definition above defined only the s-wave scattering length. One can proceed to define different kinds of scattering lengths depending on which asymptotic behavior (boundary condition) we demand of the minimizer of $\mathcal{E}_R$. We will be, for the most part, interested in different kinds of scattering lengths in dimension $d = 1$, with the masses $m_1 = m_2 = 1/2$. Thus we define the scattering lengths of interest:

Definition 2.27. *Let* $f_e \in H^1(\mathbb{R})$ *be the unique solutions of the equation*

$$-f_e''(x) + \frac{1}{2}v(x)f_e = 0, \tag{2.3.8}$$

in the sense of distributions on B_R*, with boundary conditions* $f_e(R) = 1$ *and*

$f_e(-R) = 1$. *Then we have*

$$\int_{B_R} 2\left|f_e'\right|^2 + v\left|f_e\right|^2 = \frac{4}{R - a_e}, \tag{2.3.9}$$

for some length, a_e, called the ***even wave scattering length****.*

Definition 2.28. *Let $f_o \in H^1(\mathbb{R})$ be the unique solutions of the equation*

$$-f_o''(x) + \frac{1}{2}v(x)f_o = 0, \tag{2.3.10}$$

in the sense of distributions on B_R, with boundary conditions $f_o(R) = 1$ and $f_o(-R) = -1$. Then we have

$$\int_{B_R} 2\left|f_o'\right|^2 + v\left|f_o\right|^2 = \frac{4}{R - a_o}, \tag{2.3.11}$$

for some length, a_o, called the ***odd wave scattering length****.*

Remark 2.29. *In dimension one, when the odd wave scattering length plays no role, we will often refer to the even wave scattering length, a_e, as "the scattering length" and denote it by a, as in Theorem 2.25.*

Remark 2.30. *We did not prove the uniqueness of the solutions above. In Definition 2.27, it follows from Theorem 2.25 by noting that any solution of* (2.3.8) *is a minimizer of $\mathcal{E}_R$. In Definition 2.28 it follows from the fact that by Theorem 2.25 there is a unique solution that vanishes at the origin (simply consider the solution of* (2.3.8) *with potential $v' = v + \infty\delta_0$ and multiply by sign(x)). Thus the odd part of f_o is unique. The even part of f_o vanishes at $x = R$, and since* (2.3.10) *is the Euler-Lagrange equation for $\mathcal{E}_R$, we see that $(f_o)_{even} = 0$, since this is the only local extremum of $\mathcal{E}_R$ with zero boundary conditions.*

Remark 2.31. *The even wave scattering length, a_e, need not be non-negative as is the case for the s-wave scattering length in $d \geq 2$. However, we do have $a_o \geq 0$. This is easily seen by noticing that the minimizer of*

$$\int_{B_R} 2\left|f_o'\right|^2, \tag{2.3.12}$$

with boundary condition $f(R) = -f(-R) = 1$, is $f(x) = (1/R)x$ on B_R, which has energy $\frac{4}{R}$. Thus adding a positive potential must increase the energy.

Alternatively, we may see this by noting that the odd wave scattering length is equivalent to the s-wave scattering length in $d = 3$ with potential $v(|\cdot|)$ since (2.3.10) *is exactly the radial scattering equation in $d = 3$ when restricted to* $[0, R]$.

Remark 2.32. *We also have $a_o \geq a_e$ by the fact that $|f_o|$ is a trial state for $\mathcal{E}_R$ with even boundary conditions, and its energy is $4/(R - a_o) \geq 4/(R - a_e)$.*

We give two examples of the scattering length in the following:

Example 2.33. *Consider $v = c\delta$. For the even wave scattering length, we solve, in this case, the equation*

$$f_e''(x) = 0, \tag{2.3.13}$$

on the interval $[0, R]$, with the boundary condition $f'(0_+) = \frac{c}{2} f(0)$ and $f(R) = 1$. The solution is $f_e(x) = \frac{x+2/c}{R+2/c}$, for $x \in [0, R]$. We conclude that $a_e = -2/c$. For the odd wave scattering length, we notice that having $v \neq 0$, does not change the scattering solution from the $v = 0$ case, and we have $f_o(x) = \frac{x}{R}$. We conclude that $a_o = 0$.

Example 2.34. *Consider $v = \infty \mathbb{1}_{[-R_0, R_0]}$, i.e.* the hard core. *In this case*

$$f_{e/o}''(x) = 0, \text{ for } x \in (R_0, R] \tag{2.3.14}$$

and $f_{e/o}(x) = 0$ for $x \in [0, R_0]$ constitutes scattering equation on $[0, R]$. Thus find that

$$f_{e/o}(x) = \begin{cases} 0 & x \in [0, R_0] \\ \frac{x - R_0}{R - R_0} & x \in (R_0, R] \end{cases} \tag{2.3.15}$$

solves the scattering equation. We conclude that $a_e = a_o = R_0$.

2.4 The Ground State Energy of Dilute Gases

To put the results of this thesis into context, we here summarize the currently known results about the ground state energies of dilute Bose gases. To begin with, we define what is meant by "dilute".

Definition 2.35. *For the d-dimensional ($d = 1, 2, 3$) system of bosons, with the formal Hamiltonian*

$$H = -\sum_{i=1}^{N} \Delta_i + \sum_{1 \leq i < j \leq N} v(x_i - x_j), \tag{2.4.1}$$

we say that the system is in ***the dilute limit*** *or that the Bose gas is* ***dilute*** *if $\rho^{1/d} |a| \ll 1$. Notice that the absolute value on a is only important when $d = 1$, since only then can the s-wave scattering length be negative.*

Definition 2.36. *For the one-dimensional system of fermions with the formal Hamiltonian*

$$H = -\sum_{i=1}^{N} \partial_i^2 + \sum_{1 \leq i < j \leq N} v(x_i - x_j), \tag{2.4.2}$$

we say that the system is in ***the dilute limit*** *or that the Fermi gas is* ***dilute*** *if $\rho \max(||a_e|, a_o|) \ll 1$.*

Remark 2.37. *For fermions in dimension $d = 2, 3$, one can similarly define diluteness. The diluteness parameter will in this case depend on the spin configuration. For example will the vanishing total spin-z gas have the same definition as for bosons, since the p-wave scattering contribution to the energy is sub-leading. However, for spin-polarized gases the p-wave scattering length will appear in the diluteness parameter.*

Remark 2.38. *For $d = 1$ the free Bose gas, i.e. with $v = 0$, has $|a_e| = \infty$. Hence the free Bose gas cannot be considered dilute at any density.*

In the following, we will list some of the known results about dilute gases in dimensions $d = 2, 3$. We will then in the remainder of this thesis shed light on the corresponding results in one dimension.

The dilute Bose gas in three dimensions

The three dimensional dilute Bose gas is probably the most well-studied example of a dilute quantum gas. Historically the most famous result on the three dimensional dilute Bose gas is due to Lee, Huang, and Yang [LHY57]. Interestingly, the energy was found, to second order, to depend on the potential only through the scattering length. The mathematical literature is quite rich, and we refer to the papers [Dys57, LY98, LY99, LY01, YY09, FS20, FS21, BCS21]

for more details. The latest results are very recent, and it was only in 2020 that the Lee-Huang-Yang formula was rigorously established to second order when Fournais and Solovej proved a second order lower bound. Without giving details about assumptions needed on the potential, the Lee-Huang-Yang formula takes the form

$$e^{3D}(\rho) = 4\pi\rho^2 a\left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} + o\left(\sqrt{\rho a^3}\right)\right), \tag{2.4.3}$$

where $e^{3D}(\rho) = \lim\limits_{\substack{N,L\to\infty \\ N/L^3=\rho}} \frac{E^{3D}(N,L)}{L^3}$, and $E^{3D}(N,L)$ is the ground state of the Bose gas with N bosons in $\Omega = [0,L]^3$ with dynamics given by the Hamiltonian $H = -\sum_{i=1}^N \Delta_i + \sum_{1\leq i<j\leq N} v(|x_i - x_j|)$.

The dilute Bose gas in two dimensions

In the two dimensional scenario, the ground state energy of the dilute Bose gas again possesses an expansion that, to second order, only depends on the potential through the scattering length, analogous to the Lee-Huang-Yang result in three dimensions. The first derivation of this expansion to leading order was given for the hard sphere case in [Sch71] and higher order terms were first given in [HFM78]. To leading order, a rigorous understanding was only reached in 2001 by Lieb and Yngvason in [LY01], and very recently the full proof was given at next to leading order by Fournais *et al.* in [FGJ$^+$22]. Without giving details on assumptions on the potential, the formula takes the form

$$e^{2D}(\rho) = 4\pi\rho^2 Y\left(1 - Y\left|\ln(Y)\right| + \left(2\gamma + \frac{1}{2} + \ln(\pi)\right)Y + o(Y)\right), \tag{2.4.4}$$

with γ being the Euler-Mascheroni constant and $Y := \left|\ln(\rho a^2)\right|^{-1}$. Above $e^{2D}(\rho) = \lim\limits_{\substack{N,L\to\infty \\ N/L^2=\rho}} \frac{E^{2D}(N,L)}{L^2}$, and $E^{2D}(N,L)$ is the ground state of the Bose gas with N bosons in $\Omega = [0,L]^2$ with dynamics given by the Hamiltonian $H = -\sum_{i=1}^N \Delta_i + \sum_{1\leq i<j\leq N} v(|x_i - x_j|)$.

The dilute spin–S Fermi gas in three dimensions

The establishment of expansions for the ground state energy of the dilute Bose gas in terms of the scattering length led to the natural question of whether

a similar expansion exists for the spin–1/2 Fermi gas. The asymptotics were first derived in [HY57, LY57], however, it was not until 2004 that the result was rigorously proven in [LSS05]. Recently the error has been improved to be almost "optimal" [Lau23], i.e. the order of magnitude is almost equal to that of the conjectured next term in the expansion. Furthermore, for smooth potentials, the error was recently improved in [FGHP21] and a proof with optimal error was given in [Gia22]. Without giving details on the assumptions on the potential, the formula takes the form

$$e^{3D}_{F,S}(\rho) = \frac{3}{5}(6\pi)^{2/3}\sum_{i=-S}^{S}\rho_i^{5/3} + 8\pi a \sum_{-S\leq i<j\leq S}\rho_i\rho_j + o\left(\rho^2 a\right). \tag{2.4.5}$$

where ρ_i denotes the density of particles with spin-z i and the index i runs over integers or half integers. Furthermore, $e^{3D}_{F,S}(\rho) = \lim\limits_{\substack{N,L\to\infty \\ N/L^3=\rho}} \frac{E^{3D}_{F,S}(N,L)}{L^3}$, and $E^{3D}_{F,S}(N,L)$ is the ground state of the spin–S Fermi gas with N spin–S fermions in $\Omega = [0,L]^3$ with dynamics given by the Hamiltonian $H = -\sum_{i=1}^{N}\Delta_i + \sum_{1\leq i<j\leq N} v(|x_i - x_j|)$.

We may note, that a, denotes the s-wave scattering length. The p-wave scattering length is relevant when two Fermions of the same species/spin interact, however, this is lower order since fermions of the same spin tend to localize away from each other due to the Pauli exclusion principle. Recently an upper bound was proven in the spin-polarized case in [LS23], in which the relevant scattering length is the *p-wave scattering length*, analogous to the *odd-wave scattering length* in one dimension defined above in Definition 2.28.

The dilute spin–S Fermi gas in two dimensions

In [LSS05], the two dimensional result was also proved. The intuition behind the two dimensional result is, in this case, understood by considering the bosonic result, where to first order one replaces the scattering length a with $\ln(|\rho a^2|)^{-1}$. Furthermore, the kinetic energy term is of course replaced by the free Fermi energy in two dimensions. Without giving details on the assumptions on the potential, the formula takes the form

$$e^{2D}_{F,S}(\rho) = 2\pi\sum_{i=-S}^{S}\rho_i^2 + \frac{8\pi}{\ln(|\rho a^2|)}\sum_{-S\leq i<j\leq S}\rho_i\rho_j + o\left(\rho^2\ln(|\rho a^2|)^{-1}\right). \tag{2.4.6}$$

where ρ_i denotes the density of particles with spin i and the index i runs over integers or half integers. Furthermore, $e^{2D}_{F,S}(\rho) = \lim_{\substack{N,L\to\infty \\ N/L^2=\rho}} \frac{E^{2D}_{F,S}(N,L)}{L^2}$ and $E^{2D}_{F,S}(N,L)$ is the ground state of the spin–S Fermi gas with N spin–S fermions in $\Omega = [0,L]^2$ with dynamics given by the Hamiltonian $H = -\sum_{i=1}^{N} \Delta_i + \sum_{1\le i<j\le N} v(|x_i - x_j|)$.

2.5 The Lieb-Liniger Model: A Solvable Model in One Dimension

In 1960 a one-dimensional model of impenetrable bosons was solved by Girardeau [Gir60]. This initialized the study of solvable models of particles in the continuum in one dimension. The next major breakthrough was in this context made in 1963 by Lieb and Liniger, who posed and solved a model of one-dimensional point interacting bosons [LL63]. Their solution generalized the solution of the impenetrable bosons by Girardeau. The technique that was used is known as *Bethe ansatz* or *Bethe's hypothesis* after it was invented by Bethe to solve the one-dimensional Heisenberg chain [Bet31]. We will in this section, for self-containment, go through the solution of the Lieb-Liniger model, as the solution and more generally the ground state energy is of importance later in the thesis when studying the ground state energy of the dilute one-dimensional Bose gas. We follow the steps given in [LL63] and present a few more general results.

The Lieb-Liniger model is a model of bosons in $\Omega = [0,L]$ with dynamics given by the Hamiltonian

$$H_{LL} = -\sum_{i=1}^{N} \Delta_i + 2c \sum_{1\le i<j\le N} \delta(x_i - x_j), \tag{2.5.1}$$

where the right-hand side is defined in the sense of quadratic forms. More precisely on a *sector*, $\{\sigma\} = \{\sigma_1, \sigma_2, \ldots, \sigma_N\} := \{0 < x_{\sigma_1} < x_{\sigma_2} < \ldots < x_{\sigma_N} < L\}$, where $\sigma \in S_N$ is a permutation of $\{1,\ldots,N\}$, the Hamiltonian acts as $-\sum_{i=1}^{N} \Delta_i$, and by elliptic regularity, ([Gri11], Theorem 3.2.3.1), the

domain is given by

$$\mathcal{D}(H_{LL}) = \Big\{\psi \in H^1_s([0,L]^N) \;\Big|\; \psi\big|_\sigma \in H^2(\{\sigma\}) \text{ for any } \sigma \in S_N, \\ \text{and } (\partial_i - \partial_j)\psi|_{x_i=x_j^+} = c\psi|_{x_i=x_j}\Big\}.$$

The Bethe ansatz then prescribes that we, on a sector $\{1,2,\ldots,N\}$, seek solutions to the eigenvalue equation, $H_{LL}\psi = E\psi$, of the form

$$\psi(x) = \sum_{P\in S_N} a(P)\exp\left(i\sum_{i=1}^N k_{P_i}x_i\right), \tag{2.5.2}$$

where $a(P) \in \mathbb{C}$ are suitably chosen coefficients and $(k_i)_{i=1,2,\ldots,N}$ are non-equal real numbers.
The boundary conditions

$$(\partial_{j+1} - \partial_j)\psi|_{x_{j+1}=x_j} = c\psi|_{x_i=x_j},$$

are satisfied if for $P = (P_1, P_2, \ldots, P_j = \alpha, P_{j+1} = \beta, \ldots, P_N)$ and $Q = (P_1, P_2, \ldots, Q_j = \beta, Q_{j+1} = \alpha, \ldots, P_N)$, we have $i(k_\beta - k_\alpha)(a(P) - a(Q)) = c(a(P) + a(Q))$ implying

$$a(Q) = -\frac{c - i(k_\beta - k_\alpha)}{c + i(k_\beta - k_\alpha)}a(P) = -\exp(i\theta_{\beta,\alpha})a(P) \tag{2.5.3}$$

where we have defined

$$\theta_{i,j} \coloneqq -2\arctan\left(\frac{k_i - k_j}{c}\right). \tag{2.5.4}$$

We note that we require $k_i \neq k_j$ for $i \neq j$ in order for ψ to be non-vanishing. Defining $a(I) = 1$, it is simple to see that by the relations (2.5.3), all $a(P)$ are fixed. In fact that $a(P)$ is uniquely determined by (2.5.3) follows from the fact that in going from the identity I to some permutation P, the same elements are eventually transposed, by any path of transpositions.
The values of the pseudo momenta k_i are now determined by the periodic boundary conditions, which on the sector $\{1,2,\ldots,N\}$ take the form

$$\begin{aligned} \psi(0,x_2,x_3,\ldots,x_N) &= \psi(x_2,x_3,\ldots,x_N,L), \\ (\partial_x\psi(x,x_2,x_3,\ldots,x_N))\big|_{x=0} &= (\partial_x\psi(x_2,x_3,\ldots,x_N,x))\big|_{x=L}. \end{aligned} \tag{2.5.5}$$

With the ansatz state above, these equations correspond to the N equation

$$(-1)^{N-1}\exp(-ik_jL) = \exp\left(i\sum_{i=1}^{N}\theta_{i,j}\right), \tag{2.5.6}$$

with the definition $\theta_{i,i} := 0$. Although the "pseudo" momenta k_i cannot be regarded as being true momenta, one can construct the total momentum of a state. We notice that $P_{\text{tot.}} := \sum_{i=1}^{N} k_i$ is constant across different sectors, and hence it may be regarded as the true total momentum. Furthermore, we see that if the set $(k_i)_{i\in\{1,\ldots,N\}}$ solves the equations (2.5.6), then the set $(k_i' = k_i + 2\pi n_0/L)_{i\in\{1,\ldots,N\}}$, with any $n_0 \in \mathbb{Z}$, solves it as well. This corresponds to changing the total momentum to $P'_{\text{tot.}} = P_{\text{tot.}} + 2\pi n_0\rho$, with $\rho := N/L$. Thus we may restrict to finding all solutions with $-\pi\rho < P_{\text{tot.}} \leq \pi\rho$, then all other solutions are related by a constant change in "pseudo" momenta. Ordering the "pseudo" momenta such that $k_1 < k_2 < \ldots < k_N$, another consequence of (2.5.6) is that $\sum_{i=1}^{N} k_i = 2\pi n/L$ for some integer $-N/2 < n \leq N/2$, since $\theta_{i,j} = -\theta_{j,i}$.
Now we define

$$\delta_i = (k_{i+1} - k_i)L = \sum_{s=1}^{N}(\theta_{s,i} - \theta_{s,i+1}) + 2\pi n_i, \tag{2.5.7}$$

where n_i are integers and the second equality follows from (2.5.6). Since $\theta_{s,i}$ is strictly increasing in i, we see that $n_i \geq 1$. Notice that $k_j - k_i = \frac{1}{L}\sum_{s=i}^{j-1}\delta_i$ for $j > i$, hence (2.5.7) is a set of equations determining $(\delta_i)_{i\in\{1,\ldots,N-1\}}$. Given a set of $(n_i)_{i\in\{1,\ldots,N-1\}}$ and a solution of (2.5.7), $(\delta_i)_{i\in\{1,\ldots,N-1\}}$, we merely choose k_1 to satisfy (2.5.6) by having

$$k_1 = -\frac{1}{L}\sum_{i=1}^{N}\theta_{i,1} - \frac{2\pi m}{L} + \frac{\epsilon(N)}{L}, \tag{2.5.8}$$

where m is some integer determined by $-\pi\rho < P_{\text{tot.}} \leq \pi\rho$ and

$$\epsilon(N) = \begin{cases} 0 & \text{if } N \text{ is odd,} \\ \pi & \text{if } N \text{ is even} \end{cases}.$$

The right-hand side of (2.5.8) depends only on the δs. The proof of existence of solutions for (2.5.7) that varies continuously with c, was given in [YY69].

The Ground State

It is clear that within the set of ansatz states, the variational ground state must have $n_i = 1$ for all $i = 1, \dots, N-1$, this is to pack the pseudo-momenta k_i as closely as possible. In this case, we have by symmetry and uniqueness of the ground state that $k_i = -k_{N-i+1}$. Thus, since $P_{\text{tot.}} = \sum_{i=1}^{N} k_i = Nk_1 + \frac{1}{L}\sum_{j=1}^{N-1}(N-j)\delta_j = 0$ we find

$$k_1 = -k_N = -\frac{1}{NL}\sum_{j=1}^{N-1}(N-j)\delta_j.$$

We may also ask whether the true ground state is attained among these ansatz states. This turns out to be the case, which may be seen by the following results. We denote in this section by E_F the periodic spin-polarized (spinless) free Fermi ground state energy $E_F = \inf\left(\mathcal{E}_{0,0}(\psi)|\psi \in C^{\infty}_{a,\text{per}}\left([0,L]^N\right)\right)$, with $C^{\infty}_{a,\text{per}}\left([0,L]^N\right)$ denoting anti-symmetric periodic smooth functions.

Lemma 2.39. *Let Ψ_c denote the (true) ground state and E_c denote the (true) ground state energy of H_{LL} with coupling $c > 0$. Then $\lim_{c\to\infty} E_c = E_F = E_\infty$, where E_F is the free Fermi ground state energy and $\Psi_c \to \Psi_\infty$ in $L^2([0,L]^N)$ as $c \to \infty$.*

Proof. By going to the quadratic form representation of H_{LL}, it is clear by a trial state argument that $E_c \leq E_F$ for any $c < \infty$. Now assume that $E_c < \mathcal{E} < E_F$ for all $c < \infty$ where $\mathcal{E}$ is independent of c. Then the ground state at coupling Ψ_c of H_{LL}, is uniformly (in c) bounded in H^1. Hence for any sequence $(c_n)_{n\in\mathbb{N}} \subset \mathbb{R}_+$, we find that Ψ_{c_n} is, by possibly passing to a subsequence, weakly convergent in H^1 to some $\Psi \in H^1$. By the Rellich–Kondrachov theorem Ψ_{c_n} converges in L^2 norm to the same limit. Now assuming $c_n \to \infty$ as $n \to \infty$ we have $\Psi_{c_n}(x_i = x_j) \to 0$ in $L^2([0,L]^{N-1})$ as $n \to \infty$ for any $i \neq j$ in order for the potential energy to stay finite. But then the limit Ψ also satisfies $\Psi(x_i = x_j) = 0$ (in $L^2([0,L]^{N-1})$) for any $i \neq j$. This follows from the fact that $\delta(x_i - x_j)f(\overline{x^j}) \in H^{-1}([0,L]^N)$ for any $f \in L^2([0,L]^{N-1})$ and from weak H^1 convergence of Ψ_{c_n}. Notice that Ψ is a trial state for the impenetrable boson model ($c = \infty$). However, clearly we have $E_\Psi \leq \mathcal{E} < E_F$ by weak lower semi-continuity of the H^1–norm, which contradicts E_F being

the ground state energy of the impenetrable boson model. Hence we conclude $E_\Psi = E_F = E_\infty$, but then by uniqueness of the ground state in the impenetrable bosons model, $\Psi = \Psi_\infty$. Since $c_n \to \infty$ as $n \to \infty$ was arbitrary, we conclude that any subsequence of Ψ_{c_n} has a further subsequence $\Psi_{c_{n_i}}$ such that $\Psi_{c_{n_i}} \to \Psi_\infty$ as $i \to \infty$, and the proof is complete. □

Proposition 2.40. *Let $\Psi_V(c)$ be the variational ground state (in the Bethe ansatz class, as given above) of H_{LL}, then $\Psi_V(c)$ is the true ground state.*

Proof. Consider first the limit $c \to \infty$. Here it is easily verified that $\Psi_V(c) \to |\Psi_F|$ in L^2, where Ψ_F is the free Fermi ground state, i.e. a Slater determinant state and that $E_V(c) \to E_F$, where E_F is the free Fermi energy. This is the non-degenerate ground state energy at $c = \infty$, i.e. the impenetrable bosons. Now by the uniqueness of the bosonic ground state and continuity of the (true and variational) ground state energy in $1/c$, as well as the fact that $\Psi_V(c)$ is an eigenstate, we conclude that the variational ground state must remain the true ground state, as $1/c$ varies. If this was not the case, there would be an orthogonal true ground state, implying a degeneracy either at $c = \infty$ or at some $c > 0$.
Continuity of the true ground state energy, in c, can be seen by perturbation theory [RS78], or by a simple trial state argument, using Ψ_c (the ground state of $H_{LL}(c)$) as a trial state for $\mathcal{E}_{H_{LL}(c+\epsilon)}$.

□

We note that while Proposition 2.40 holds for the ground state, its proof cannot be generalized to excited states, since there is no unique nth excited state in the Bose gas. In this case, we refer to the more involved proof of completeness of the Bethe ansatz states by Dorlas [Dor93]. Proposition 2.40 of course follows from this result as well.
Although it is not needed for our analysis, we note that one may strengthen the result regarding convergence of Ψ_c as $c \to \infty$. This is shown in the following result.

Proposition 2.41. *Let Ψ_c denote the (true) ground state of H_{LL} with coupling c. If $(c_n > 0)_{n\in\mathbb{N}}$ is a sequence of couplings then there exist a subsequence $\Psi_{c_{n_i}}$, such that $\Psi_{c_{n_i}}$ converges in $C^\infty(\overline{\{1,2,\ldots,N\}})$ as $i \to \infty$.*

Proof. Since Ψ_{c_n} are ground states we know $-\Delta\Psi_{c_n} = \lambda_n \Psi_{c_n}$, with $\lambda_n \leq E_F$ for all $n \in \mathbb{N}$. Since $\overline{\{1,2,\ldots,N\}}$ is convex, we have by elliptic regularity

([Gri11], Theorem 3.2.3.1) that

$$\|\Psi_{c_n}\|_{H^{2m}(\{1,2,\dots,N\})} \leq C_m \lambda_n^m \|\Psi_{c_n}\|_{L^2(\{1,2,\dots,N\})} \leq C_m E_F^m.$$

By the Rellich–Kondrachov theorem [Ada75], there exist for each $m \in \mathbb{N}$ a subsequence $\Psi^m_{c_{n_i}}$ such that $\Psi^m_{c_{n_i}}$ converges in $H^{2m-1}(\{1,2,\dots,N\})$. By a diagonal argument we find a subsequence, $\Psi^i_{c_{n_i}}$, which converges in $H^k(\{1,2,\dots,N\})$ for all $k \in \mathbb{N}$. Hence, by the Sobolev embedding theorem ([Ada75], Theorem 5.4), $\Psi^i_{c_{n_i}}$ converges to Ψ in $C^\infty(\overline{\{1,2,\dots,N\}})$. □

Proposition 2.41 generalizes to exited states, by bounding $\lambda_n^{(i)} \leq E_F^{(i)}$, with $\lambda^{(i)}$ and $E_F^{(i)}$ denoting the ith exited eigenvalues in the proof.

Interestingly, it is possible to study the thermodynamic limit ($N, L \to \infty$ with $N/L = \rho$) of the system by the use of the Bethe ansatz solution. To do this, we define $K(\gamma) := \lim_{\substack{N,L\to\infty \\ N/L=\rho}} k_N$ where $\gamma = c/\rho$. Of course, the energy will grow with the particle number, so we are, in this case, interested in the energy per volume (length)

$$e(\gamma) := \lim_{\substack{N,L\to\infty \\ N/L=\rho}} \frac{1}{L} E_N. \tag{2.5.9}$$

Since we have $k_{i+1} - k_i < 2\pi/L$, we conclude

$$\theta_{s,i} - \theta_{s,i+1} = -\frac{2c(k_{i+1} - k_i)}{c^2 + (k_s - k_i)^2} + \mathcal{O}(1/(cL)^2). \tag{2.5.10}$$

So by (2.5.7) we see for the ground state ($n_i = 1$) that

$$k_{i+1} - k_i = \frac{2\pi}{L} - \frac{1}{L} \sum_{s=1}^{N} \frac{2c(k_{i+1} - k_i)}{c^2 + (k_s - k_i)^2} + \rho O(1/(cL)^2). \tag{2.5.11}$$

Now let f be such that $k_{i+1} - k_i = 1/(Lf(k_i))$. Then we may approximate the sum by an integral in the $L \to \infty$ limit, and we have

$$2\pi f(k) - 1 = 2c \int_{-K}^{K} \frac{f(p)}{c^2 + (p-k)^2} \, \mathrm{d}p + \varepsilon(1/(cL)), \tag{2.5.12}$$

with $\varepsilon(x) \to 0$ as $x \to 0$. The very definition of f implies $\int_{-K}^{K} f(p) \, \mathrm{d}p = \rho$,

with ground state energy

$$E = \sum_i k_i^2 = \frac{N}{\rho} \int_{-K}^{K} k^2 f(k) \, \mathrm{d}k, \tag{2.5.13}$$

and it follows from the definition of f and $k_i < k_{i+1}$ that $f \geq 0$.
It is now a matter of a simple coordinate transformation

$$g(x) \coloneqq f(Kx), \quad c \coloneqq K\lambda \tag{2.5.14}$$

to find the equations for the ground state energy in the thermodynamic limit:

$$2\pi g(x) - 1 = 2\lambda \int_{-1}^{1} \frac{g(y)}{\lambda^2 + (y-x)^2} \, \mathrm{d}y, \tag{2.5.15}$$

$$e(\gamma) = \rho^3 \frac{\gamma^3}{\lambda^3} \int_{-1}^{1} x^2 g(x) \, \mathrm{d}x, \tag{2.5.16}$$

$$1 = \frac{\gamma}{\lambda} \int_{-1}^{1} g(x) \, \mathrm{d}x. \tag{2.5.17}$$

The first equation is an inhomogeneous Fredholm equation of the second kind which is solved by the Liouville-Neumann series. Notice that our equation for $e(\gamma)$ differs from that of Lieb and Liniger by a factor ρ^3, since we have absorbed this factor as part of $e(\gamma)$. This difference is also present when comparing to Chapter 3, where the convention of Lieb and Liniger is followed. In Lemma 16 of Chapter 3 we prove the following lemma on the thermodynamic ground state energy of the Lieb-Liniger model. This lemma will be important in the proof of a lower bound on the ground state energy for the dilute Bose gas.

Lemma 2.42 (Lemma 16 in Chapter 3 ([ARS22]))**.** *Let $e(\gamma)$ be the solution of* (2.5.15)–(2.5.17)*. Then for $\gamma > 0$ we have*

$$e(\gamma) \geq \frac{\pi^2}{3} \rho^3 \left(\frac{\gamma}{\gamma + 2} \right)^2. \tag{2.5.18}$$

Here we would like to give the equivalent result for a finite number of particles.

Lemma 2.43. *Let $(k_i)_{i=1}^N$ satisfy $k_1 < k_2 < \ldots < k_N$ and* (2.5.11)*. Then we*

have

$$\sum_{n=1}^{N} k_n^2 \geq N\left(\rho^2 - \frac{1}{L^2}\right)\frac{\pi^2}{3}\left(1+2\frac{\rho}{c}\right)^{-2} + \mathcal{O}\left(\frac{\rho}{c}\frac{\rho^2}{cL}\right). \tag{2.5.19}$$

Proof. By discarding the term $(k_s - k_i)^2$ in the denominator inside the sum in (2.5.11) we find straightaway that

$$k_{i+1} - k_i \geq \frac{2\pi}{L}\left(1+2\frac{\rho}{c}\right)^{-1} + \rho\mathcal{O}\left(1/(cL)^2\right).$$

For the ground state where $k_i = -k_{N-i+1}$ it follows that

$$|k_i| \geq \frac{2\pi}{L}\left(1+2\frac{\rho}{c}\right)^{-1}(i-(N+1)/2) + \rho\mathcal{O}\left(1/(cL)^2\right), \text{ for all } i = 1, ..., N. \tag{2.5.20}$$

Therefore we find the lower bound on the energy

$$\sum_{i=1}^{N} k_i^2 \geq N\left(\rho^2 - \frac{1}{L^2}\right)\frac{\pi^2}{3}\left(1+2\frac{\rho}{c}\right)^{-2} + \mathcal{O}\left(\frac{\rho}{c}\frac{\rho^2}{cL}\right). \tag{2.5.21}$$

□

2.6 The Yang-Gaudin Model

Similarly to the Lieb-Liniger model, the Yang-Gaudin model is exactly solvable, by use of a generalized Bethe ansatz. This was originally done in [Yan67], and we shall briefly review the methods in this section. The model of interest describes N spin–1/2 fermions and is given using the same formal Hamiltonian as for the Lieb-Liniger model

$$H_{YG} = -\sum_{i=1}^{N}\partial_i^2 + 2c\sum_{1\leq i<j\leq N}\delta(x_i - x_j), \tag{2.6.1}$$

however, the domain is not, for the moment being, taken to have any given spatial symmetry.

Labeling the symmetries

To analyze the problem, Yang considers the possible spatial symmetries that may appear in the problem. Having combined spin-space anti-symmetry re-

quires that any irreducible representation of S_N determining the spatial symmetry must have a corresponding conjugate spin symmetry. As an example consider the two particle case where the wave function is either symmetric and the spin state is the singlet, *or* the wave function is anti-symmetric and the spin state is in the triplet. If you have more particles, the picture is more complicated, although similar. Notice that one cannot have 3 spin–1/2 particles that are mutually in the singlet state with each other. It turns out, that one way to label the symmetry of a spin state is by Young tableaux, i.e. a diagram of boxes with numbers obeying the rule that numbers increase along all rows and columns. A tableau labels a subspace of spin states. To construct the subspace consider all states that are symmetrized in particle labels in the same rows. Next anti-symmetrize, in these states, all particle labels in the same columns. For example:

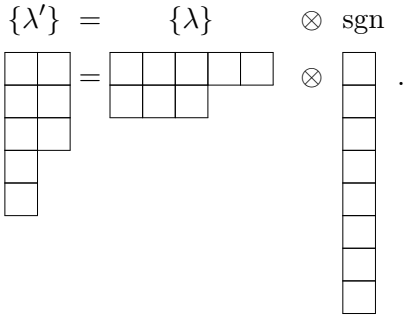
$$\begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 \\ \cline{1-1}\end{array} = \text{span}\left(|\uparrow\uparrow\downarrow\rangle - |\downarrow\uparrow\uparrow\rangle, |\downarrow\downarrow\uparrow\rangle - |\uparrow\downarrow\downarrow\rangle\right), \tag{2.6.2}$$

$$\begin{array}{|c|c|}\hline 1 & 3 \\ \hline 2 \\ \cline{1-1}\end{array} = \text{span}\left(|\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\rangle, |\downarrow\uparrow\downarrow\rangle - |\uparrow\downarrow\downarrow\rangle\right), \tag{2.6.3}$$

$$\begin{array}{|c|c|c|}\hline 1 & 2 & 3 \\ \hline\end{array} = \text{span}\left(|\uparrow\uparrow\uparrow\rangle, |\downarrow\downarrow\downarrow\rangle, |\uparrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\rangle + |\uparrow\uparrow\downarrow\rangle, |\uparrow\downarrow\downarrow\rangle + |\downarrow\downarrow\uparrow\rangle + |\downarrow\uparrow\downarrow\rangle\right). \tag{2.6.4}$$

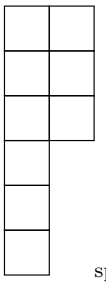
By the before mentioned fact that one cannot anti-symmetrize three 1/2–spins, Young tableaux of spin–1/2 states have at most two rows. An interesting fact with this labeling of spin states is that the structure of a given tableau is related to the total spin of the state. To see this, notice that all columns of lengths two carry vanishing total spin because they form a singlet state. On the other hand, all columns of length one are symmetrized with each other. Hence it is well known that they carry maximal total spin. In the subspace labeled by a tableau with M columns of length 2 and $N-2M$ columns of length 1, all states are of the form $|S_0\rangle \otimes |S_{(N-2M)/2}\rangle$, where $|S_0\rangle$ is some spin state of total spin 0 and $|S_{(N-2M)/2}\rangle$ is some spin state of total spin $(N-2M)/2$. Remembering that irreducible representations of $SU(2)$ are labeled by the total spin, we conclude that a Young diagram, which is just a Young tableau with blank entries, labels the irreducible $SU(2)$ representations.

Remember that we may label the irreducible representation of S_N determining the spatial symmetry also by Young diagrams, [WJ91]. Recall that for irreducible representations of S_N we have the relation



(2.6.5)

Thus we see that a wave function, which is anti-symmetric under (spin-space) permutations, and which spatially transforms in the irreducible representation



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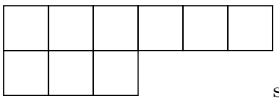
must be defined in the spin subspace



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We notice that this restricts the spatial symmetries that spin–1/2 fermions can possess, since the spin diagrams have at most two rows. In the following, we will denote the diagram consisting of a row with $N-M$ boxes and a row with M boxes by $[N-M, M]$, and diagrams consisting of a column of $N-M$ boxes and a column of M boxes by $[2^M, 1^{N-2M}]$.

Recap of the findings of Yang: Solution by Bethe-Yang ansatz

The solution found by Yang in [Yan67], relies on a generalization of the Bethe ansatz, which we saw in the previous section solved the Lieb-Liniger model. The generalized Bethe ansatz is also known as the Yang-Bethe hypothesis or

Yang-Bethe ansatz. We recap here, without proof, the findings of Yang. For references on these results, we point to [Gau67, Yan67, Sut68, Fun81, Gau14]. The model is solved by applying a standard Bethe ansatz state: On the sector $\{\sigma\}$ define

$$\psi = \sum_{P \in S_N} \xi_{P,\sigma} \exp\left(k_{P_1} x_{\sigma_1} + \ldots + k_{P_N} x_{\sigma_N}\right), \tag{2.6.6}$$

with energy $E = \sum_{i=1}^{N} k_i^2$. Similarly to in the Lieb-Liniger case, in order to satisfy the right boundary condition, we have

$$\xi_{P,\sigma} = Y_{ij}^{1,2} \xi_{Q,\sigma}, \tag{2.6.7}$$

when $Q = (P_1, \ldots, \underbrace{2}_{i}, \ldots, \underbrace{1}_{j}, \ldots, P_N)$ and
$P = (P_1, \ldots, \underbrace{1}_{i}, \ldots, \underbrace{2}_{j}, \ldots, P_N)$, where we defined

$$Y_{ij}^{12} = \frac{(k_i - k_j)(12) - ic}{(k_i - k_j) + ic}, \tag{2.6.8}$$

with (12) acting by interchanging σ_1 and σ_2. We see that we recover the Lieb-Liniger result if ψ is symmetric and a Slater determinant if ψ is anti-symmetric.
A crucial observation by Yang is that we have the following identities, of which the second is famously known as the Yang-Baxter equation.

$$\begin{aligned} Y_{ij}^{ab} Y_{ji}^{ab} &= 1 \\ Y_{jk}^{ab} Y_{ik}^{bc} Y_{ij}^{ab} &= Y_{ij}^{bc} Y_{ik}^{ab} Y_{jk}^{bc}. \end{aligned} \tag{2.6.9}$$

These make the equations (2.6.7) mutually consistent.
The condition of periodic boundary conditions may now be written

$$\lambda_j \xi_{I,\sigma} = X_{(j+1)j} X_{(j+2)j} \ldots X_{Nj} X_{1j}, \ldots X_{(j-1)j} \xi_{I,\sigma}, \tag{2.6.10}$$

with $\lambda_j = \exp(ik_j L)$ and $X_{ij} = P_{ij} Y_{ij}^{ij}$.
Now, restricting to ψ in some irreducible representation $R = [2^M, 1^{N-2M}]$, one easily sees that, using $X_{ij} = (1 - P_{ij} x_{ij})/(1 + x_{ij})$, we may equivalently consider a spin state, Φ, of total spin $N - 2M$, satisfying the equation

$$\mu_j \Phi = X'_{(j+1)j} X'_{(j+2)j} \ldots X'_{Nj} X'_{1j}, \ldots X'_{(j-1)j} \Phi, \tag{2.6.11}$$

with $X'_{ij} = (1 + P_{ij}^{\tilde{R}} x_{ij})/(1 + x_{ij})$, where $\tilde{R}$ denotes the conjugate representation, so $P_{ij}^{\tilde{R}}$ is acting on the spins i.e. $P_{ij}^{\tilde{R}} = -P_{ij}$.
Now considering instead a spin chain of total z–spin $(N-2M)/2$, we know that this chain can have components with total spin $N/2$, $(N-1)/2, \ldots (N-2M)/2$. Notice that $P_{ij} = 1/2 + 2S_i \cdot S_j$, for spin–1/2 particles, which commute with the total spin operator. Hence we may find eigenvalues, μ_j, in each total spin sector separately. However, since these eigenvalues correspond to eigenvalues of (2.6.1), the theorem of Lieb and Mattis [LM62b][2] tells us that the eigenvalue μ_j yielding the smallest eigenvalue of (2.6.1) must come from the total spin sector $N - 2M$, i.e. minimal total spin in the case when $N/2$ is an odd integer.
The Bethe-Yang hypothesis states that

$$\Phi(y_1, \ldots, y_M) = \sum_{P \in S_N} A_P \prod_{i=1}^{M} F(\Lambda_{P_i}, y_i), \tag{2.6.12}$$

where y_i denotes the positions of the spin downs, and with

$$F(\Lambda, y) = \prod_{j=1}^{y-1} \frac{ik_j - i\Lambda - c/2}{ik_{j+1} - i\Lambda + c/2}, \tag{2.6.13}$$

[2] **A detail often left out in the literature:** This theorem is only proved in the paper [LM62b] for Dirichlet or Neumann boundary conditions. One may prove that the absolute ground state is in the total spin $S = 0$ subspace even with periodic boundary conditions when $N/2$ is an odd integer. The proof requires $N/2$ to be an odd integer in order to have a positive periodic ground state on an ordered sector

$$\{x_1 < x_2 < \ldots < x_{N/2} \text{ and } x_{N/2+1} < x_{N/2+2} < \ldots < x_N\}.$$

Furthermore, in this case, the ground state is unique.
The exact statement of the theorem is then: Denote by $E(S)$ the lowest energy of any state with total spin S. Then the following theorem holds:

Theorem 2.44 (Lieb and Mattis, [LM62b], for periodic boundary conditions, $d = 1$)**.** *If $N/2$ is an odd integer and $S > 2n$ for some integer n then $E(S) > E(2n)$, unless the potential, V, is pathological, in which $E(S) \geq E(2n)$. Furthermore, when V is not pathological, the ground state with energy $E(0)$ is unique.*

Proof. The proof follows the proof of Theorem I in [LM62b] with $M = 2n$ and $N/2$ odd, in order for $\left|\varphi_0(x_1, \ldots, x_{N/2-2n} | x_{N/2-2n+1}, \ldots, x_N)\right|$ to be a *continuous* anti-symmetric periodic wave function on the above mentioned sector. □

For more details on the notion of "pathological" and the proof, we refer to the original paper by Lieb and Mattis.

and

$$-\prod_{j=1}^{N}\frac{ik_j-i\Lambda_\alpha-c/2}{ik_j-i\Lambda_\alpha+c/2}=\prod_{\beta=1}^{M}\frac{-i\Lambda_\beta+i\Lambda_\alpha-c}{-i\Lambda_\beta+i\Lambda_\alpha+c}. \tag{2.6.14}$$

One may verify that Φ has total spin $N-2M$. Yang then finds

$$\mu_j(k,c,[N-M,M])=\prod_{\beta=1}^{M}\frac{ik_j-i\Lambda_\beta-c/2}{ik_j-i\Lambda_\beta+c/2}. \tag{2.6.15}$$

Thus the energy is determined by the equation

$$\exp(ik_jL)=\prod_{\beta=1}^{M}\frac{ik_j-i\Lambda_\beta-c/2}{ik_j-i\Lambda_\beta+c/2}. \tag{2.6.16}$$

Taking the logarithm of (2.6.14) and (2.6.16) and adding certain integers to get a well defined $c\to\infty$ limit, as we did in Section 2.5, one finds

$$\begin{aligned}-\sum_{k\in\{k_j\}_j}\theta(2\Lambda-2k)&=2\pi J_\Lambda-\sum_{\Lambda'\in(\Lambda_\alpha)_\alpha}\theta(\Lambda-\Lambda'),\\ kL&=2\pi I_k-\sum_{\Lambda'\in(\Lambda_\alpha)_\alpha}\theta(2k-2\Lambda'),\end{aligned} \tag{2.6.17}$$

with the usual $\theta(x)\coloneqq-2\arctan(x/c)$. For N even and M odd we have for ground state (among the ansatz states)

$$\begin{aligned}J_\Lambda&\in\{-(M-1)/2,\dots,(M-1)/2\},\\ I_k&\in\{1-N/2,\dots,N/2\}.\end{aligned} \tag{2.6.18}$$

Going to the thermodynamic limit, i.e. $N,M,L\to\infty$ proportionally, one then find the equations for the energy

$$2\pi\sigma(\Lambda)=-\int_{-B}^{B}\frac{2c\sigma(\Lambda')\,\mathrm{d}\Lambda'}{c^2+(\Lambda-\Lambda')^2}+\int_{-Q}^{Q}\frac{4cf(k)\,\mathrm{d}k}{c^2+4(k-\Lambda)^2}, \tag{2.6.19}$$

$$2\pi f(k)=1+\int_{-B}^{B}\frac{4c\sigma(\Lambda')\,\mathrm{d}\Lambda'}{c^2+4(k-\Lambda')^2}, \tag{2.6.20}$$

$$\rho=N/L=\int_{-Q}^{Q}f(k)\,\mathrm{d}k,\quad M/L=\int_{-B}^{B}\sigma(\Lambda)\,\mathrm{d}\Lambda, \tag{2.6.21}$$

$$e=E/L=\int_{-Q}^{Q}k^2f(k)\,\mathrm{d}k, \tag{2.6.22}$$

with $f, \sigma \geq 0$. We see that taking $B = \infty$, and integrating over (2.6.19), one finds by interchanging the order of integration

$$2\pi M/L = -\int_{-\infty}^{\infty} 2\pi\sigma(\Lambda')\,\mathrm{d}\Lambda' + 2\pi\int_{-Q}^{Q} f(k)\,\mathrm{d}k, \tag{2.6.23}$$

where we used $\int_{-\infty}^{\infty}\frac{\mathrm{d}x}{1+x^2} = \pi$. So using (2.6.21) we find $2M = N$, and thus the total spin is $S_{\text{tot.}} = 0$. By a theorem of Lieb and Mattis [LM62b], this is then the total ground state.

Lower bound of the Yang-Gaudin model

Now the following lemma will prove useful in obtaining a lower bound for the thermodynamic "ground state energy" (in the sense that it comes from a solution of integral equations (2.6.19)–(2.6.22)) of the Yang-Gaudin model.

Lemma 2.45. *For any $m \in \mathbb{N}_+$, the equations* (2.6.19)–(2.6.22) *imply that*

$$\begin{aligned} 2\pi f(k) = 1 &+ (-1)^{m+1} 4\int_{-\infty}^{\infty} \frac{(2m-1)c\sigma(\Lambda'')}{((2m-1)^2c^2 + 4(k-\Lambda'')^2)}\,\mathrm{d}\Lambda'' \\ &+ 2\sum_{n=0}^{m-1}(-1)^{n+1}\int_{-Q}^{Q}\frac{2c(2n)f(k')}{((2n)^2c^2+4(k-k')^2)}\,\mathrm{d}k', \end{aligned} \tag{2.6.24}$$

,

Proof. We give a proof by induction: For the induction base case, we notice that the $m = 1$ statement is simply (2.6.20). For the induction step, assume that (2.6.24) hold for $m = m_0$, we may plug the right-hand side of (2.6.19) into (2.6.24). By Tonelli's theorem, we may interchange the order of integration and we find

$$\begin{aligned} &2\pi f(k) - 1 = \\ &\frac{(-1)^{m_0+2}}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{8c^2(2m_0-1)\sigma(\Lambda'')}{(c^2+(\Lambda'-\Lambda'')^2)((2m_0-1)^2c^2+4(k-\Lambda')^2)}\,\mathrm{d}\Lambda'\,\mathrm{d}\Lambda'' \\ &+\frac{(-1)^{m_0+1}}{2\pi}\int_{-Q}^{Q}\int_{-\infty}^{\infty}\frac{4^2c^2(2m_0-1)f(k')}{(c^2+4(k'-\Lambda')^2)((2m_0-1)^2c^2+4(k-\Lambda')^2)}\,\mathrm{d}\Lambda'\,\mathrm{d}k' \\ &+2\sum_{n=0}^{m_0-1}(-1)^{n+1}\int_{-Q}^{Q}\frac{2c(2n)f(k')}{((2n)^2c^2+4(k-k')^2)}\,\mathrm{d}k'. \end{aligned} \tag{2.6.25}$$

Using the formulas

$$\int_{-\infty}^{\infty} \frac{m}{(1+(x'-x'')^2)(m^2+4(y-x'))}\,\mathrm{d}x' = \frac{(m+2)\pi}{(2+m)^2+4(y-x'')^2}, \tag{2.6.26}$$

$$\int_{-\infty}^{\infty} \frac{m}{(1+4(y'-x')^2)(m^2+4(y-x'))}\,\mathrm{d}x' = \frac{(m+1)\pi}{2((m+1)^2+4(y-y')^2)}, \tag{2.6.27}$$

for any $x'', y, y' \in \mathbb{R}$ and $m \in \mathbb{N}_+$, we find

$$\begin{aligned} 2\pi f(k) = 1 + (-1)^{m_0+2} 4 \int_{-\infty}^{\infty} \frac{(2(m_0+1)-1)c\sigma(\Lambda'')}{((2(m_0+1)-1)^2c^2+4(k-\Lambda'')^2)}\,\mathrm{d}\Lambda'' \\ +2\sum_{n=0}^{m_0}(-1)^{n+1}\int_{-Q}^{Q} \frac{2c(2n)f(k')}{((2n)^2c^2+4(k-k')^2)}\,\mathrm{d}k', \end{aligned} \tag{2.6.28}$$

which proves the required result. □

We will aim at proving a lower bound. To do this, notice that in Lemma 2.45 the second term in (2.6.24) vanishes in the limit $m \to \infty$ by the estimate

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{(2m-1)c\sigma(\Lambda'')}{((2m-1)^2c^2+4(k-\Lambda'')^2)}\,\mathrm{d}\Lambda'' &\leq \frac{1}{(2m-1)c}\int_{-\infty}^{\infty}\sigma(\Lambda'')\,\mathrm{d}\Lambda'' \\ &= \frac{M/L}{(2m-1)c}. \end{aligned} \tag{2.6.29}$$

For the third term in (2.6.24), we need the estimate of the following lemma:

Lemma 2.46. *For any $m_0 \in \mathbb{N}_+$ we have*

$$\sum_{n=0}^{m_0}(-1)^{n+1}\int_{-Q}^{Q} \frac{2c(2n)f(k')}{((2n)^2c^2+4(k-k')^2)}\,\mathrm{d}k' \leq \sum_{n=0}^{m_0}(-1)^{n+1}\int_{-Q}^{Q}\frac{2f(k')}{2nc}\,\mathrm{d}k'. \tag{2.6.30}$$

Proof. Essentially we want to throw away the $(k-k')^2$ in the denominator on the left-hand side of (2.6.30) to get an upper bound. For all terms with positive coefficients, this can be done by the inequality

$$\int_{-Q}^{Q}\frac{2f(k')}{2nc}\,\mathrm{d}k' \geq \int_{-Q}^{Q}\frac{2c(2n)f(k')}{((2n)^2c^2+4(k-k')^2)}\,\mathrm{d}k'. \tag{2.6.31}$$

However, for the terms with a negative sign, this estimate cannot be used. Thus we use the following strategy instead: In order to deal with the signs we estimate the differences

$$\begin{aligned}\Delta_n = &\left(\int_{-Q}^{Q} \frac{2f(k')}{2nc}\,\mathrm{d}k' - \int_{-Q}^{Q} \frac{2c(2n)f(k')}{((2n)^2c^2+4(k-k')^2)}\,\mathrm{d}k'\right)\\ &-\left(\int_{-Q}^{Q} \frac{2f(k')}{2(n+1)c}\,\mathrm{d}k' - \int_{-Q}^{Q} \frac{2c(2(n+1))f(k')}{((2(n+1))^2c^2+4(k-k')^2)}\,\mathrm{d}k'\right).\end{aligned} \tag{2.6.32}$$

A straightforward computation shows

$$\begin{aligned}&\Delta_n = \\ &\int_{-Q}^{Q} \frac{2f(k')}{2n(n+1)c}\\ &-\left(\frac{2c(2n)\left[(2(n+1))^2c^2+4(k-k')^2\right]}{\left[(2n)^2c^2+4(k-k')^2\right]\left[(2(n+1))^2c^2+4(k-k')^2\right]}\right.\\ &\qquad\left.\frac{-2c(2(n+1))\left[(2n)^2c^2+4(k-k')^2\right]}{\left[(2n)^2c^2+4(k-k')^2\right]\left[(2(n+1))^2c^2+4(k-k')^2\right]}\right)f(k')\,\mathrm{d}k'\\ &=\int_{-Q}^{Q} \frac{2f(k')}{2n(n+1)c}\\ &\quad-\frac{2c\cdot 8n(n+1)c^2-4c\cdot 4(k-k')^2}{\left[(2n)^2c^2+4(k-k')^2\right]\left[(2(n+1))^2c^2+4(k-k')^2\right]}f(k')\,\mathrm{d}k'\\ &\geq\int_{-Q}^{Q} \frac{4c\cdot 4(k-k')^2}{\left[(2n)^2c^2+4(k-k')^2\right]\left[(2(n+1))^2c^2+4(k-k')^2\right]}f(k')\,\mathrm{d}k'\\ &\geq 0\end{aligned} \tag{2.6.33}$$

It follows for any m_0 that

$$\begin{aligned}&\sum_{n=0}^{m_0}(-1)^{n+1}\int_{-Q}^{Q} \frac{2c(2n)f(k')}{((2n)^2c^2+4(k-k')^2)}\,\mathrm{d}k'\\ &\leq\sum_{n=1}^{m_0}(-1)^{n+1}\int_{-Q}^{Q} \frac{2f(k')}{2nc}\,\mathrm{d}k' - \sum_{l=1}^{\lfloor m_0/2\rfloor}\Delta_{(2l-1)}\\ &\leq\sum_{n=0}^{m_0}(-1)^{n+1}\int_{-Q}^{Q} \frac{2f(k')}{2nc}\,\mathrm{d}k'.\end{aligned} \tag{2.6.34}$$

Here the first inequality is an *equality* if m_0 is even, and the inequality when m_0 is odd follows from (2.6.31) with $n = m_0$. □

We notice that we may upper bound f:

Lemma 2.47. *Let f be a solution of* (2.6.19)–(2.6.21)*, then*

$$2\pi f(k) \leq 1 + 2\sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \int_{-Q}^{Q} \frac{f(k')}{c}\,\mathrm{d}k' = 1 + \frac{2\ln(2)}{c}\rho. \tag{2.6.35}$$

Proof. By Lemma 2.45 with $m \to \infty$ using (2.6.29) and Lemma 2.46 the result follows. □

We are ready to give a lower bound for the "ground state" energy of the Yang-Gaudin model.

Proposition 2.48. *Let e be a solution of* (2.6.19)–(2.6.22)*, then*

$$e \geq \frac{\pi^2}{3}\rho^3 \left(\frac{1}{1+\frac{2\ln(2)}{c}\rho}\right)^2. \tag{2.6.36}$$

Proof. We notice that the expression for $e = \int_{-Q}^{Q} f(k)k^2\,\mathrm{d}k$, given $\int_{-Q}^{Q} f(k)\,\mathrm{d}k = \rho$ *and* $f \leq K$, is minimized by having $f = K\mathbb{1}_{[-\rho/(2K),\rho/(2K)]}$, in which case $\int_{-Q}^{Q} f(k)k^2\,\mathrm{d}k = \frac{2}{3}K\left(\frac{\rho}{2K}\right)^3$. That $\rho/(2K) \leq Q$ follows straight away from $\rho = \int_{-Q}^{Q} f(k)\,\mathrm{d}k \leq 2KQ$. By Lemma 2.47, we find $f \leq \frac{1}{2\pi}\left(1 + \frac{2\ln(2)}{c}\rho\right)$, so it follows that $e \geq \frac{\pi^2}{3}\rho^3\left(\frac{1}{1+\frac{2\ln(2)}{c}\rho}\right)^2$. □

We will, in Chapter 4, find a matching upper bound for the Yang-Gaudin ground state energy in the dilute limit.

A Small Caveat

There is an issue in the analysis of the Yang-Gaudin model: It is safe to say that in the physics/integrability literature, the "ground state" of (2.6.1) is widely believed to be the one found above. However, there is, to the best of our knowledge, no rigorous proof in the literature that the true ground state of (2.6.1) is among the Yang-Bethe ansatz states. In fact, there seems to be no proof of the existence of a solution to the equations (2.6.17) given two sets of integers $(I_j)_{j=1}^N$ and $(J_a)_{a=1}^M$. This is in contrast to the analysis of the Lieb-Liniger model, in which both the existence of solutions as well as the completeness of the Bethe ansatz states is known, [Dor93]. Since we will not use the results from this section for any rigorous analysis in the remainder of

the thesis, we leave the establishment of these facts for future work. We will in Chapter 4 refer to the e coming from a solution of (2.6.19)–(2.6.22) as the ground state energy of the Yang–Gaudin model, however this non-rigorous use of the terminology is never used in any rigorous setting.
We may state, for good measure, what is needed to make statements about the ground state rigorous:

- Establish existence of solutions of (2.6.17) for any two sets of integers $(I_j, J_a)_{j,a}$, at any $c > 0$ such that k_j, Λ_a varies continuously with c.
- Either of the two:
    1. Establish that Yang finds full multiplicity of solution converging to the ground state in the limit $c \to \infty$. (In this case the theorem of Lieb and Mattis [Theorem 2.44]) implies that no extra ground state can exist.
    2. Justify rigorously Gaudin's findings in the $c \to 0$ limit, where the ground state is unique [Gau67]. In this case, the ground state is of Bethe-Yang ansatz form in this limit. It is then implied that this is the case for all $c > 0$ again by the theorem of Lieb and Mattis.

Chapter 3

The Ground State Energy of the One-dimensional Dilute Bose Gas (Preprint)

This chapter contains a revised edition of the preprint, [ARS22], written as part of a collaboration with Robin Reuvers and Jan Philip Solovej. To emphasize the independence of this preprint from the rest of thesis, the title page with abstract and authors is included. Furthermore, the labeling of equations, theorems, lemma, and references is kept separate from the rest of the thesis. Repetitions from the preceding chapters of this thesis might occur, and repetitions of the content in this preprint may also occur in the following chapters. When referring to the results of this preprint, we shall state "from Chapter 3" explicitly and refer to the labeling in this chapter.

Ground state energy of dilute Bose gases in 1D

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Abstract

We study the ground state energy of a gas of 1D bosons with density ρ, interacting through a general, repulsive 2-body potential with scattering length a, in the dilute limit $\rho|a| \ll 1$. The first terms in the expansion of the thermodynamic energy density are $\pi^2\rho^3/3(1+2\rho a)$, where the leading order is the 1D free Fermi gas. This result covers the Tonks–Girardeau limit of the Lieb–Liniger model as a special case, but given the possibility that $a > 0$, it also applies to potentials that differ significantly from a delta function. We include extensions to spinless fermions and 1D anyonic symmetries, and discuss an application to confined 3D gases.

1 Introduction

The ground state energy of interacting, dilute Bose gases in 2 and 3 dimensions has long been a topic of study. Usually, a Hamiltonian of the form

$$-\sum_{i=1}^{N}\Delta_{x_i}+\sum_{1\leq i<j\leq N}v(x_i-x_j) \tag{1.1}$$

is considered ($\hbar = 2m = 1$), in a box $[0,L]^d$ of dimension $d = 2, 3$, and with a repulsive 2-body interaction $v \geq 0$ between the bosons. Diluteness is defined by saying the density $\rho = N/L^d$ of the gas is low compared to the scale set by the scattering length a of the potential (see Appendix C in [30] for a discussion, and also Section 1.2 for $d = 1$ below). That is, $\rho a^2 \ll 1$ in 2D, and $\rho a^3 \ll 1$ in 3D.

In the thermodynamic limit, the diluteness assumption allows for surprisingly general expressions for the ground state energy. Take, for example, the famous energy expansion to second

order in $\rho a^3 \ll 1$ by Lee–Huang–Yang [27], derived for 3D bosons with a hard core of diameter a,

$$4\pi N\rho^{2/3}(\rho a^3)^{1/3}\left(1+\frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3}+o\left(\sqrt{\rho a^3}\right)\right). \tag{1.2}$$

After early rigorous work by Dyson [11], Lieb and Yngvason [31] proved that the leading term in this expansion holds for a very general class of potentials v, and a similar result was obtained for the second-order term [3, 14, 15, 50].

The situation is similar in 2D. The leading order in the energy expansion for $\rho a^2 \ll 1$ derived by Schick [43] was proved rigorously by Lieb and Yngvason [36]. A second-order term has also been derived and was equally predicted to be general [1, 13, 38], resulting in the expansion

$$\frac{4\pi N\rho}{|\ln(\rho a^2)|}\left(1-\frac{\ln\left|\ln(\rho a^2)\right|}{|\ln(\rho a^2)|}+\frac{C}{|\ln(\rho a^2)|}+o\left(\left|\ln(\rho a^2)\right|^{-1}\right)\right), \tag{1.3}$$

for some constant C. This was recently shown rigorously [12].

Remarkably, it seems the existence of a similar, general expansion in 1D was never studied in similar depth. It was, however, suggested in [2] by considering two exactly-known special cases, as we will do now as well.

The first is the famous Lieb–Liniger model [33]. Many of its features can be calculated explicitly with Bethe ansatz wave functions, but for our purpose we return to something basic: the ground state energy. Consider Lieb and Liniger's Hamiltonian for a gas of N one-dimensional bosons on an interval of length L (periodic b.c.), with a repulsive point interaction of strength $2c > 0$,

$$-\sum_{i=1}^{N}\partial_{x_i}^2+2c\sum_{1\le i<j\le N}\delta(x_i-x_j). \tag{1.4}$$

The ground state can be found explicitly [33], and in the thermodynamic limit $L\to\infty$ with density $\rho = N/L$ fixed, its energy is

$$E_{\mathrm{LL}} = N\rho^2 e(c/\rho), \tag{1.5}$$

where $e(c/\rho)$ is described by integral equations. Since c/ρ is the only relevant parameter, diluteness, or low density ρ, should imply $c/\rho \gg 1$. In this case, the ground state energy can be expanded as ([33]; see, for example, [21, 25]),

$$E_{\mathrm{LL}} = N\rho^2 e(c/\rho) = N\frac{\pi^2}{3}\rho^2\left(\left(1+2\frac{\rho}{c}\right)^{-2}+\mathcal{O}\left(\frac{\rho}{c}\right)^3\right). \tag{1.6}$$

Recall that the dilute limit is $\rho a^2 \ll 1$ in 2D and $\rho a^3 \ll 1$ in 3D. This seems easy to generalize

to 1D, but it turns out the Lieb–Liniger potential $2c\delta$ has scattering length $a = -2/c$. That is, in 1D the scattering length can be negative even if the potential is positive, and we should be careful to define the dilute limit as $\rho|a| \ll 1$. This then matches the limit $c/\rho \gg 1$ mentioned above, and we can write (1.6) as

$$\begin{aligned} E_{\mathrm{LL}} &= N\frac{\pi^2}{3}\rho^2\left((1-\rho a)^{-2} + \mathcal{O}(\rho a)^3\right) \\ &= N\frac{\pi^2}{3}\rho^2\left(1 + 2\rho a + 3(\rho a)^2 + \mathcal{O}(\rho a)^3\right). \end{aligned} \tag{1.7}$$

This expansion should now be a good candidate for the 1D equivalent of (1.2) and (1.3). This is supported by the fact that 1D bosons with a hard core of diameter a have an exact thermodynamic ground state energy of [2, 17]

$$N\frac{\pi^2}{3}\left(\frac{N}{L-Na}\right)^2 = N\frac{\pi^2}{3}\rho^2(1-\rho a)^{-2}. \tag{1.8}$$

This is the 1D free Fermi energy on an interval shortened by the space taken up by the hard cores (the ground state is of Girardeau type; see Remark 2 and the discussion of the Girardeau wave function in Section 1.2).

With two explicit examples satisfying (1.7) to second order, it seems likely we can expect this expansion to be general [2], just like (1.2) and (1.3) in three and two dimensions. Indeed, our main result confirms the validity of (1.7) to first order, for a wide class of interaction potentials.

1.1 Main theorem

Throughout the paper, we will assume that the 2-body potential v is a symmetric measure with a finite range, $\mathrm{supp}(v) \subset [-R_0, R_0]$. Furthermore, we assume $v = v_{\mathrm{reg}} + v_{\mathrm{h.c.}}$, where v_{reg} is a finite measure, and $v_{\mathrm{h.c.}}$ is a positive linear combination of 'hard-core' potentials of the form

$$v_{[x_1,x_2]}(x) := \begin{cases} \infty & |x| \in [x_1, x_2] \\ 0 & \text{otherwise} \end{cases}, \tag{1.9}$$

for $0 \le x_1 \le x_2 \le R_0$.[1] We will consider the N-body Hamiltonian

$$H_N = -\sum_{i=1}^{N} \partial_{x_i}^2 + \sum_{1\le i<j\le N} v(x_i - x_j) \tag{1.10}$$

[1] Note we allow $0 \le x_1 = x_2 \le R_0$, by which we mean that impenetrable delta potentials of the form $h(\delta_{-x_1} + \delta_{x_1})$ with $h \to \infty$ can freely be included. This amounts to a zero boundary condition at $|x| = x_1$.

on the interval $[0, L]$ with any choice of (local, self-adjoint) boundary conditions. Let $\mathcal{D}(H_N)$ be the appropriate bosonic domain of symmetric wave functions with these boundary conditions. The ground state energy is then

$$E(N, L) := \inf_{\substack{\Psi \in \mathcal{D}(H_N) \\ \|\Psi\|=1}} \langle \Psi | H_N | \Psi \rangle = \inf_{\substack{\Psi \in \mathcal{D}(H_N) \\ \|\Psi\|=1}} \mathcal{E}(\Psi), \tag{1.11}$$

with energy functional

$$\mathcal{E}(\Psi) = \int_{[0,L]^N} \sum_{i=1}^{N} |\partial_i \Psi|^2 + \sum_{1 \le i < j \le N} v_{ij} |\Psi|^2 . \tag{1.12}$$

Theorem 1 (bosons)**.** *Consider a Bose gas with repulsive interaction $v = v_{reg} + v_{h.c.}$ as defined above. Write $\rho = N/L$. For $\rho|a|$ and ρR_0 sufficiently small, the ground state energy can be expanded as*

$$E(N, L) = N \frac{\pi^2}{3} \rho^2 \left(1 + 2\rho a + \mathcal{O}\left((\rho|a|)^{6/5} + (\rho R_0)^{6/5} + N^{-2/3} \right) \right), \tag{1.13}$$

where a is the scattering length of v (see Lemma 4 below). A precise expression for the error is given in the upper and lower bounds (2.1) *and* (3.1)*.*

To obtain this result, we prove an upper bound in the form of Proposition 8 in Section 2, and a matching lower bound in the form of Proposition 15 in Section 3. We use Dirichlet boundary conditions for the upper bound and Neumann boundary conditions for the lower bound, as these produce the highest and lowest ground state energy respectively. This way, Theorem 1 holds for a wide range of boundary conditions.

Remark 2. *As a special case, Theorem 1 covers the ground state energy expansion* (1.6) *of the Lieb–Liniger model* (1.4) *in the limit $c/\rho \gg 1$, as discussed in the introduction. This is known as the Tonks–Girardeau limit. Crucially, in this limit, the leading order term is the energy of the 1D free Fermi gas $N\pi^2\rho^2/3$, as first understood by Girardeau [17] (see also the discussion around* (1.15) *and* (1.16) *below).*[2] *Theorem 1 shows this holds for general potentials as well. That means that the dilute limit in 1D is very different from the one in two and three dimensions, where the zeroth-order term in the energy is that of a perfect condensate at zero momentum and the first-order term can be extracted using Bogoliubov theory [6]. In particular, the free Bose gas ($v = 0$) in 1D cannot be considered dilute, because it has infinite $|a|$.*

Remark 3. *An interesting feature of Theorem 1 is that the scattering length, a, can be both*

[2]Note that Girardeau studied the $c/\rho \to \infty$ case before Lieb and Liniger, who then generalized his work to obtain and solve the complete Lieb-Liniger model (1.4).

positive and negative. In this sense, our result covers cases that do not necessarily resemble the Lieb–Liniger model, which always has a negative scattering length. We discuss this further in Section 1.4.

Note that zero scattering length can be achieved, which means the error in (1.13) *cannot just be written in terms of* $(\rho|a|)^s$ *for some* $s > 1$*, but that* $(\rho R_0)^s$ *also appears.*

1.2 Proof strategy

The most important ingredient in our proof is the following lemma, which follows from straightforward variational calculus. It is based on work by Dyson on the 3D Bose gas [11] and is present in Appendix C in [30].

Lemma 4 (The 2-body scattering solution and scattering length)**.** *Suppose* v *is a repulsive interaction* $v = v_{\text{h.c.}} + v_{\text{reg}}$ *as defined in the previous section. In particular,* v *is symmetric and* $\text{supp}(v) \subset [-R_0, R_0]$*. Let* $R > R_0$*. For all* $f \in H^1[-R, R]$ *subject to* $f(R) = f(-R) = 1$*,*

$$\int_{-R}^{R} 2|\partial_x f|^2 + v(x)|f(x)|^2 \,\mathrm{d}x \geq \frac{4}{R-a}. \tag{1.14}$$

There is a unique f_0 *attaining the minimum energy: the scattering solution. It satisfies the scattering equation* $\partial_x^2 f_0 = \frac{1}{2} v f_0$ *in the sense of distributions, and* $f_0(x) = (x-a)/(R-a)$ *for* $x \in [R_0, R]$*. The parameter* a *is called the scattering length, which need not be positive in 1D.*

Similar lemmas play an important role in the understanding of the ground state energy expansions (1.2) and (1.3) in higher dimensions [11, 31, 36], but there are a number of things we need to do differently. These relate to the fermionic behaviour of the bosons in the limit $\rho|a| \ll 1$ (see Remark 2 above).

What does this mean in practice? For the upper bound in Section 2, it suffices to find a suitable trial state by the variational principle (1.11). Good trial states for dilute bosons in 2D and 3D are close to a pure condensate, but in 1D the state will have to be close to the free Fermi ground state obtained in the limit $\rho|a| \to 0$. To achieve this, we can rely on Girardeau's solution [17] of the $c/\rho \to \infty$ limit of the Lieb–Liniger model. In that case, the delta function in (1.4) enforces a zero boundary condition whenever two bosons meet, so the bosons are impenetrable. The wave function is then found by minimizing the kinetic energy subject to this boundary condition. If we only consider the sector $0 \leq x_1 \leq \cdots \leq x_N \leq L$ (which suffices by symmetry), this is exactly the free Fermi problem. For periodic boundary conditions on the interval $[0, L]$,

the (unnormalized) free Fermi ground state is[3]

$$\Psi_F^{\mathrm{per}}(x_1,\dots,x_N) = \prod_{1\le i<j\le N} \sin\left(\pi\frac{x_i-x_j}{L}\right). \tag{1.15}$$

Of course, the ground state for impenetrable bosons should be symmetric rather than antisymmetric, and to correctly extend it beyond $0 \le x_1 \le \cdots \le x_N \le L$ we need to remove the signs,

$$\left|\Psi_F^{\mathrm{per}}\right|(x_1,\dots,x_N) = \prod_{1\le i<j\le N} \left|\sin\left(\pi\frac{x_i-x_j}{L}\right)\right|. \tag{1.16}$$

This is Girardeau's ground state for impenetrable bosons, and it still produces the free Fermi kinetic energy $N\pi^2/3\rho^2$ in the thermodynamic limit.[4]

Returning to the problem of finding a suitable trial state, (1.16) should be a good departure point. To account for the effect of the interaction potential, we should modify the $\sin(\pi(x_i - x_j)/L)$ terms in (1.16) on the scale set by a. Lemma 4, and the scattering solution f_0, are designed to provide the right 2-body wave function in the presence of the potential, so it seems natural to replace the sine by

$$\begin{cases} f_0(x)\sin(\pi b/L) & |x| \le b \\ \sin(\pi\,|x|\,/L) & |x| > b \end{cases} \tag{1.17}$$

on some suitable scale $|a| \ll b \ll L$. This is the idea we rely upon for the upper bound proved in Section 2.

For the lower bound in Section 3, we equally need to find a way to obtain the free Fermi energy to leading order. We use Lemma 4 in combination with the known expansion (1.6) for the Lieb–Liniger model. Choosing a suitable $R > R_0$, the idea is that (1.14) can be written as

$$\int_{-R}^{R} 2|\partial_x f|^2 + v(x)|f(x)|^2\,\mathrm{d}x \ge \frac{2}{R-a}\int (\delta_R(x)+\delta_{-R}(x))|f(x)|^2\,\mathrm{d}x, \tag{1.18}$$

thus lower bounding the kinetic and potential energy on $[-R,R]$ by a symmetric delta potential at radius R. Heuristically, we proceed by repeatedly applying (1.18) to an N-body wave function Ψ to obtain the symmetric delta potential for any neighbouring pairs of bosons. Then—crucially—we throw away the regions where $|x_{i+1}-x_i| \le R$, which is inspired by a similar step in [35]. This produces a lower bound since v is repulsive. With these regions removed, the two delta functions at radius $|x_{i+1}-x_i| = R$ collapse into a single delta at $|x_{i+1}-x_i| = 0$, with value

[3]This expression can be found by creating a Slater determinant of momentum eigenstates, and noting this is a Vandermonde determinant. See Section 2.1 for the calculation for Dirichlet boundary conditions.

[4]The wave functions Ψ_F^{per} and $|\Psi_F^{\mathrm{per}}|$ have the same energy and that is all we will need in this paper. However, their momentum distributions are very different, which is discussed further in Section 1.5.

$4/(R-a)$. This gives the Lieb–Liniger model on a reduced interval, evaluated on some wave function, which can then be lower bounded using the Lieb–Liniger ground state energy (1.6) (appropriately corrected for finite N, and the loss of norm of Ψ from the thrown-out regions).

All this may seem rather radical, but the heuristics work out: starting with an interval of length L, we cut it back to length $L-(N-1)R$, so that the Lieb–Liniger expansion (1.6) with $c=2/(R-a)$ and new density $N/(L-(N-1)R)=\rho(1+\rho R+\dots)$ produce

$$N\frac{\pi^2}{3}\rho^2(1+2\rho R+\dots)(1-2\rho(R-a)+\dots)=N\frac{\pi^2}{3}\rho^2(1+2\rho a+\dots). \tag{1.19}$$

We show that, a priori, the ground state wave function has little weight in the regions that get thrown out, so that (1.19) is accurate. The rigorous procedure used to obtain the Lieb–Liniger model and the expansion (1.19) are outlined in Section 3.

1.3 Spinless fermions and anyons

The expansion in Theorem 1 generalizes to spinless fermions in 1D. Given the antisymmetry of the fermionic wave function, the result involves the odd-wave scattering length a_{odd} of v, obtained from Lemma 4 by replacing the symmetric boundary condition $f(R)=f(-R)=1$ by an antisymmetric one, $f(R)=-f(-R)=1$.

Theorem 5 (spinless fermions)**.** *Consider a Fermi gas with repulsive interaction $v=v_{reg}+v_{h.c.}$ as defined before Theorem 1. Let a_{odd} be the odd-wave scattering length of v. Define $\mathcal{D}_F(H_N)$ to be the appropriate domain of antisymmetric wave functions, and let $E_F(N,L)$ be its associated ground state energy. Write $\rho=N/L$. For ρa_{odd} and ρR_0 sufficiently small, the ground state energy can be expanded as*

$$E_F(N,L)=N\frac{\pi^2}{3}\rho^2\left(1+2\rho a_{odd}+\mathcal{O}\left((\rho R_0)^{6/5}+N^{-2/3}\right)\right). \tag{1.20}$$

This theorem follows from Theorem 1 by using Girardeau's insight [17] that fermions and impenetrable bosons in 1D are unitarily equivalent, and hence have the same energy. It suffices to know the wave function on a single sector $0\le x_1\le\dots\le x_N\le L$, after which we can extend to any other sector by adding the correct sign for either bosons or fermions (note, any acceptable wave function is zero whenever $x_i=x_j$). Flipping these signs is exactly the nature of the unitary operator; see for example the equivalence between (1.15) and (1.16) discussed above. Given that Theorem 1 holds for impenetrable bosons, we can apply it as long as we use a zero boundary condition at $x=0$ in Lemma 4. By similar reasoning, this produces the same scattering length as using the fermionic boundary condition $f(R)=-f(-R)=1$ in Lemma 4. Theorem 5 is therefore a corollary of Theorem 1.

Remark 6 (spin-1/2 fermions)**.** *Consider the case of spin-*1/2 *fermions. If we study the usual, spin-independent Lieb–Liniger Hamiltonian* (1.4)*, the ground state will have a fixed total spin* S*. In fact, it is possible to study the ground state energy in each spin sector, and it will be monotone increasing in* S *according to work by Lieb and Mattis [32]. For each of these sectors, an explicit solution in terms of the Bethe ansatz exists [16, 49]. In certain cases, these can be expanded in the limit* $c/\rho \gg 1$ *[22], and the analogue to* (1.6) *and* (1.7) *can be obtained. The ground state energy for spin-*1/2 *fermions (*$S = 0$ *by Lieb–Mattis) gives [18, 22]*

$$N\frac{\pi^2}{3}\rho^2\left(1 - 4\frac{\rho}{c}\ln(2) + \mathcal{O}(\rho/c)^2\right) = N\frac{\pi^2}{3}\rho^2\left(1 + 2\ln(2)\rho a + \mathcal{O}(\rho a)^2\right). \tag{1.21}$$

Both the Lieb–Liniger exact solution and the expansions can be generalized to higher spins (or Young diagrams) [23, 47]. Note the leading order will be the free Fermi $N\pi^2\rho^2/3$ *in all cases, since the delta potential does not influence the energy for impenetrable particles.*

For general potentials, the zeroth-order Fermi term is still expected to be correct, but the first-order term in (1.21) *has to be more complicated. Given that two spin-*1/2 *fermions can form symmetric and antisymmetric combinations, both the even-wave scattering length* $a_{even} = a$ *and the odd-wave scattering length* a_{odd} *of the potential will play a role. In the Lieb–Liniger example* (1.21)*,* $a_{odd} = 0$*, since the delta interaction does not affect antisymmetric wave functions. However, for hard-core fermions of diameter* a*,* $a_{odd} = a_{even} = a$*, and the energy should be* (1.8) *since the spin symmetry plays no role. These two examples suggest that the correct formula is*

$$N\frac{\pi^2}{3}\rho^2\big(1 + 2\ln(2)\rho a_{even} + 2(1 - \ln(2))\rho a_{odd} + \mathcal{O}(\rho\max(|a_{even}|, a_{odd}))^2\big). \tag{1.22}$$

We will discuss this expansion in a future publication.

The approach followed to obtain Theorem 5 can actually be taken further. What if, starting from some wave function on a sector $0 \leq x_1 < \cdots < x_N \leq L$, we want to add anyonic phases $e^{i\kappa}$ with $0 \leq \kappa \leq \pi$, whenever two particles are interchanged? It turns out this can be made to work, going back to, amongst others, [26, 28] (see [7, 41] for a historical overview of this approach, comparisons with other versions of 1D anyonic statistics, and a discussion of experimental relevance). Just like fermions are unitarily equivalent to impenetrable bosons, these 1D anyons are equivalent to bosons with a certain choice of boundary conditions whenever two bosons meet. This can be related to the Lieb–Liniger model with certain c [41], since the delta function potential in (1.4) also imposes boundary conditions whenever two bosons meet. Hence, the (bosonic) Lieb–Liniger model can be viewed as a description of a non-interacting gas of anyons, with the $c/\rho \to \infty$ case being equivalent to fermions ($\kappa = \pi$) as understood by Girardeau.

Somewhat confusingly, this does not complete the picture, because many authors study gases of 1D anyons themselves interacting through a Lieb–Liniger potential, see for example [4, 24]. In this case, there are two parameters: the statistical parameter κ describing the phase $e^{i\kappa}$ upon particle exchange, and the Lieb–Liniger parameter c. Not surprisingly, this set-up is again unitarily equivalent to the bosonic Lieb–Liniger model, with an interaction potential of $2c\delta_0/\cos(\kappa/2)$.[5] This means Theorem 1 can be applied. We provide more details about the set-up, and prove the following theorem as a corollary of Theorem 1, in Section 4.

Theorem 7 (anyons)**.** *Let $c \geq 0$ and consider 1D anyons with statistical parameter $\kappa \in [0, \pi]$ and repulsive interaction $v = v_{\mathrm{reg}} + v_{\mathrm{h.c.}} + 2c\delta_0$, where $v_{\mathrm{h.c.}}$ is defined before Theorem 1, and v_{reg} is a finite measure with $v_{\mathrm{reg}}(\{0\}) = 0$. Define a_κ to be the scattering length associated with potential $v_\kappa = v_{h.c.} + v_{reg} + \frac{2c}{\cos(\kappa/2)}\delta_0$. Write $\rho = N/L$. For $\rho|a_\kappa|$ and ρR_0 sufficiently small, the ground state energy $E_{(\kappa,c)}(N, L)$ of the anyon gas can be expanded as*

$$E_{(\kappa,c)}(N, L) = N\frac{\pi^2}{3}\rho^2\left(1 + 2\rho a_\kappa + \mathcal{O}\left((\rho|a_\kappa|)^{6/5} + (\rho R_0)^{6/5} + N^{-2/3}\right)\right). \tag{1.23}$$

1.4 Physical applications and confinement from 3D to 1D

Given the general expansions (1.2) and (1.3) for the energy of dilute Bose gases in three and two dimensions, it is perhaps surprising that the possibility of a 1D equivalent was only hinted at in [2], and never studied in depth. On the other hand, given the existence of the Lieb–Liniger model, this is perhaps not surprising at all. Not only can we calculate everything explicitly in that case, Lieb–Liniger physics also naturally shows up in experimental settings in which 3D particles are confined to a 1D environment [34, 35, 40, 45]. Nevertheless, we would like to argue that our result adds something that goes beyond the Lieb–Liniger model: it allows for positive scattering lengths a.

Mathematically, this seems clear. The scattering length of the Lieb–Liniger model with $c > 0$ is $a = -2/c < 0$, but Theorem 1 is also valid for potentials with a positive scattering length. There are plenty of interesting potentials with this property, and the energy shift has the opposite sign compared to the Lieb–Liniger case. (Note the Lieb–Liniger model with $c < 0$ can be solved explicitly [8], but that it has a clustered ground state of energy $-\mathcal{O}(N^2)$ [33, 37], so that scattering is irrelevant.)

Physically, the issue can seem more subtle. In the lab, 1D physics can be obtained by confining 3D particles with 3D potentials to a one-dimensional setting [19, 20, 39, 44]. As mentioned, the Lieb–Liniger model is very relevant to such set-ups [34, 35, 40, 45], but only in certain parameter regimes. In these references, the confinement length $l_\perp$ in the trapping

[5] From the viewpoint of the energy, the combination $2c/\cos(\kappa/2)$ is the only relevant parameter. This is different for the momentum distribution, see Section 1.5.

direction (a length that is necessarily small on some scale to create 1D physics) is much bigger than the range of atomic forces (or 3D scattering length). This allows excited states in the trapping direction to play a role in the problem, making the mathematical analysis complicated. The assumption that $l_\perp \gg a_{3D}$ is sometimes referred to as weak confinement [5].

There should also be a 'strong confinement' regime $l_\perp \ll a_{3D}$, in which the excited states in the trapping direction play no role at all (presumably simplifying the mathematical steps needed to go from 3D to 1D). The problem would then essentially be 1D, and take on the form considered in Theorem 1, thus allowing for positive 1D scattering lengths. We do not know whether the strong confinement regime is currently experimentally accessible.

1.5 Open problems

1. **The second-order term.** The second-order expansions (1.2) and (1.3) of the ground state energy of the dilute Bose gas in 3D and 2D hold for a wide class of potentials. As motivated in the introduction, the same might be true in the 1D expansion (1.7), but the techniques used in higher dimensions are not expected to be applicable to 1D.

2. **Momentum distribution.** As mentioned in Footnote 4, even though the 1D free Fermi ground state (1.15) and Girardeau's bosonic equivalent (1.16) have the same energy, their momentum distributions differ. In the thermodynamic limit, the free Fermi ground state has a uniform momentum distribution, up to the Fermi momentum $|k| \leq k_F = \pi\rho$. Girardeau's state has the same quasi-momentum distribution, but the momentum distribution itself diverges like $1/\sqrt{k}$ for small k [29, 48]. At finite N, the $k = 0$ occupation is $O(1)$ for fermions, while it is $O(\sqrt{N})$ for bosons.
   It is also possible to study the Lieb–Liniger ground state in this way [9]. The bosonic zero-momentum occupation λ_0 in the limit $c/\rho \gg 1$ is predicted to be

$$\lambda_0 \sim N^{\frac{1}{2}+\frac{2\rho}{c}+\mathcal{O}(\rho/c)^2} = N^{\frac{1}{2}-\rho a+\mathcal{O}(\rho a)^2}, \tag{1.24}$$

   and one can ask if this holds for general potentials as well. The same question can be posed in the context of anyons [9], as the full prediction seems to be [4, 9]

$$\lambda_0 \sim N^{\left(\frac{1}{2}+\frac{2\rho}{c}\cos\left(\frac{\kappa}{2}\right)\right)\left(1-\left(\frac{\kappa}{\pi}\right)^2\right)+\mathcal{O}(\rho\cos(\kappa/2)/c)^2} = N^{\left(\frac{1}{2}-\rho a_\kappa\right)\left(1-\left(\frac{\kappa}{\pi}\right)^2\right)+\mathcal{O}(\rho a_\kappa)^2}. \tag{1.25}$$

3. **Positive temperature.** For $T > 0$, one can again ask if quantities like the chemical potential and free energy only depend on ρa to lowest orders. Starting from the ideal Fermi gas and excluding volume as in the case of hard-core bosons (the equivalent of (1.8)), it is possible to generate appropriate expressions that might be universal [10].

Proving these for a wide class of potentials is an open problem.

2 Upper bound in Theorem 1

Proposition 8 (Upper bound in Theorem 1)**.** *Consider a Bose gas with repulsive interaction $v = v_{reg} + v_{h.c.}$ as defined above Theorem 1, with Dirichlet boundary conditions. Write $\rho = N/L$. There exists a constant $C_U > 0$ such that for $\rho|a|$, $\rho R_0 \leq C_U^{-1}$, the ground state energy $E^D(N, L)$ satisfies*

$$E^D(N,L) \leq N\frac{\pi^2}{3}\rho^2\left(1 + 2\rho a + C_U\left(\left((\rho\,|a|)^{6/5} + (\rho R_0)^{3/2}\right)\left(1 + \rho R_0^2 \int v_{\mathrm{reg}}\right)^{1/2} + N^{-1}\right)\right). \tag{2.1}$$

As explained in Section 1.2, the proof relies on a trial state constructed from the free Fermi ground state. With Dirichlet boundary conditions, we cannot use $\left|\Psi_F^{\mathrm{per}}\right|$ from (1.16), and shall instead have to construct its Dirichlet equivalent, denoted by $|\Psi_F|$ in this section. This will be done in Section 2.1. Given a suitable scale $b > R_0$ to be fixed later on, the trial state will be

$$\Psi_\omega(x) = \begin{cases} \omega(\mathcal{R}(x))\frac{|\Psi_F(x)|}{\mathcal{R}(x)} & \text{if } \mathcal{R}(x) < b \\ |\Psi_F(x)| & \text{if } \mathcal{R}(x) \geq b, \end{cases} \tag{2.2}$$

where $\omega(x) = f_0(x)b$ is constructed from the scattering solution f_0 from Lemma 4 ($R = b$), and $\mathcal{R}(x) := \min_{i<j}(|x_i - x_j|)$ is the distance between the closest pair of particles (uniquely defined almost everywhere). In other words, we only modify $|\Psi_F|$ with the scattering solution for the closest pair. This is convenient for technical reasons, and will turn out to suffice if the number of particles N is not too big.

For this and other reasons, we will need another technical step: an argument that produces a trial state for arbitrary N (and L) using the Ψ_ω defined in (2.2). This is done in Section 2.4 by dividing $[0, L]$ into small intervals, and patching copies of Ψ_ω.

First, we focus on the small-N trial state Ψ_ω. Our goal will be the following lemma. In the following we will take b to satisfy $b > \max(2a, R_0)$.

Lemma 9. *Let $E_0 = N\frac{\pi^2}{3}\rho^2(1 + \mathcal{O}(1/N))$ the ground state energy of the (Dirichlet) free Fermi gas. The energy of the trial state Ψ_ω defined in* (2.2) *can be estimated as*

$$\begin{aligned} \mathcal{E}(\Psi_\omega) &:= \int_{[0,L]^N} \sum_{i=1}^N |\partial_i \Psi_\omega|^2 + \sum_{1\leq i<j\leq N} v_{ij}\,|\Psi_\omega|^2 \\ &\leq E_0\left(1 + 2\rho a\frac{b}{b-a} + \text{const.}\ \left(N(\rho b)^3\left[1 + \rho b^2\int v_{\mathrm{reg}}\right] + \rho a\frac{\ln(N)}{N}\right)\right). \end{aligned} \tag{2.3}$$

To prove this lemma, it is useful divide the configuration space into various sets. For $i < j$, define

$$\begin{aligned} B &:= \{x \in \mathbb{R}^N \mid \mathcal{R}(x) < b\} \\ A_{ij} &:= \{x \in \mathbb{R}^N | \, |x_i - x_j| < b\} \\ B_{ij} &:= \{x \in \mathbb{R}^N | \mathcal{R}(x) < b, \ \mathcal{R}(x) = |x_i - x_j|\} \subset A_{ij}. \end{aligned} \tag{2.4}$$

Note that Ψ_ω equals $|\Psi_F|$ on the complement of B, and that B_{ij} equals B intersected with the set {"particles i and j are closer than any other pair"}. On the set A_{12}, we will use the shorthand $\Psi_{12} := \omega(x_1 - x_2)\frac{\Psi_F(x)}{(x_1 - x_2)}$, and define the energies

$$\begin{aligned} E_1 &:= \binom{N}{2} \int_{A_{12}} \sum_{i=1}^N |\partial_i \Psi_{12}|^2 + \sum_{1 \le i < j \le N} (v_{\mathrm{reg}})_{ij} \, |\Psi_{12}|^2 - \sum_{i=1}^N |\partial_i \Psi_F|^2 \,, \\ E_2^{(1)} &:= \binom{N}{2} 2N \int_{A_{12} \cap A_{13}} \sum_{i=1}^N |\partial_i \Psi_F|^2 \,, \\ E_2^{(2)} &:= \binom{N}{2} \binom{N-2}{2} \int_{A_{12} \cap A_{34}} \sum_{i=1}^N |\partial_i \Psi_F|^2 \,. \end{aligned} \tag{2.5}$$

Recall $E_0 = N\frac{\pi^2}{3}\rho^2(1 + \mathcal{O}(1/N))$ is the ground state energy of the (Dirichlet) free Fermi gas. The following estimate then holds.

Lemma 10.

$$\mathcal{E}(\Psi_\omega) \le E_0 + E_1 + E_2^{(1)} + E_2^{(2)}. \tag{2.6}$$

The plan to prove the upper bound for Theorem 1 (Proposition 8) is as follows. We first prove Lemma 10 below. We then study the Dirichlet free Fermi ground state Ψ_F in Section 2.1, laying the ground work for the estimates of E_1, $E_2^{(1)}$ and $E_2^{(2)}$. We estimate E_1 in Section 2.2 and $E_2^{(1)}$ and $E_2^{(2)}$ in Section 2.3. Altogether, these prove Lemma 9, which will then be used to construct a successful trial state for large in N in Section 2.4.

Proof of Lemma 10. Since v has supported in the interval $[-b, b]$, and $\Psi_\omega = |\Psi_F|$ except in the region $B = \{x \in \mathbb{R}^N | \mathcal{R}(x) < b\}$, we can write, using the diamagnetic inequality[6],

$$\mathcal{E}(\Psi_\omega) \le E_0 + \int_B \sum_{i=1}^N |\partial_i \Psi_\omega|^2 + \sum_{1 \le i < j \le N} v_{ij} \, |\Psi_\omega|^2 - \sum_{i=1}^N |\partial_i \Psi_F|^2 \,, \tag{2.7}$$

with $E_0 = N\frac{\pi^2}{3}\rho^2(1 + \mathcal{O}(1/N))$ the ground state energy of the free Fermi gas. Using symmetry under the exchange of particles and the fact that $B_{ij} \cap B_{kl} = \emptyset$ for $(i, j) \neq (k, l)$ and $(i, j) \neq (l, k)$,

[6]Strictly speaking, the diamagnetic inequality is not needed, as the estimate can be shown to be an equality in this case.

and using diamagnetic inequality in the first sum in the second line, we find

$$\begin{aligned}\mathcal{E}(\Psi_\omega) &\leq E_0 + \binom{N}{2}\int_{B_{12}} \sum_{i=1}^N |\partial_i \Psi_\omega|^2 + \sum_{1\leq i<j\leq N} v_{ij}\,|\Psi_\omega|^2 - \sum_{i=1}^N |\partial_i \Psi_F|^2 \\ &\leq E_0 + \binom{N}{2}\int_{B_{12}} \sum_{i=1}^N |\partial_i \Psi_{12}|^2 + \sum_{1\leq i<j\leq N} (v_{\mathrm{reg}})_{ij}\,|\Psi_{12}|^2 - \sum_{i=1}^N |\partial_i \Psi_F|^2 .\end{aligned} \tag{2.8}$$

where we have used that $\Psi_\omega = 0$ on the support of $(v_{\mathrm{h.c.}})_{ij}$ for all i, j. Since we have $v_{\mathrm{reg}} \geq 0$, it follows that

$$\begin{aligned}\mathcal{E}(\Psi_\omega) &\leq E_0 + \binom{N}{2}\int_{A_{12}} \sum_{i=1}^N |\partial_i \Psi_{12}|^2 + \sum_{1\leq i<j\leq N} (v_{\mathrm{reg}})_{ij}\,|\Psi_{12}|^2 - \sum_{i=1}^N |\partial_i \Psi_F|^2 \\ &\quad - \binom{N}{2}\int_{A_{12}\setminus B_{12}} \sum_{i=1}^N |\partial_i \Psi_{12}|^2 + \sum_{1\leq i<j\leq N} (v_{\mathrm{reg}})_{ij}\,|\Psi_{12}|^2 - \sum_{i=1}^N |\partial_i \Psi_F|^2 \\ &\leq E_0 + E_1 + \binom{N}{2}\int_{A_{12}\setminus B_{12}} \sum_{i=1}^N |\partial_i \Psi_F|^2 .\end{aligned} \tag{2.9}$$

Noting that $x \in A_{12} \setminus B_{12}$ implies $x \in A_{ij}$ for some $(i, j) \neq (1, 2)$, we may, by antisymmetry of Ψ_F, estimate

$$\begin{aligned}\int_{A_{12}\setminus B_{12}} \sum_{i=1}^N |\partial_i \Psi_F|^2 &\leq 2N \int_{(A_{12}\setminus B_{12})\cap A_{13}} \sum_{i=1}^N |\partial_i \Psi_F|^2 + \binom{N-2}{2}\int_{(A_{12}\setminus B_{12})\cap A_{34}} \sum_{i=1}^N |\partial_i \Psi_F|^2 \\ &\leq 2N \int_{A_{12}\cap A_{13}} \sum_{i=1}^N |\partial_i \Psi_F|^2 + \binom{N-2}{2}\int_{A_{12}\cap A_{34}} \sum_{i=1}^N |\partial_i \Psi_F|^2 .\end{aligned} \tag{2.10}$$

Thus we find $\mathcal{E}(\Psi_\omega) \leq E_0 + E_1 + E_2^{(1)} + E_2^{(2)}$ as desired. □

2.1 The free Fermi ground state with Dirichlet b.c.

The Dirichlet eigenstates of the Laplacian are $\phi_j(x) = \sqrt{2/L}\sin(\pi j x/L)$. Thus, the Dirichlet free Fermi ground state is

$$\Psi_F(x) = \det\left(\phi_j(x_i)\right)_{i,j=1}^N = \sqrt{\frac{2}{L}}^N \left(\frac{1}{2i}\right)^N \begin{vmatrix} \mathrm{e}^{iy_1} - \mathrm{e}^{-iy_1} & \mathrm{e}^{i2y_1} - \mathrm{e}^{-i2y_1} & \dots & \mathrm{e}^{iNy_1} - \mathrm{e}^{-iNy_1} \\ \mathrm{e}^{iy_2} - \mathrm{e}^{-iy_2} & \mathrm{e}^{i2y_2} - \mathrm{e}^{-i2y_2} & \dots & \mathrm{e}^{iNy_2} - \mathrm{e}^{-iNy_2} \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{e}^{iy_N} - \mathrm{e}^{-iy_N} & \mathrm{e}^{i2y_N} - \mathrm{e}^{-i2y_N} & \dots & \mathrm{e}^{iNy_N} - \mathrm{e}^{-iNy_N} \end{vmatrix}, \tag{2.11}$$

where we defined $y_i = \frac{\pi}{L}x_i$. Defining $z = \mathrm{e}^{iy}$ and using the relation $(x^n - y^n)/(x-y) = \sum_{k=0}^{n-1} x^k y^{n-1-k}$, we find

$$\Psi_F(x) = \sqrt{\frac{2}{L}}^N \left(\frac{1}{2i}\right)^N \prod_{i=1}^N (z_i - z_i^{-1}) \begin{vmatrix} 1 & z_1 + z_1^{-1} & \dots & \sum_{k=0}^{N-1} z_1^{2k-N+1} \\ 1 & z_2 + z_2^{-1} & \dots & \sum_{k=0}^{N-1} z_2^{2k-N+1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & z_N + z_N^{-1} & \dots & \sum_{k=0}^{N-1} z_N^{2k-N+1} \end{vmatrix}. \tag{2.12}$$

Notice that $(z+z^{-1})^n = \sum_{k=0}^n \binom{n}{k} z^{2k-n}$. For $1 \le i \le N-1$, we add $\left(\binom{N-1}{i} - \binom{N-1}{i-1}\right)$ times column $N-i$ to column N. This does not change the determinant, so

$$\Psi_F(x) = \sqrt{\frac{2}{L}}^N \left(\frac{1}{2i}\right)^N \prod_{i=1}^N (z_i - z_i^{-1}) \begin{vmatrix} 1 & z_1 + z_1^{-1} & \dots & \sum_{k=0}^{N-2} z_1^{2k-N+1} & (z_1 + z_1^{-1})^{N-1} \\ 1 & z_2 + z_2^{-1} & \dots & \sum_{k=0}^{N-2} z_2^{2k-N+1} & (z_2 + z_2^{-1})^{N-1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & z_N + z_N^{-1} & \dots & \sum_{k=0}^{N-2} z_N^{2k-N+1} & (z_N + z_N^{-1})^{N-1} \end{vmatrix}. \tag{2.13}$$

For $1 \le i \le N-2$, we add $\left(\binom{N-2}{i} - \binom{N-2}{i-1}\right)$ times column $N-1-i$ to column $N-1$, and continue this process. That is, for $3 \le j \le N$ and $1 \le i \le N-j$, we add $\left(\binom{N-j}{i} - \binom{N-j}{i-1}\right)$ times column $N-1-i$ to column $N-j+1$. This gives

$$\Psi_F(x) = \sqrt{\frac{2}{L}}^N \left(\frac{1}{2i}\right)^N \prod_{i=1}^N (z_i - z_i^{-1}) \begin{vmatrix} 1 & z_1 + z_1^{-1} & (z_1 + z_1^{-1})^2 & \dots & (z_1 + z_1^{-1})^{N-1} \\ 1 & z_2 + z_2^{-1} & (z_2 + z_2^{-1})^2 & \dots & (z_2 + z_2^{-1})^{N-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & z_N + z_N^{-1} & (z_N + z_N^{-1})^2 & \dots & (z_N + z_N^{-1})^{N-1} \end{vmatrix}. \tag{2.14}$$

This is a Vandermonde determinant and we conclude

$$\begin{aligned} \Psi_F(x) &= \sqrt{\frac{2}{L}}^N \left(\frac{1}{2i}\right)^N \prod_{k=1}^N (z_k - z_k^{-1}) \prod_{i<j}^N \Big((z_i + z_i^{-1}) - (z_j + z_j^{-1}) \Big) \\ &= 2^{\binom{N}{2}} \sqrt{\frac{2}{L}}^N \prod_{k=1}^N \sin\left(\frac{\pi}{L}x_k\right) \prod_{i<j}^N \left[\cos\left(\frac{\pi}{L}x_i\right) - \cos\left(\frac{\pi}{L}x_j\right) \right] \\ &= -2^{\binom{N}{2}+1} \sqrt{\frac{2}{L}}^N \prod_{k=1}^N \sin\left(\frac{\pi}{L}x_k\right) \prod_{i<j}^N \sin\left(\frac{\pi(x_i - x_j)}{2L}\right) \sin\left(\frac{\pi(x_i + x_j)}{2L}\right). \end{aligned} \tag{2.15}$$

2.1.1 1-body reduced density matrix

The 1-particle reduced density matrix of the Dirichlet free Fermi ground state is

$$\gamma^{(1)}(x;y) = \frac{2}{L}\sum_{j=1}^{N} \sin\left(\frac{\pi}{L}jx\right)\sin\left(\frac{\pi}{L}jy\right) = \frac{\sin\left(\pi\left(\rho+\frac{1}{2L}\right)(x-y)\right)}{2L\sin\left(\frac{\pi}{2L}(x-y)\right)} - \frac{\sin\left(\pi\left(\rho+\frac{1}{2L}\right)(x+y)\right)}{2L\sin\left(\frac{\pi}{2L}(x+y)\right)}. \tag{2.16}$$

We can write $\gamma^{(1)}(x;y)$, as well as its translation invariant part $\tilde{\gamma}^{(1)}(x;y)$, in terms of the Dirichlet kernel $D_n(x) = \frac{1}{2\pi}\sum_{j=-n}^{n} \mathrm{e}^{ijx} = \frac{\sin((n+1/2)x)}{2\pi\sin(x/2)}$,

$$\begin{aligned} \gamma^{(1)}(x;y) &= \frac{\pi}{L}\left(D_N\left(\pi\frac{x-y}{L}\right) - D_N\left(\pi\frac{x+y}{L}\right)\right), \\ \tilde{\gamma}^{(1)}(x;y) &\coloneqq \frac{\pi}{L}D_N\left(\pi\frac{x-y}{L}\right). \end{aligned} \tag{2.17}$$

A consequence is that

$$\left|\partial_x^{k_1}\partial_y^{k_2}\gamma^{(1)}(x;y)\right| \leq \frac{1}{\pi}(2N)^{k_1+k_2+1}\left(\frac{\pi}{L}\right)^{k_1+k_2+1} = \pi^{k_1+k_2}(2\rho)^{k_1+k_2+1}. \tag{2.18}$$

Combined with Wick's theorem, which we discuss in the next subsection, (2.18) implies bounds on (derivatives of) higher-order reduced density matrices of the free Fermi ground state, that are uniform in all coordinates. Note the relevant power of ρ can be obtained directly from dimensional analysis. This will be used later on to do Taylor expansions.
Other useful bounds, which will be used in the proof of Lemma 11 are

$$\begin{aligned} \int_{[0,L]}\left|\rho^{(1)\prime}\right| &\leq \text{const. } \rho\ln(N), \\ \int_{[0,L]}\left|\rho^{(1)\prime\prime}\right| &\leq \text{const. } \rho^2\ln(N), \end{aligned} \tag{2.19}$$

which follow from the textbook bound on the L^1-norm of the mth derivative of Dirichlet's kernel

$$\|\partial^m D_N\|_{L^1([0,2\pi])} \leq \text{const. } N^m\ln(N).$$

2.1.2 k-body reduced density matrices and Wick's theorem

Given a wave function $\Psi \in L^2([0,L]^N)$, its k-particle reduced density matrix is given by

$$\gamma_\Psi^{(k)}(x_1,...,x_k;y_1,...,y_k) = \frac{N!}{(N-k)!}\int_{[0,L]^{N-k}} \overline{\Psi(x_1,...,x_N)}\Psi(y_1,...,y_k,x_{k+1},x_N)\,\mathrm{d}x_{k+1}\ldots\mathrm{d}x_N. \tag{2.20}$$

Similarly, we define the the k-particle reduced density by

$$\rho_{\Psi}^{(k)}(x_1,...,x_k) = \gamma_{\Psi}^{(k)}(x_1,...,x_k;x_1,...,x_k). \tag{2.21}$$

We will frequently abbreviate $\gamma_{\Psi_F}^{(k)}$ as $\gamma^{(k)}$ and $\rho_{\Psi_F}^{(k)}$ as $\rho^{(k)}$. For a quasi-free state, Wick's theorem states that the k-point function may be expressed solely in terms of sums of products of two-point functions, with appropriate signs (see e.g. [46], Theorem 10.2). For the free Fermi ground state (which has a fixed particle number), it implies

$$\gamma^{(k)}(x_1,...,x_k;y_1,...,y_k) = \begin{vmatrix} \gamma^{(1)}(x_1;y_1) & \gamma^{(1)}(x_1;y_2) & \cdots & \gamma^{(1)}(x_1;y_k) \\ \gamma^{(1)}(x_2;y_1) & \gamma^{(1)}(x_2;y_2) & \cdots & \gamma^{(1)}(x_2;y_k) \\ \vdots & \vdots & \ddots & \vdots \\ \gamma^{(1)}(x_k;y_1) & \gamma^{(1)}(x_k;y_2) & \cdots & \gamma^{(1)}(x_k;y_k) \end{vmatrix}. \tag{2.22}$$

We use this to compute $\rho^{(2)}$ below. Using Taylor expansion and (2.18), it will also be used to bound various reduced densities and density matrices.

2.1.3 Useful bounds on various reduced density matrices of Ψ_F

Lemma 11. *For the 2-body reduced density $\rho^{(2)}$ of the free Fermi ground state, it holds that*

$$\rho^{(2)}(x_1,x_2) = \left(\frac{\pi^2}{3}\rho^4 + f(x_2)\right)(x_1-x_2)^2 + \mathcal{O}(\rho^6(x_1-x_2)^4), \tag{2.23}$$

with $\int_{[0,L]} |f(x_2)|\,\mathrm{d}x_2 \leq$ const. $\rho^3 \ln(N)$.

Proof. Note that by translation invariance, we may Taylor expand $\tilde{\gamma}^{(1)}(x;y)$, defined in (2.17), in $x-y$ around 0. Only even terms can appear as D_N is even. Using (2.18), we find

$$\tilde{\gamma}^{(1)}(x;y) - (\rho + 1/(2L)) = \frac{\pi^2}{6}(\rho^3 + \rho^2\mathcal{O}(1/L))(x_1-x_2)^2 + \mathcal{O}(\rho^5(x_1-x_2)^4). \tag{2.24}$$

Furthermore, it is easy to check that $\gamma^{(1)}(x_1;x_2) - \rho^{(1)}((x_1+x_2)/2) = \tilde{\gamma}^{(1)}(x_1;x_2) - (\rho + 1/(2L))$. Now, by Wick's theorem (2.22),

$$\rho^{(2)}(x_1,x_2) = \rho^{(1)}(x_1)\rho^{(1)}(x_2) - \gamma^{(1)}(x_1;x_2)\gamma^{(1)}(x_2;x_1). \tag{2.25}$$

Note that by Taylor's theorem and (2.18),

$$\begin{aligned}\rho^{(1)}(x_1) = \rho^{(1)}((x_1+x_2)/2) + \rho^{(1)\prime}((x_1+x_2)/2)\frac{x_1-x_2}{2} \\ + \frac{1}{2}\rho^{(1)\prime\prime}((x_1+x_2)/2)\left(\frac{x_1-x_2}{2}\right)^2 + \mathcal{O}(\rho^4(x_1-x_2)^3),\end{aligned} \tag{2.26}$$

$$\begin{aligned}\rho^{(1)}(x_2) = \rho^{(1)}((x_1+x_2)/2) + \rho^{(1)\prime}((x_1+x_2)/2)\frac{x_2-x_1}{2} \\ + \frac{1}{2}\rho^{(1)\prime\prime}((x_1+x_2)/2)\left(\frac{x_1-x_2}{2}\right)^2 + \mathcal{O}(\rho^4(x_1-x_2)^3),\end{aligned} \tag{2.27}$$

where both expressions can be expanded further if needed. Using that $\gamma^{(1)}$ is symmetric in its coordinates, we conclude from the previous three equations that

$$\begin{aligned}\rho^{(2)}(x_1,x_2) = \rho^{(1)}((x_1+x_2)/2)^2 - \gamma^{(1)}(x_1;x_2)^2 - \left[\rho^{(1)\prime}((x_1+x_2)/2)\right]^2\left(\frac{x_1-x_2}{2}\right)^2 \\ +\rho^{(1)}((x_1+x_2)/2)\rho^{(1)\prime\prime}((x_1+x_2)/2)\left(\frac{x_1-x_2}{2}\right)^2 + \mathcal{O}(\rho^6(x_1-x_2)^4).\end{aligned} \tag{2.28}$$

Terms of order $\mathcal{O}(\rho^5(x_1-x_2)^3)$ must cancel due to symmetry.
Now, notice that $0 \le \rho^{(1)} \le 2\rho$ and $\left|\rho^{(1)\prime}\right| \le 8\pi\rho^2$ by (2.18). Together with (2.19), this implies,

$$\rho^{(2)}(x_1,x_2) = \rho^{(1)}((x_1+x_2)/2)^2 - \gamma^{(1)}(x_1;x_2)^2 + g_1(x_1+x_2)(x_1-x_2)^2 + \mathcal{O}(\rho^6(x_1-x_2)^4), \tag{2.29}$$

for some function g_1 satisfying $\int_{[0,L]}|g_1| \le$ const. $\rho^3\ln(N)$. Furthermore, notice that by (2.24) and the remark below it, we have

$$\begin{aligned}&\rho^{(1)}((x_1+x_2)/2)^2 - \gamma^{(1)}(x_1;x_2)^2 \\ &\quad= (\rho^{(1)}((x_1+x_2)/2) - \gamma^{(1)}(x_1;x_2))(\rho^{(1)}((x_1+x_2)/2) + \gamma^{(1)}(x_1;x_2)) \\ &\quad= \left[\rho + 1/(2L) - \tilde{\gamma}^{(1)}(x_1;x_2)\right]\left[-\rho - 1/(2L) + \tilde{\gamma}^{(1)}(x_1;x_2) + 2\rho^{(1)}((x_1+x_2)/2)\right] \\ &\quad= -\left[\rho + 1/(2L) - \tilde{\gamma}^{(1)}(x_1;x_2)\right]^2 + 2\left[\rho + 1/(2L) - \tilde{\gamma}^{(1)}(x_1;x_2)\right]\rho^{(1)}((x_1+x_2)/2) \\ &\quad= 2\left(\frac{\pi^2}{6}(\rho+1/(2L))^3(x_1-x_2)^2 + \mathcal{O}(\rho^5(x_1-x_2)^4)\right)\left(\rho + \frac{1}{2L} - \frac{\pi}{L}D_N((x_1+x_2)/(2L))\right) \\ &\quad= \frac{\pi^2}{3}\rho^4(x_1-x_2)^2 + g_2(x_1-x_2)(x_1-x_2)^2 + \mathcal{O}(\rho^6(x_1-x_2)^4),\end{aligned} \tag{2.30}$$

where we have chosen $g_2(x) = \frac{\pi^2}{3}\rho^3\left(\frac{\text{const.}}{2L} + \left|\frac{\pi}{L}D_N(x/(2L))\right|\right)$ which clearly satisfies $\int_{[0,L]} g_2 \le$ const. $\rho^3\ln(N)$. Combining (2.29) and (2.30) now proves the lemma. □

Lemma 12.

$$\begin{aligned}
\rho^{(3)}(x_1,x_2,x_3) &\le \text{const. } \rho^7(x_1-x_2)^2(x_3-x_2)^2,\\
\rho^{(4)}(x_1,x_2,x_3,x_4) &\le \text{const. } \rho^8(x_1-x_2)^2(x_3-x_4)^2,\\
\left|\sum_{i=1}^{2}\partial_{y_i}^2\gamma^{(2)}(x_1,x_2;y_1,y_2)|_{y=x}\right| &\le \text{const. } \rho^6(x_1-x_2)^2,\\
\left|\partial_{y_1}^2\left(\frac{\gamma^{(2)}(x_1,x_2;y_1,y_2)}{y_1-y_2}\right)\Big|_{y=x}\right| &\le \text{const. } \rho^6\,|x_1-x_2|\,,\\
\left|\sum_{i=1}^{2}(-1)^{i-1}\partial_{y_i}\left(\frac{\gamma^{(2)}(x_1,x_2;y_1,y_2)}{y_1-y_2}\right)\Big|_{y=x}\right| &\le \text{const. } \rho^6(x_1-x_2)^2, \qquad (2.31)\\
\sum_{i=1}^{3}\left(\partial_{x_i}\partial_{y_i}\gamma^{(3)}(x_1,x_2,x_3;y_1,y_2,y_3)\right)\Big|_{y=x} &\le \text{const. } \rho^9(x_1-x_2)^2(x_3-x_2)^2,\\
\left|\sum_{i=1}^{3}\left(\partial_{y_i}^2\gamma^{(3)}(x_1,x_2,x_3;y_1,y_2,y_3)\right)\Big|_{y=x}\right| &\le \text{const. } \rho^9(x_1-x_2)^2(x_3-x_2)^2,\\
\left|\left[\partial_y\gamma^{(4)}(x_1,x_2,x_3,x_4;y,x_2,x_3,x_4)\Big|_{y=x_1}\right]_{x_1=x_2-b}^{x_1=x_2+b}\right| &\le \text{const. } \rho^8 b(x_3-x_4)^2.
\end{aligned}$$

Proof. The bounds follow straightforwardly from Taylor's theorem and the symmetries of the left-hand sides. We give, in the following, two examples which we find to be representative for the general strategy.

Example 1: Consider $\sum_{i=1}^{2}\partial_{y_i}^2\gamma^{(2)}(x_1,x_2;y_1,y_2)|_{y=x}$. Notice first that $\sum_{i=1}^{2}\partial_{y_i}^2\gamma^{(2)}(x_1,x_2;y_1,y_2)$ is antisymmetric in (x_1,x_2) and in (y_1,y_2). As we discussed after (2.18), all derivatives of $\gamma^{(k)}$ are bounded uniformly in its coordinates by a constant times ρ^k for some $k\in\mathbb{N}$, we can Taylor expand $\partial^2\gamma^{(2)}$. By expanding x_1 around x_2 and y_1 around y_2, we see that antisymmetry implies $\sum_{i=1}^{2}\partial_{y_i}^2\gamma^{(2)}(x_1,x_2;y_1,y_2)\le \text{const. } \rho^6(x_1-x_2)(y_1-y_2)$, where the power of ρ can be found by dimensional analysis.

Example 2: Consider $\left|\sum_{i=1}^{2}(-1)^{i-1}\partial_{y_i}\left(\frac{\gamma^{(2)}(x_1,x_2;y_1,y_2)}{y_1-y_2}\right)\Big|_{y=x}\right|$. We start by defining the coordinates $z_y\coloneqq(y_1-y_2)/2$, $z_y'\coloneqq(y_1+y_2)/2$, $z_x\coloneqq(x_1-x_2)/2$, and $z_x'\coloneqq(x_1+x_2)/2$. Furthermore, define $\hat\gamma^{(2)}(z_x,z_x';z_y,z_y')\coloneqq\gamma^{(2)}(z_x+z_x',z_x'-z_x;z_y+z_y',z_y'-z_y)$. By the antisymmetry of $\gamma^{(2)}$ in x_1,x_2 and y_1,y_2, we see that $\hat\gamma^{(2)}$ is odd in z_x and z_y.

In this case, we notice that $\sum_{i=1}^{2}(-1)^{i-1}\partial_{y_i}=\partial_{z_y}$ and thus we find

$$\partial_{z_y}\left(\frac{\hat\gamma^{(2)}(z_x,z_x';z_y,z_y')}{z_y}\right)=\frac{z_y\partial_{z_y}\hat\gamma^{(2)}(z_x,z_x';z_y,z_y')-\hat\gamma^{(2)}(z_x,z_x';z_y,z_y')}{z_y^2}.$$

Taylor expanding both terms the numerator in z_y and z_x around 0 to order $z_x z_y^3$ gives

$$\begin{aligned}\Big| z_x z_y \partial_{z_x}\left[\partial_{z_y}\hat{\gamma}^{(2)}(z_x,z_x';z_y,z_y')\right]\Big|_{z_x=z_y=0} + z_x z_y^3 \partial_{z_x}\partial_{z_y}^2\left[\partial_{z_y}\hat{\gamma}^{(2)}(z_x,z_x';z_y,z_y')\right]\Big|_{z_x=z_y=0} \\ - z_x z_y \partial_{z_x}\partial_{z_y}\left[\hat{\gamma}^{(2)}(z_x,z_x';z_y,z_y')\right]\Big|_{z_x=z_y=0} - \frac{1}{2} z_x z_y^3 \partial_{z_x}\partial_{z_y}^3\left[\hat{\gamma}^{(2)}(z_x,z_x';z_y,z_y')\right]\Big|_{z_x=z_y=0} \\ + \mathcal{O}\left(\rho^8 (z_x z_y^5 + z_x^3 z_y^3)\right)\Big| \\ \leq \text{const. } \rho^6 \left| z_x z_y^3 \right|,\end{aligned} \tag{2.32}$$

where we used that $\hat{\gamma}^{(2)}(z_x, z_x'; z_y, z_y')$ is odd in z_x and z_y, to conclude that all even order terms vanish when Taylor exanding in these variables around 0. The desired result follows.

□

2.2 Estimating E_1

Recall $A_{12} = \{x \in \mathbb{R}^N | \, |x_1 - x_2| < b\}$ and $\Psi_{12}(x) = \frac{\omega(x_1-x_2)}{(x_1-x_2)}\Psi_F(x)$, as well as

$$E_1 \coloneqq \binom{N}{2} \int_{A_{12}} \sum_{i=1}^N |\partial_i \Psi_{12}|^2 + \sum_{1\leq i<j\leq N} (v_{\text{reg}})_{ij} |\Psi_{12}|^2 - \sum_{i=1}^N |\partial_i \Psi_F|^2 . \tag{2.33}$$

We prove the following bound.

Lemma 13. *For $b > \max(2a, R_0)$ we have*

$$E_1 \leq E_0 \left(2\rho a \frac{b}{b-a} + \text{const.} \left(N(\rho b)^3 \left[1 + \rho b^2 \int v_{\text{reg}} \right] + \rho a \frac{\ln(N)}{N} \right) \right). \tag{2.34}$$

Proof. We estimate E_1 by splitting it into four terms $E_1 = E_1^{(1)} + E_1^{(2)} + E_1^{(3)} + E_1^{(4)}$, with

$$\begin{aligned} E_1^{(1)} &\coloneqq \binom{N}{2} \int_{A_{12}} 2 |\partial_1 \Psi_{12}|^2 , \\ E_1^{(2)} &\coloneqq -\binom{N}{2} \int_{A_{12}} \left(2 |\partial_1 \Psi_F|^2 + \sum_{i=3}^N |\partial_i \Psi_F|^2 \right), \\ E_1^{(3)} &\coloneqq \binom{N}{2} \int_{A_{12}} \sum_{1\leq i<j\leq N} (v_{\text{reg}})_{ij} |\Psi_{12}|^2 , \\ E_1^{(4)} &\coloneqq \binom{N}{2} \int_{A_{12}} \sum_{i=3}^N |\partial_i \Psi_{12}|^2 . \end{aligned} \tag{2.35}$$

By partial integration of x_1 in $E_1^{(1)}$, we find

$$E_1^{(1)} = 2\binom{N}{2}\int_{A_{12}} \overline{\Psi_{12}}\left(-\partial_1^2\Psi_{12}\right) + 2\binom{N}{2}\int \left[\overline{\Psi_{12}}\partial_1\Psi_{12}\right]_{x_1=x_2-b}^{x_1=x_2+b} \mathrm{d}x_2\ldots\mathrm{d}x_N. \tag{2.36}$$

The boundary term can be calculated explicitly, and we find

$$\begin{aligned} 2\binom{N}{2}\int \left[\overline{\Psi_{12}}\partial_1\Psi_{12}\right]_{x_1=x_2-b}^{x_1=x_2+b} \mathrm{d}x_2\ldots\mathrm{d}x_N &= \int \left[\frac{\omega(x_1-x_2)}{|x_1-x_2|}\partial_1\left(\frac{\omega(x_1-x_2)}{|x_1-x_2|}\right)\rho^{(2)}(x_1,x_2)\right]_{x_2-b}^{x_2+b}\mathrm{d}x_2 \\ &\quad + \int \left[\left(\frac{\omega(x_1-x_2)}{|x_1-x_2|}\right)^2\partial_1\left(\gamma^{(2)}(x_1,x_2;y,x_2)\right)\Big|_{y=x_1}\right]_{x_2-b}^{x_2+b}\mathrm{d}x_2. \end{aligned} \tag{2.37}$$

Since the function $\frac{\omega(x_1-x_2)}{|x_1-x_2|}$ is continuously differentiable and satisfies $\frac{\omega(x_1-x_2)}{|x_1-x_2|} = \frac{|x_1-x_2|-a}{b-a}\frac{b}{|x_1-x_2|}$ for $|x_1-x_2|>b$, we see that

$$\partial_1\left(\frac{\omega(x_1-x_2)}{|x_1-x_2|}\right)\Big|_{x_1=x_2\pm b} = \pm\frac{a}{b(b-a)}. \tag{2.38}$$

Using Lemma 11, we find

$$\int \left[\frac{\omega(x_1-x_2)}{|x_1-x_2|}\partial_1\left(\frac{\omega(x_1-x_2)}{|x_1-x_2|}\right)\rho^{(2)}(x_1,x_2)\right]_{x_2-b}^{x_2+b}\mathrm{d}x_2 \leq 2a\frac{b}{b-a}N\frac{\pi^2}{3}\rho^3\left(1+\text{const.}\ \frac{\ln(N)}{N}\right). \tag{2.39}$$

Furthermore, we denote

$$\begin{aligned} &\int \left[\left(\frac{\omega(x_1-x_2)}{|x_1-x_2|}\right)^2\partial_1\left(\gamma^{(2)}(x_1,x_2;y,x_2)\right)\Big|_{y=x_1}\right]_{x_2-b}^{x_2+b}\mathrm{d}x_2 \\ &\quad = \int \left[\partial_1\left(\gamma^{(2)}(x_1,x_2;y,x_2)\right)\Big|_{y=x_1}\right]_{x_2-b}^{x_2+b}\mathrm{d}x_2 =: \kappa_1. \end{aligned} \tag{2.40}$$

Thus, we have

$$E_1^{(1)} \leq \frac{\pi^2}{3}N\rho^3(2a)\frac{b}{b-a}\left(1+\text{const.}\ \frac{\ln(N)}{N}\right) + \kappa_1 + 2\binom{N}{2}\int_{A_{12}}\overline{\Psi_{12}}(-\partial_1^2\Psi_{12}). \tag{2.41}$$

For $E_1^{(2)}$, we find

$$\begin{aligned} E_1^{(2)} &= -\binom{N}{2}\int_{A_{12}}\left(2\left|\partial_1\Psi_F\right|^2+\sum_{i=3}^{N}\left|\partial_i\Psi_F\right|^2\right) \\ &= -\binom{N}{2}\int_{A_{12}}\sum_{i=1}^{N}\overline{\Psi_F}(-\partial_i^2\Psi_F)-2\binom{N}{2}\int\left[\overline{\Psi_F}\partial_1\Psi_F\right]_{x_1=x_2-b}^{x_1=x_2+b} \\ &= -E_0\binom{N}{2}\int_{A_{12}}|\Psi_F|^2-\underbrace{\int\left[\partial_y\gamma^{(2)}(x_1,x_2;y,x_2)|_{y=x_1}\right]_{x_2-b}^{x_2+b}\mathrm{d}x_2}_{\kappa_1} \\ &\leq -\kappa_1, \end{aligned} \tag{2.42}$$

Part of $E_1^{(3)}$ can be estimated as follows. First, notice that using $|\omega|\leq b$, we find

$$\begin{aligned} &\binom{N}{2}\int_{A_{12}}\left(\sum_{2\leq i<j}^{N}(v_{\mathrm{reg}})_{ij}\left|\Psi_{12}\right|^2+\sum_{k=3}^{N}(v_{\mathrm{reg}})_{1k}\left|\Psi_{12}\right|^2\right) \\ &\quad\leq \text{const. } b^2\left(\int_{\{|x_1-x_2|<b\}\cap\mathrm{supp}((v_{\mathrm{reg}})_{34})}v_{\mathrm{reg}}(|x_3-x_4|)\frac{1}{(x_1-x_2)^2}\rho^{(4)}(x_1,x_2,x_3,x_4)\right. \\ &\qquad\left.+\int_{\{|x_1-x_2|<b\}\cap\mathrm{supp}((v_{\mathrm{reg}})_{23})}v_{\mathrm{reg}}(|x_2-x_3|)\frac{1}{(x_1-x_2)^2}\rho^{(3)}(x_1,x_2,x_3)\right). \end{aligned} \tag{2.43}$$

Hence, by Lemma 12,

$$\begin{aligned} &\binom{N}{2}\int_{A_{12}}\left(\sum_{2\leq i<j}^{N}(v_{\mathrm{reg}})_{ij}\left|\Psi_{12}\right|^2+\sum_{k=3}^{N}(v_{\mathrm{reg}})_{1k}\left|\Psi_{12}\right|^2\right) \\ &\quad\leq \text{const. } \left(N^2(\rho b)^3\rho^3\int x^2v_{\mathrm{reg}}(x)\,\mathrm{d}x+N(\rho b)^3\rho^3\int x^2v_{\mathrm{reg}}(x)\,\mathrm{d}x\right) \\ &\quad\leq \text{const. } N^2(\rho b)^5\rho\int v_{\mathrm{reg}}=\text{const. } E_0N(\rho b)^3\left(\rho b^2\int v_{\mathrm{reg}}\right), \end{aligned} \tag{2.44}$$

and so

$$\begin{aligned} E_1 &= E_1^{(1)}+E_1^{(2)}+E_1^{(3)}+E_1^{(4)} \\ &\leq \frac{2\pi^2}{3}N\rho^3a\frac{b}{b-a}+2\binom{N}{2}\int_{A_{12}}\left(\overline{\Psi_{12}}(-\partial_1^2)\Psi_{12}+\frac{1}{2}\sum_{i=3}^{N}\left|\partial_i\Psi_{12}\right|^2+\frac{1}{2}v_{12}\left|\Psi_{12}\right|^2\right) \\ &\quad+\text{const. } E_0\left(N(\rho b)^3\left(\rho b^2\int v_{\mathrm{reg}}\right)+\rho a\frac{\ln(N)}{N}\right). \end{aligned} \tag{2.45}$$

Using the two-body scattering equation $\partial^2\omega = \frac{1}{2}v\omega$ from Lemma 4, this implies

$$\begin{aligned} E_1 \leq \frac{2\pi^2}{3}N\rho^3 a\frac{b}{b-a} &+ 2\binom{N}{2}\int_{A_{12}}\frac{\overline{\Psi_F}}{(x_1-x_2)}\omega^2(-\partial_1^2)\frac{\Psi_F}{(x_1-x_2)} \\ &+ 4\binom{N}{2}\int_{A_{12}}\frac{\overline{\Psi_F}}{(x_1-x_2)}\omega(\partial_1\omega)\partial_1\frac{\Psi_F}{(x_1-x_2)} \\ &+ \binom{N}{2}\int_{A_{12}}\sum_{i=3}^{N}\overline{\Psi_F}\frac{\omega^2}{(x_1-x_2)^2}(-\partial_i^2)\Psi_F \\ &+ \text{const. } E_0\left(N(\rho b)^3\left(\rho b^2\int v_{\text{reg}}\right)+\rho a\frac{\ln(N)}{N}\right). \end{aligned} \tag{2.46}$$

Furthermore, we have

$$\begin{aligned} &\binom{N}{2}\int_{A_{12}}\sum_{i=3}^{N}\overline{\Psi_F}\frac{\omega^2}{(x_1-x_2)^2}(-\partial_i^2)\Psi_F \\ &= E_0\binom{N}{2}\int_{A_{12}}\left|\frac{\omega}{(x_1-x_2)}\Psi_F\right|^2 - 2\binom{N}{2}\int_{A_{12}}\overline{\Psi_F}\frac{\omega^2}{(x_1-x_2)^2}(-\partial_1^2)\Psi_F. \end{aligned} \tag{2.47}$$

By Lemma 11 and $|\omega| \leq b$, it follows that, it follows that

$$\binom{N}{2}\int_{A_{12}}\left|\frac{\omega}{(x_1-x_2)}\Psi_F\right|^2 \leq b^2\int_{\{|x_1-x_2|<b\}}\frac{\rho^{(2)}(x_1,x_2)}{|x_1-x_2|^2}\,\mathrm{d}x_1\,\mathrm{d}x_2 \leq \text{const. } N(\rho b)^3, \tag{2.48}$$

and by Lemma 12

$$\begin{aligned} 2\binom{N}{2}\left|\int_{A_{12}}\overline{\Psi_F}\frac{\omega^2}{(x_1-x_2)^2}(-\partial_1^2)\Psi_F\right| &\leq \frac{1}{2}\left|\sum_{i=1}^{2}\int_{A_{12}}\frac{\omega^2}{(x_1-x_2)^2}\partial_{y_i}^2\gamma^{(2)}(x_1,x_2;y_1,y_2)\Big|_{y=x}\right| \\ &\leq \text{const. } N\rho^2(\rho b)^3, \end{aligned} \tag{2.49}$$

so that we find that the third line of (2.46) is bounded by const. $E_0N(\rho b)^3$.

For the first line, again by Lemma 12, we find that

$$\begin{aligned} 2\binom{N}{2}\int_{A_{12}}\frac{\overline{\Psi_F}}{(x_1-x_2)}\omega^2(-\partial_1^2)\frac{\Psi_F}{(x_1-x_2)} &= \int_{A_{12}}\left|\frac{\omega^2}{x_1-x_2}\right|\left[\partial_{y_1}^2\left(\frac{\gamma^{(2)}(x_1,x_2;y_1,y_2)}{(y_1-y_2)}\right)\right]\Big|_{y=x} \\ &\leq \text{const. } N\rho^2(\rho b)^3. \end{aligned} \tag{2.50}$$

For the second line of (2.46), by using the scattering equation $\partial^2\omega = \frac{1}{2}v\omega \geq 0$ which implies

$0 \leq \omega'(x) \leq \omega'(b) = \frac{b}{b-a}$ for $|x| < b$, we find that

$$\begin{aligned}
&\left| 4\binom{N}{2} \int_{A_{12}} \frac{\overline{\Psi_F}}{(x_1 - x_2)} \omega(\partial_1 \omega) \partial_1 \left(\frac{\Psi_F}{(x_1 - x_2)} \right) \right| \\
&\qquad = 2 \left| \frac{1}{2} \sum_{i=1}^{2} \int_{A_{12}} \frac{\omega}{x_1 - x_2} (-1)^{i-1} \omega'(x_1 - x_2) \partial_{y_i} \left(\frac{\gamma^{(2)}(x_1, x_2; y_1, y_2)}{y_1 - y_2} \right) \Bigg|_{y=x} \right| \\
&\qquad \leq \text{const.} \ \frac{b}{b-a} N \rho^2 (\rho b)^3.
\end{aligned} \tag{2.51}$$

Combining everything, we get the desired result.

□

2.3 Estimating $E_2^{(1)} + E_2^{(2)}$

Recall that

$$\begin{aligned}
E_2^{(1)} &= \binom{N}{2} 2N \int_{A_{12} \cap A_{13}} \sum_{i=1}^{N} |\partial_i \Psi_F|^2 , \\
E_2^{(2)} &= \binom{N}{2} \binom{N-2}{2} \int_{A_{12} \cap A_{34}} \sum_{i=1}^{N} |\partial_i \Psi_F|^2 ,
\end{aligned} \tag{2.52}$$

with $A_{ij} := \{x \in \mathbb{R}^N | \, |x_i - x_j| < b\}$. We prove the following bound.

Lemma 14.

$$E_2^{(1)} + E_2^{(2)} \leq E_0 \left(N(\rho b)^4 + N^2 (\rho b)^6 \right). \tag{2.53}$$

Proof. We start by splitting $E_2^{(1)}$ and $E_2^{(2)}$ in two terms each and using partial integration. Consider first $E_2^{(1)}$,

$$\begin{aligned}
E_2^{(1)} &= \binom{N}{2} 2N \int_{A_{12} \cap A_{23}} \sum_{i=1}^{N} |\partial_i \Psi_F|^2 \\
&= \binom{N}{2} 2N \int_{A_{12} \cap A_{23}} \sum_{i=1}^{3} |\partial_i \Psi_F|^2 + \binom{N}{2} 2N \int_{A_{12} \cap A_{23}} \sum_{i=4}^{N} |\partial_i \Psi_F|^2 .
\end{aligned} \tag{2.54}$$

For the second term, we perform partial integration to find

$$\begin{aligned}\binom{N}{2}2N\int_{A_{12}\cap A_{23}}\sum_{i=4}^{N}|\partial_i\Psi_F|^2 &= \binom{N}{2}2N\int_{A_{12}\cap A_{23}}\sum_{i=4}^{N}\overline{\Psi_F}(-\partial_i^2\Psi_F)\\ &\leq E_0\binom{N}{2}2N\int_{A_{12}\cap A_{23}}|\Psi_F|^2-\binom{N}{2}2N\int_{A_{12}\cap A_{23}}\sum_{i=1}^{3}\overline{\Psi_F}(-\partial_i^2\Psi_F)\\ &\leq 3E_0\int_{[0,L]}\int_{[x_2-b,x_2+b]}\int_{[x_2-b,x_2+b]}\rho^{(3)}(x_1,x_2,x_3)\,\mathrm{d}x_3\,\mathrm{d}x_1\,\mathrm{d}x_2\\ &\quad-\binom{N}{2}2N\int_{A_{12}\cap A_{23}}\sum_{i=1}^{3}\overline{\Psi_F}(-\partial_i^2\Psi_F).\end{aligned} \tag{2.55}$$

Lemma 12 implies

$$3E_0\int_{[0,L]}\int_{[x_2-b,x_2+b]}\int_{[x_2-b,x_2+b]}\rho^{(3)}(x_1,x_2,x_3)\,\mathrm{d}x_3\,\mathrm{d}x_1\,\mathrm{d}x_2\leq\text{const. }NE_0(\rho b)^6. \tag{2.56}$$

Furthermore, Lemma 12 and antisymmetry imply

$$\binom{N}{2}2N\int_{A_{12}\cap A_{23}}\sum_{i=1}^{3}\left(|\partial_i\Psi_F|^2-\overline{\Psi_F}(-\partial_i^2\Psi_F)\right)\leq\text{const. }\rho^9Lb^6=\text{const. }E_0(\rho b)^6. \tag{2.57}$$

Collecting everything, we find

$$E_2^{(1)}\leq\text{const. }NE_0(\rho b)^6. \tag{2.58}$$

To estimate $E_2^{(2)}$, we use an identical strategy. Integration by parts and antisymmetry give

$$\begin{aligned}E_2^{(2)} &= \binom{N}{2}\binom{N-2}{2}\int_{A_{12}\cap A_{34}}\left(\sum_{i=1}^{4}|\partial_i\Psi_F|^2+\sum_{i=5}^{N}|\partial_i\Psi_F|^2\right)\\ &= \binom{N}{2}\binom{N-2}{2}\left(4\int_{|x_3-x_4|<b}\left[\overline{\Psi_F}\partial_1\Psi_F\right]_{x_1=x_2-b}^{x_1=x_2+b}+\int_{A_{12}\cap A_{34}}\sum_{i=1}^{N}\overline{\Psi_F}(-\partial_i^2\Psi_F)\right)\\ &= 4\int_{x_2\in[0,L]}\int_{|x_3-x_4|<b}\left[\partial_{y_1}\gamma^{(4)}(x_1,x_2,x_3,x_4;y_1,x_2,x_3,x_4)\Big|_{y_1=x_1}\right]_{x_1=x_2-b}^{x_1=x_2+b}\\ &\quad+E_0\int_{A_{12}\cap A_{34}}\rho^{(4)}(x_1,\ldots,x_4).\end{aligned} \tag{2.59}$$

Lemma 12 implies

$$4\int_{x_2\in[0,L]}\int_{|x_3-x_4|<b}\left[\partial_{y_1}\gamma^{(4)}(x_1,x_2,x_3,x_4;y_1,x_2,x_3,x_4)\Big|_{y_1=x_1}\right]_{x_1=x_2-b}^{x_1=x_2+b}\leq\text{const. }E_0N(\rho b)^4, \tag{2.60}$$

and

$$E_0 \int_{A_{12}\cap A_{34}} \rho^{(4)}(x_1,\dots,x_4) \leq \text{const. } E_0 N^2 (\rho b)^6, \tag{2.61}$$

which finishes the estimate of $E_2^{(2)}$. □

2.4 Constructing the trial state for arbitrary N

Together, Lemmas 10, 13 and 14 provide a proof of Lemma 9, which is the upper bound for small N obtained from the trial state Ψ_ω (2.2). To construct a trial state for arbitrary N, we glue together copies of Ψ_ω on small intervals. This is straightforward with Dirichlet boundary conditions since the wave functions vanish at the boundaries. We therefore consider the state $\Psi_{\text{full}} = \prod_{i=1}^M \Psi_{\omega,\ell}(x_1^i,\dots,x_{\tilde{N}}^i)$, where $(x_1^i,\dots,x_{\tilde{N}}^i)$ are the positions of the particles in box i and ℓ is the length of each box. Of course, $\cup_{i=1}^M \{x_1^i,\dots,x_{\tilde{N}}^i\} = \{x_1,\dots,x_N\}$ and $\{x_1^i,\dots,x_{\tilde{N}}^i\} \cap \{x_1^j,\dots,x_{\tilde{N}}^j\} = \emptyset$ for $i \neq j$, such that[7] $M\tilde{N} = N$. The boxes are of length[8] $\ell = L/M - b$, and are equally spaced throughout $[0, L]$, leaving a distance of b between each box. This is to prevent particles in different boxes from interacting.

We can now prove the upper bound needed for Theorem 1.

Proof of Proposition 8. From Lemma 9, the energy of the full trial state described above is bounded by

$$E \leq M e_0 \left(1 + 2\tilde{\rho}a\frac{b}{b-a} + \text{const. } \left(\tilde{N}(\tilde{\rho}b)^3\left[1 + \tilde{\rho}b^2\int v_{\text{reg}}\right] + \tilde{\rho}a\frac{\ln(\tilde{N})}{\tilde{N}}\right)\right) / \left\|\Psi_\omega\right\|^2, \tag{2.62}$$

with $e_0 = \frac{\pi^2}{3}\tilde{N}\tilde{\rho}^2(1 + \text{const. } \frac{1}{\tilde{N}})$ and $\tilde{\rho} = \tilde{N}/\ell = \rho/(1 - \frac{bM}{L}) \leq \rho(1 + 2bM/L)$ for $bM/L \leq 1/2$. Notice that $\tilde{\rho}a\frac{\ln(\tilde{N})}{\tilde{N}} \leq C_\epsilon \max(\tilde{N}^{-1}, (\tilde{\rho}a)^{2-\epsilon})$ with some ϵ dependent constant C_ϵ. This is easily seen by considering the cases $N \leq (\tilde{\rho}a)^{-1}$ and $N > (\tilde{\rho}a)^{-1}$ separately. Thus this term is sub-leading, and we will absorb it into other error terms. Clearly, we have $\|\Psi_\omega\|^2 \geq 1 - \int_B |\Psi_F|^2 \geq 1 - \int_{|x_1-x_2|<b} \rho^{(2)}(x_1,x_2) \geq 1 - \text{const. } \tilde{N}(\rho b)^3$, where the last inequality follows from Lemma 11. Thus, choosing M such that $bM/L \ll 1$, we have

$$E \leq N\frac{\pi^2}{3}\rho^2 \frac{\left(1 + \frac{2\rho ab}{b-a} + \text{const. } \frac{M}{N} + \text{const. } 2\rho abM/L + \text{const. } \tilde{N}(\rho b)^3\left(1 + \rho b^2\int v_{\text{reg}}\right)\right)}{1 - \tilde{N}(\tilde{\rho}b)^3}. \tag{2.63}$$

[7] Of course there might not, for a given N, exist desirable integers $\tilde{N}$ and M such that this relation is satisfied. However, below when choosing $\tilde{N}$, we think of M as being $\left\lceil N/\tilde{N}\right\rceil$. In this case the number of particles in each box will be $\lceil N/M\rceil$ or $\lceil N/M - 1\rceil$. The energy, in the two cases, will differ only at sub-leading order, and the difference may be absorbed in the error terms.

[8] In fact, given that a boxes can have $\lceil N/M\rceil$ or $\lceil N/M - 1\rceil$ particles, we may choose the respective length of these boxes as $\ell_{\lceil N/M\rceil} = \rho^{-1}\lceil N/M\rceil - b$ and $\ell_{\lceil N/M-1\rceil} = \rho^{-1}\lceil N/M - 1\rceil - b$.

First assume that $N \geq (\rho b)^{-3/2} \left(1 + \rho b^2 \int v_{\mathrm{reg}}\right)^{1/2}$. Now, we would choose $\tilde{N} = N/M = \rho L/M \gg 1$, or equivalently $M/L \ll \rho$. Setting $x = M/N$, we see that the error is

$$\text{const.} \quad \left[(1 + 2\rho^2 ab^2/(b-a))x + x^{-1}(b\rho)^3 \left(1 + \rho b^2 \int v_{\mathrm{reg}}\right)\right], \tag{2.64}$$

Here, we used the fact that $\tilde{N}(\rho b)^3 \leq 1/2$, so that we have $1/(1 - \tilde{N}(\rho b)^3) \leq 1 + 2\tilde{N}(\rho b)^3$. Optimizing in x, we find $x = M/N = \frac{(b\rho)^{3/2}\left(1+\rho b^2 \int v_{\mathrm{reg}}\right)^{1/2}}{1+2\rho^2 ab} \simeq (b\rho)^{3/2} \left(1 + \rho b^2 \int v_{\mathrm{reg}}\right)^{1/2}$, which gives the error

$$\text{const.} \ (b\rho)^{3/2} \left(1 + \rho b^2 \int v_{\mathrm{reg}}\right)^{1/2}. \tag{2.65}$$

Now, choose $b = \max(\rho^{-1/5} |a|^{4/5}, R_0)$. Then, for $(\rho |a|)^{1/5} \leq 1/2$,

$$\frac{b}{b-a} \leq 1 + 2a/b \leq 1 + 2(\rho |a|)^{1/5}. \tag{2.66}$$

Notice that

$$(\rho b)^{3/2} = \max\left((\rho |a|)^{6/5}, (\rho R_0)^{3/2}\right) \leq (\rho |a|)^{6/5} + (\rho R_0)^{3/2}. \tag{2.67}$$

Now, for $N < (\rho b)^{-3/2} \left(1 + \rho b^2 \int v_{\mathrm{reg}}\right)^{1/2}$, the result follows from (2.62) with $M = 1$, as well as $\rho a \frac{\ln(N)}{N} \leq C_\epsilon \max(N^{-1}, (\rho a)^{2-\epsilon})$. □

3 Lower bound in Theorem 1

Proposition 15 (Lower bound in Theorem 1)**.** *Consider a Bose gas with repulsive interaction $v = v_{reg} + v_{h.c.}$ as defined above Theorem 1, with Neumann boundary conditions. Write $\rho = N/L$. There exists a constant $C_L > 0$ such that the ground state energy $E^N(N, L)$ satisfies*

$$E^N(N, L) \geq N \frac{\pi^2}{3} \rho^2 \left(1 + 2\rho a - C_L \left((\rho |a|)^{6/5} + (\rho R_0)^{6/5} + N^{-2/3}\right)\right). \tag{3.1}$$

As mentioned in Section 1.2, the proof is based on a reduction to the Lieb-Liniger model combined with Lemma 4. Similar to the upper bound, this idea only provides a useful lower bound for small N, which we obtain in Proposition 24 and Corollary 25 at the end Section 3.2, after preparatory estimates on the Lieb–Liniger model in Section 3.1. Then, in Section 3.3, this lower bound will be generalized to arbitrary N, proving Proposition 15.

3.1 Lieb-Liniger model: preparatory facts

The thermodynamic ground state energy of the Lieb-Liniger model is determined by the system of equations [33]

$$e(\gamma) = \frac{\gamma^3}{\lambda^3} \int_{-1}^{1} g(x) x^2 \, \mathrm{d}x, \tag{3.2}$$

$$2\pi g(y) = 1 + 2\lambda \int_{-1}^{1} \frac{g(x)}{\lambda^2 + (x-y)^2} \, \mathrm{d}x, \tag{3.3}$$

$$\lambda = \gamma \int_{-1}^{1} g(x) \, \mathrm{d}x, \tag{3.4}$$

with $g \geq 0$. This allows for a rigorous lower bound.

Lemma 16 (Lieb-Liniger lower bound)**.** *For $\gamma > 0$,*

$$e(\gamma) \geq \frac{\pi^2}{3} \left(\frac{\gamma}{\gamma + 2} \right)^2 \geq \frac{\pi^2}{3} \left(1 - \frac{4}{\gamma} \right). \tag{3.5}$$

Proof. Neglecting $(x-y)^2$ in the denominator of (3.3), we see that $g \leq \frac{1}{2\pi} + \frac{1}{\pi\lambda} \int_{-1}^{1} g(x) \, \mathrm{d}x$. On the other hand, (3.2) and (3.4) imply $e(\gamma) = \frac{\int_{-1}^{1} g(x) x^2 \, \mathrm{d}x}{\left(\int_{-1}^{1} g(x) \, \mathrm{d}x \right)^3}$. Denote $\int_{-1}^{1} g(x) \, \mathrm{d}x = M$, so that $g \leq \frac{1}{2\pi} \left(1 + \frac{2M}{\lambda} \right) = \frac{1}{2\pi} \left(1 + \frac{2}{\gamma} \right)$. Now, we minimize the expression for $e(\gamma)$ in g subject to this bound. This gives $g = K \mathbb{1}_{[-\frac{M}{2K}, \frac{M}{2K}]}$ with $K = \frac{1}{2\pi} \left(1 + \frac{2}{\gamma} \right)$, resulting in $\int_{-1}^{1} g(x) x^2 \, \mathrm{d}x = \frac{1}{3} \frac{M^3}{4K^2}$. Now, $e(\gamma) \geq \frac{1}{3} \frac{1}{4K^2}$ for $\gamma > 0$, and (3.5) follows. □

The thermodynamic Lieb–Liniger energy behaves like $n\rho^2 e(c/\rho)$, and the next result corrects the lower bound from (3.5) to obtain an estimate for finite particle numbers n.

Lemma 17 (Lieb-Liniger lower bound for finite n)**.** *The Lieb–Liniger ground state energy with Neumann boundary conditions can be estimated by*

$$E_{LL}^N(n, \ell, c) \geq \frac{\pi^2}{3} n\rho^2 \left(1 - 4\rho/c - \text{const.} \ \frac{1}{n^{2/3}} \right). \tag{3.6}$$

This will be proved after the following lemma due to Robinson. Note we use the superscripts N and D to denote Neumann and Dirichlet boundary conditions, respectively. For simplicity, we will consider the Lieb-Liniger model on $[-L/2, L/2]$ in this subsection, and use the notation $\Lambda_s := [-s/2, s/2]$.

Lemma 18 (Robinson [42])**.** *Let v be symmetric and decreasing (that is, $v \circ \mathfrak{c} \geq v$ for any contraction $\mathfrak{c}$). For any $b > 0$,*

$$E_{\Lambda_{L+2b}}^D \leq E_{\Lambda_L}^N + \frac{2n}{b^2}. \tag{3.7}$$

Proof. The idea of the proof is given on page 66 of [42], but we shall give a more explicit proof here. In order to compare energies with different boundary conditions, consider a cut-off function h with the property that

1. h is real, symmetric, and continuously differentiable on Λ_{3L},
2. $h(x) = 0$ for $|x| > L/2 + b$,
3. $h(x) = 1$ for $|x| < L/2 - b$,
4. $h(L/2 - x)^2 + h(L/2 + x)^2 = 1$ for $0 < x < b$,
5. $\left|\frac{\mathrm{d}h}{\mathrm{d}x}\right|^2 \leq \frac{1}{b^2}$, and $h^2 \leq 1$.

Let $f \in \mathcal{D}(\mathcal{E}^N_{\Lambda_L})$. Define $\tilde{f}$ by extending f to Λ_{3L} by reflecting f across each face of its domain in Λ_{3L}. Define then $V : L^2(\Lambda_L) \to L^2(\Lambda_{L+2b})$ by $Vf(x) := \tilde{f}(x)\prod_{i=1}^n h(x_i)$. It is not hard to show that V is an isometry, this is shown in Lemma 2.1.12 of [42]. Also, we clearly have $Vf \in \mathcal{D}(\mathcal{E}^D_{\Lambda_{L+2b}})$. Let ψ be the ground state for $\mathcal{E}^N_{\Lambda_L}$, and define the trial state $\psi_{\text{trial}} = V\psi$. Without the potential, the bound (3.7) is obtained in Lemma 2.1.13 of [42]. Hence, we need only prove that no energy is gained by the potential in the trial state. To see this, define $\tilde{\psi}$ to be ψ extended by reflection as above and notice that for $|x_2| < L/2 - b$, we have

$$\begin{aligned}
&\int_{-L/2-b}^{L/2+b} v(|x_1 - x_2|)\left|\tilde{\psi}(x)\right|^2 h(x_1)^2 h(x_2)^2\,\mathrm{d}x_1 \leq \\
&\int_{-L/2+b}^{L/2-b} v(|x_1 - x_2|)\left|\tilde{\psi}(x)\right|^2 \mathrm{d}x_1 + \sum_{s\in\{-1,1\}} s\int_{s(L/2-b)}^{s(L/2)} v(|x_1 - x_2|)\left|\tilde{\psi}(x)\right|^2 (h(x_1)^2 + h(L - x_1)^2)\,\mathrm{d}x_1 \\
&= \int_{-L/2}^{L/2} v(|x_1 - x_2|)\left|\tilde{\psi}(x)\right|^2 \mathrm{d}x_1,
\end{aligned} \tag{3.8}$$

where we used that v is symmetric decreasing in the first inequality, as well as the fact that $h(x)^2 + h(L-x)^2 = 1$ for $L/2 - b \leq x \leq L/2$, which is just property 4 of h. Furthermore, when

$|x_2| \geq L/2 - b$ we find

$$\begin{aligned}
&\int_{L/2-b}^{L/2+b}\int_{L/2-b}^{L/2+b} v(|x_1-x_2|)\left|\tilde{\psi}(x)\right|^2 h(x_1)^2 h(x_2)^2 \,\mathrm{d}x_2\,\mathrm{d}x_1 \\
&\quad= \sum_{(s_1,s_2)\in\{-1,1\}^2} s_1 s_2 \int_{L/2-s_1 b}^{L/2}\int_{L/2-s_2 b}^{L/2} v(|x_1-x_2|)\left|\tilde{\psi}(x)\right|^2 h(x_1)^2 h(x_2)^2 \,\mathrm{d}x_2\,\mathrm{d}x_1 \\
&\quad= \sum_{(s_1,s_2)\in\{-1,1\}^2} \int_0^b\int_0^b v(|s_1y_1 - s_2y_2|)\left|\tilde{\psi}(L/2-s_1y_1, L/2-s_2y_2, \bar{x}^{1,2})\right|^2 \\
&\qquad\qquad \times h(L/2-s_1y_1)^2 h(L/2-s_2y_2)^2 \,\mathrm{d}y_2\,\mathrm{d}y_1 \\
&\quad\leq \int_0^b\int_0^b v(|y_1-y_2|)\left|\tilde{\psi}(L/2-y_1, L/2-y_2, \bar{x}^{1,2})\right|^2 \\
&\qquad\qquad \times \sum_{(s_1,s_2)\in\{-1,1\}^2} h(L/2-s_1y_1)^2 h(L/2-s_2y_2)^2 \,\mathrm{d}y_2\,\mathrm{d}y_1 \\
&\quad= \int_0^b\int_0^b v(|y_1-y_2|)\left|\tilde{\psi}(L/2-y_1, L/2-y_2, \bar{x}^{1,2})\right|^2 \mathrm{d}y_2\,\mathrm{d}y_1,
\end{aligned} \tag{3.9}$$

where we write $\bar{x}^{1,2}$ as shorthand for $(x_3, \ldots, x_N)$. In the third line, we use the definition of $\tilde{\psi}$, as well as the fact that $|s_1y_1 - s_2y_2| \geq |y_1 - y_2|$ for $y_1, y_2 \geq 0$. In the last, line we used property 4 of h. By combining the two bounds above, we clearly have

$$\begin{aligned}
&\int_{-L/2-b}^{L/2+b}\int_{-L/2-b}^{L/2+b} v(|x_1-x_2|)\left|\tilde{\psi}(x)\right|^2 h(x_1)^2 h(x_2)^2 \,\mathrm{d}x_1\,\mathrm{d}x_2 \\
&\qquad\qquad \leq \int_{-L/2}^{L/2}\int_{-L/2}^{L/2} v(|x_1-x_2|)\left|\tilde{\psi}(x)\right|^2 \mathrm{d}x_1\,\mathrm{d}x_2.
\end{aligned} \tag{3.10}$$

The result now follows from the fact that V is an isometry. □

Proof of Lemma 17. Lemma 18 implies that for any $b > 0$

$$E^N_{LL}(n,\ell,c) \geq E^D_{LL}(n,\ell+b,c) - \text{const.}\ \frac{n}{b^2}. \tag{3.11}$$

Since the range of the interaction in the Lieb-Liniger model is zero, we see that $e^D_{LL}(2^m n, 2^m\ell, c) := \frac{1}{2^m\ell}E^D_{LL}(2^m n, 2^m\ell, c)$ is a decreasing sequence. To see this, simply split the box of size $2^m\ell$ in two boxes of size $2^{m-1}\ell$. Now, there are no interactions between the boxes so by using the product state of the two $2^{m-1}n$-particle ground states in each box as a trial state, we see that $E^D_{LL}(2^m n, 2^m\ell) \leq 2E^D_{LL}(2^{m-1}n, 2^{m-1}\ell)$. Since we also have $e^D_{LL}(2^m n, 2^m\ell, c) \geq$

$e_{LL}(2^m n, 2^m \ell, c) \to e_{LL}(n/\ell, c)$ as $m \to \infty$ [33], we see that

$$\begin{aligned} E^N_{LL}(n,\ell,c) &\geq e_{LL}(n/(\ell+b),c)(\ell+b) - \text{const.}\ \frac{n}{b^2} \\ &\geq \frac{\pi^2}{3} n\rho^2 \left(1 - 4\rho/c - \text{const.}\ \left(3b/\ell - \frac{1}{\rho^2 b^2}\right)\right). \end{aligned} \tag{3.12}$$

Here, $\rho = n/\ell$, and the second inequality follows from Lemma 16. Optimizing in b, we find

$$E^N_{LL}(n,\ell,c) \geq \frac{\pi^2}{3} n\rho^2 \left(1 - 4\rho/c - \text{const.}\ \frac{1}{n^{2/3}}\right). \tag{3.13}$$

□

3.2 Lower bound for small particle numbers n

In this subsection, we work our way towards Proposition 24 and Corollary 25, which provide lower bounds on the Neumann ground state energy. The proof strategy followed is that in Section 1.2.

We start by removing the relevant regions of the wave function. Throughout this section, let Ψ be the Neumann ground state of $\mathcal{E}$ and let $R > \max(R_0, 2|a|)$ be a length, to be fixed later. Define the continuous function $\psi \in L^2([0, \ell - (n-1)R]^n)$ by

$$\psi(x_1, x_2, \ldots, x_n) := \Psi(x_1, R + x_2, \ldots, (n-1)R + x_n) \quad \text{for} \quad 0 \leq x_1 \leq \cdots \leq x_n \leq \ell - (n-1)R, \tag{3.14}$$

extended symmetrically to other orderings of the particles. Our first goal is to prove that almost no weight is lost in going from Ψ to ψ, so that the heuristic calculation (1.19) has a chance of success. The following lemma will be useful.

Lemma 19. *For any function $\phi \in H^1(\mathbb{R})$ such that $\phi(0) = 0$,*

$$\int_{[0,R]} |\partial\phi|^2 \geq \max_{[0,R]} |\phi|^2 / R. \tag{3.15}$$

Proof. Write $\phi(x) = \int_0^x \phi'(t)\,\mathrm{d}t$, and find that

$$|\phi(x)| \leq \int_0^x \left|\phi'(t)\right| \mathrm{d}t. \tag{3.16}$$

Hence $\max_{x\in[0,R]} |\phi(x)| \leq \int_0^R |\phi'(t)|\,\mathrm{d}t \leq \sqrt{R}\left(\int |\phi'(t)|^2\,\mathrm{d}t\right)^{1/2}$. □

We can estimate the norm loss in the following way

$$\langle\psi|\psi\rangle = 1 - \int_B |\Psi|^2 \geq 1 - \sum_{i<j} \int_{D_{ij}} |\Psi|^2 , \tag{3.17}$$

where $B := \{x \in \mathbb{R}^n | \min_{i,j} |x_i - x_j| < R\}$ and $D_{ij} := \{x \in \mathbb{R}^n | \mathfrak{r}_i(x) = |x_i - x_j| < R\}$ with $\mathfrak{r}_i(x) := \min_{j\neq i}(|x_i - x_j|)$. Note D_{ij} is not symmetric in i and j, and that for $j \neq j'$, $D_{ij} \cap D_{ij'} = \emptyset$ up to sets of measure zero. Also note $B = \cup_{i<j} D_{ij}$. To give a good bound on the right-hand side of (3.17), we need the following lemma, upper bounding the norm loss to an energy.

Lemma 20. *For ψ defined in* (3.14)*, we have*

$$1 - \langle\psi|\psi\rangle \leq 8 \left(R^2 \sum_{i<j} \int_{D_{ij}} |\partial_i \Psi|^2 + R(R-a) \sum_{i<j} \int v_{ij} |\Psi|^2 \right). \tag{3.18}$$

Proof. Note that (3.15) implies that for any $\phi \in H^1$,

$$\left| |\phi(x)| - |\phi(x')| \right|^2 \leq \left| \phi(x) - \phi(x') \right|^2 \leq R \left(\int_{[0,R]} |\partial\phi|^2 \right), \tag{3.19}$$

for $x, x' \in [0, R]$. Furthermore,

$$\begin{aligned} |\phi(x)|^2 - |\phi(x')|^2 &= \left(|\phi(x)| - |\phi(x')| \right)^2 + 2 \left(|\phi(x)| - |\phi(x')| \right) |\phi(x')| \\ &\leq 2 \left(|\phi(x)| - |\phi(x')| \right)^2 + |\phi(x')|^2 . \end{aligned} \tag{3.20}$$

It follows that

$$\max_{x\in[0,R]} |\phi(x)|^2 \leq 2R \int_{[0,R]} |\partial\phi|^2 + 2 \min_{x'\in[0,R]} |\phi(x')|^2 . \tag{3.21}$$

Viewing Ψ as a function of x_i, we have

$$2 \min_{\mathfrak{r}_i(x)=|x_i-x_j|<R} |\Psi|^2 \geq \max_{\mathfrak{r}_i(x)=|x_i-x_j|<R} |\Psi|^2 - 4R \left(\int_{\mathfrak{r}_i(x)=|x_i-x_j|<R} |\partial_i \Psi|^2 \right). \tag{3.22}$$

Hence,

$$\begin{aligned} 2 \sum_{i<j} \int v_{ij} |\Psi|^2 &\geq 2 \sum_{i<j} \int_{D_{ij}} v_{ij} |\Psi|^2 \\ &\geq \left(\int v \right) \sum_{i<j} \int \left(\max_{D'_{ij}} |\Psi|^2 - 4R \left(\int_{D'_{ij}} |\partial_i \Psi|^2 \, \mathrm{d}x_i \right) \right) \mathrm{d}\bar{x}^i \\ &\geq \frac{4}{R-a} \sum_{i<j} \left(\frac{1}{2R} \int_{D_{ij}} |\Psi|^2 - 4R \int_{D_{ij}} |\partial_i \Psi|^2 \right), \end{aligned} \tag{3.23}$$

where $D'_{ij} := \{x_i \in \mathbb{R} | \mathfrak{r}_i(x) = |x_i - x_j| < R\}$ and $\mathrm{d}\bar{x}^i$ is shorthand for integration with respect to all variables except x_i. In the last line we used $\int v \geq 4/(R-a)$. Now, rewriting and (3.17) give the result. □

To make (1.19) in the proof outlined in Section 1.2 precise, we relate the Neumann ground state energy to the Lieb–Liniger energy in Lemma 22. First, we state a direct adaptation of Lemma 4, more suited to our purpose here.

Lemma 21 (Dyson's lemma)**.** *Let $R > R_0 = \mathrm{range}(v)$ and $\varphi \in H^1(\mathbb{R})$, then for any interval $\mathcal{I} \ni 0$*

$$\int_{\mathcal{I}} |\partial\varphi|^2 + \frac{1}{2} v |\varphi|^2 \geq \int_{\mathcal{I}} \frac{1}{R-a} (\delta_R + \delta_{-R}) |\varphi|^2 , \tag{3.24}$$

where a is the scattering length.

Lemma 22. *Let $R > \max(R_0, 2|a|)$ and $\epsilon \in [0,1]$. For ψ defined in* (3.14)*,*

$$\int \sum_i |\partial_i \Psi|^2 + \sum_{i \neq j} \frac{1}{2} v_{ij} |\Psi|^2 \geq E^N_{LL}\left(n, \tilde{\ell}, \frac{2\epsilon}{R-a}\right) \langle\psi|\psi\rangle + \frac{(1-\epsilon)}{R^2} \mathrm{const.}\ (1 - \langle\psi|\psi\rangle). \tag{3.25}$$

where $\tilde{\ell} := \ell - (n-1)R$.

Proof. Splitting the energy functional into two parts, and using Lemma 21 on one term (see also (1.18)), we find

$$\begin{aligned} &\int \sum_i |\partial_i \Psi|^2 + \sum_{i \neq j} \frac{1}{2} v_{ij} |\Psi|^2 \geq \\ &\int \sum_i |\partial_i \Psi|^2 \mathbb{1}_{\mathfrak{r}_i(x) > R} + \epsilon \sum_i \frac{1}{R-a} \delta(\mathfrak{r}_i(x) - R) |\Psi|^2 \\ &\qquad + (1-\epsilon) \left(\sum_{i<j} \int_{D_{ij}} |\partial_i \Psi|^2 + \int \sum_{i<j} v_{ij} |\Psi|^2 \right), \end{aligned} \tag{3.26}$$

where $\mathfrak{r}_i(x) = \min_{j \neq i}(|x_i - x_j|)$ and the nearest neighbor delta interaction can be written $\delta(\mathfrak{r}_i(x) - R) = \left(\sum_{j \neq i} [\delta(x_i - x_j - R) + \delta(x_i - x_j + R)]\right) \mathbb{1}_{\mathfrak{r}_i(\mathfrak{x}) \geq R}$. The nearest-neighbor interaction is obtained by, for each i in the sum above, dividing the integration domain of x_i into Voronoi cells around x_k with $k \neq i$. Then, for each k, restricting to the cell around particle k and using Lemma 21 gives the desired nearest neighbor interaction. This technique is also used in [30]. With the use of Lemma 20 with $R > 2|a|$ in the last term, and by realizing that the first two terms can be obtained by using ψ as a trial state in the Lieb-Liniger model (since the two delta functions collapse to a single delta of twice the strength when volume R is removed

between particles), we obtain

$$\int \sum_i |\partial_i \Psi|^2 + \sum_{i\neq j} \frac{1}{2} v_{ij} |\Psi|^2 \geq E^N_{LL}\left(n, \tilde{\ell}, \frac{2\epsilon}{R-a}\right) \langle\psi|\psi\rangle + \frac{(1-\epsilon)}{R^2}\text{const. } (1 - \langle\psi|\psi\rangle). \quad (3.27)$$

□

The next lemma will continue the process of bounding the norm loss in going from Ψ of norm 1 to ψ in (3.14).

Lemma 23. *For $n(\rho R)^2 \leq \frac{3}{16\pi^2}\frac{1}{8}$, $\rho R \leq \frac{1}{2}$ and $R > 2|a|$ we have*

$$\langle\psi|\psi\rangle \geq 1 - \text{const. } \left(n(\rho R)^3 + n^{1/3}(\rho R)^2\right). \quad (3.28)$$

Proof. From the known upper bound, *i.e.* Proposition 8, and by Lemma 22 with $\epsilon = 1/2$, it follows that

$$n\frac{\pi^2}{3}\rho^2\left(1 + 2\rho a + \text{const. } (\rho R)^{6/5}\right) \geq E^N_{LL}\left(n, \tilde{\ell}, \frac{1}{R-a}\right)\langle\psi|\psi\rangle + \frac{1}{16R^2}(1 - \langle\psi|\psi\rangle). \quad (3.29)$$

Subtracting $E^N_{LL}\left(n, \tilde{\ell}, \frac{1}{R-a}\right)$ on both sides, and using Lemma 17 on the left-hand side, we find

$$\begin{aligned} &n\frac{\pi^2}{3}\rho^2\left(1 + 2\rho a + \text{const. } (\rho R)^{6/5}\right) - n\frac{\pi^2}{3}\tilde{\rho}^2\left(1 - 4\tilde{\rho}(R-a) - \text{const. } n^{-2/3}\right) \\ &\geq \left(\frac{1}{16R^2} - E^N_{LL}\left(n, \tilde{\ell}, \frac{1}{R-a}\right)\right)(1 - \langle\psi|\psi\rangle), \end{aligned} \quad (3.30)$$

with $\tilde{\rho} = n/\tilde{\ell} = \rho/(1 - (\rho - 1/\ell)R)$. Using the upper bound $E^N_{LL}\left(n, \tilde{\ell}, \frac{1}{R-a}\right) \leq n\frac{\pi^2}{3}\tilde{\rho}^2$ on the right-hand side, as well as $2\rho \geq \tilde{\rho} \geq \rho(1 + \rho R)$, we find

$$\text{const. } n\rho^2 R^2\left(\rho R + (\rho R)^{6/5} + n^{-2/3}\right) \geq \left(\frac{1}{16} - R^2 n\frac{4\pi^2}{3}\rho^2\right)(1 - \langle\psi|\psi\rangle). \quad (3.31)$$

It follows that we have

$$\langle\psi|\psi\rangle \geq 1 - \text{const. } \left(n(\rho R)^3 + n^{1/3}(\rho R)^2\right). \quad (3.32)$$

□

For $n \leq \kappa(\rho R)^{-9/5}$ with $\kappa = \frac{3}{16\pi^2}\frac{1}{8}$ and $\rho R \leq \frac{1}{2}$, we find

$$\langle\psi|\psi\rangle \geq 1 - \text{const. } n(\rho R)^3 = 1 - \text{const. } (\rho R)^{6/5}. \quad (3.33)$$

It is now straightforward to show the following two results, finishing the bounds for small n.

Proposition 24. *For $n(\rho R)^2 \leq \frac{3}{16\pi^2}\frac{1}{8}$, $\rho R \leq \frac{1}{2}$ and $R > 2|a|$ we have*

$$E^N(n,\ell) \geq n\frac{\pi^2}{3}\rho^2\left(1 + 2\rho a + \text{const.}\ \left(\frac{1}{n^{2/3}} + n(\rho R)^3 + n^{1/3}(\rho R)^2\right)\right). \tag{3.34}$$

Proof. By Lemma 22 with $\epsilon = 1$, we reduce to a Lieb-Liniger model with volume $\tilde{\ell}$, density $\tilde{\rho}$, and coupling c, and we have $\tilde{\ell} = \ell - (n-1)R$, $\tilde{\rho} = \frac{n}{\tilde{\ell}}$ and $c = \frac{2}{R-a}$. Notice that $\rho(1+\rho R) \leq \tilde{\rho} \leq \rho(1+2\rho R)$. Hence, by Lemmas 17 and 23,

$$\begin{aligned} E^N(n,\ell) &\geq E^N_{LL}(n,\tilde{\ell},c)\,\langle\psi|\psi\rangle \\ &\geq n\frac{\pi^2}{3}\rho^2\left(1 + 2\rho a - \text{const.}\ \frac{1}{n^{2/3}}\right)\left(1 - \text{const.}\ \left(n(\rho R)^3 + n^{1/3}(\rho R)^2\right)\right). \end{aligned} \tag{3.35}$$

□

Corollary 25. *For $\frac{\tau}{2}(\rho R)^{-9/5} \leq n \leq \tau(\rho R)^{-9/5}$ with $\tau = \frac{3}{16\pi^2}\frac{1}{8}$ and $\rho R \leq \frac{1}{2}$,*

$$E^N(n,\ell) \geq n\frac{\pi^2}{3}\rho^2\left(1 + 2\rho a - \text{const.}\ \left((\rho R)^{6/5} + (\rho R)^{7/5}\right)\right). \tag{3.36}$$

3.3 Lower bound for arbitrary N

The lower bound in Corollary 25 only applies to particle numbers of order $(\rho R)^{-9/5}$. In this subsection, we generalize to any number of particles by performing a Legendre transformation in the particle number and going to the grand canonical ensemble. First, we justify that only particle numbers of order less than or equal to $(\rho R)^{-9/5}$ are relevant for a certain choice of the chemical potential, μ.

Let C denote the constant in Corollary 25, we will then in the following, assuming $\Xi\rho a \geq -1/4$ and $C(\rho R)^{6/5} < 1/4$, fix Ξ large enough for the following bound to hold

$$\frac{\pi^2}{3}\Xi^3\ell\rho^3\left(1 + 2\Xi\rho a - C(\rho R)^{6/5}\right) \geq \pi^2\rho^2\left(1 + \frac{8}{3}\rho a\right)\Xi\rho\ell.$$

Notice $\Xi = 4$ suffices.

Lemma 26. *Assume that $C(\rho R)^{6/5} < 1/4$ and let Ξ be fixed as above. Also let $n = m\Xi\rho\ell + n_0$ with $n_0 \in [0, \Xi\rho\ell)$ for some $m \in \mathbb{N}$, with $\frac{\tau}{2\Xi}(\rho R)^{-9/5} \leq \rho\ell =: n^* \leq \frac{\tau}{\Xi}(\rho R)^{-9/5}$ and $\tau = \frac{3}{16\pi^2}\frac{1}{8}$. Furthermore, assume that $\Xi\rho a \geq -1/4$ and let $\mu = \pi^2\rho^2\left(1 + \frac{8}{3}\rho a\right)$. Then,*

$$E^N(n,\ell) - \mu n \geq E^N(n_0,\ell) - \mu n_0. \tag{3.37}$$

Proof. By Corollary 25, we have

$$E^N(\Xi\rho\ell,\ell) \geq \frac{\pi^2}{3}\Xi^3\ell\rho^3\left(1+2\Xi\rho a - C(\rho R)^{6/5}\right). \tag{3.38}$$

Superadditivity caused by the positive potential implies

$$E^N(n,\ell) - \mu n \geq m\left(E^N(\Xi\rho\ell,\ell) - \mu\Xi\rho\ell\right) + E^N(n_0,\ell) - \mu n_0. \tag{3.39}$$

The result, therefore, follows from the fact that

$$\frac{\pi^2}{3}\Xi^3\ell\rho^3\left(1+2\Xi\rho a - C(\rho R)^{6/5}\right) \geq \pi^2\rho^2\left(1+\frac{8}{3}\rho a\right)\Xi\rho\ell. \tag{3.40}$$

□

We are ready to prove the lower bound for general particle numbers.

Proof of Proposition 15. For the case $N < \tau(\rho R)^{-9/5}$, the result follows from Proposition 24. For $N \geq \tau(\rho R)^{-9/5}$, notice that

$$E^N(N,L) \geq F^N(\mu,L) + \mu N, \tag{3.41}$$

where $F^N(\mu,L) = \inf_{N'}\left(E^N(N',L) - \mu N'\right)$. Clearly, since v is repulsive, we have

$$F^N(\mu,L) \geq MF^N(\mu,\ell), \tag{3.42}$$

with $\ell = L/M$ and $M \in \mathbb{N}_+$. Now, let Ξ be fixed as above and choose M such that $\frac{\tau}{2\Xi}(\rho R)^{-9/5} \leq n^* := \rho\ell \leq \frac{\tau}{\Xi}(\rho R)^{-9/5}$ and $\mu = \pi^2\rho^2\left(1+\frac{8}{3}\rho a\right)$ (notice that $\mu = \frac{\mathrm{d}}{\mathrm{d}\rho}(\frac{\pi^2}{3}\rho^3(1+2\rho a))$). Furthermore, assume that $C(\rho R)^{6/5} < 1/4$ and $\Xi\rho a \geq -1/4$ (the cases of $C(\rho R)^{6/5} \geq 1/4$ or $\Xi\rho a < -\frac{1}{4}$ are trivial, by choosing a sufficiently large constant in the error term). By Lemma 26,

$$F^N(\mu,\ell) := \inf_n\left(E^N(n,\ell) - \mu n\right) = \inf_{n<\Xi n^*}\left(E^N(n,\ell) - \mu n\right). \tag{3.43}$$

It is known from Proposition 24 that for $n < \Xi n^*$,

$$\begin{aligned} E^N(n,\ell) &\geq n\frac{\pi^2}{3}\bar\rho^2\left(1+2\bar\rho a - \text{const.}\ \left(\frac{1}{n^{2/3}} + n(\bar\rho R)^3 + n^{1/3}(\bar\rho R)^2\right)\right) \\ &\geq \frac{\pi^2}{3}n\bar\rho^2\left(1+2\bar\rho a\right) - n^*\rho^2\mathcal{O}\left((\rho R)^{6/5}\right), \end{aligned} \tag{3.44}$$

where $\bar\rho = n/\ell$ (notice that now $\rho = N/L = n^*/\ell \neq n/\ell$) and where we used $\bar\rho < \Xi\rho$. Thus, we

have

$$F^N(\mu,\ell) \geq \inf_{\bar\rho<\Xi\rho} (g(\bar\rho)-\mu\bar\rho)\ell - n^*\rho^2\mathcal{O}\left((\rho R)^{6/5}\right), \tag{3.45}$$

where $g(\bar\rho) = \frac{\pi^2}{3}\bar\rho^3\,(1+2\bar\rho a)$ for $\bar\rho < \Xi\rho$. Note that g is a convex C^1-function with invertible derivative for $\Xi\rho a \geq -\frac{1}{4}$. Hence,

$$\begin{aligned} E^N(N,L) \geq M(F^N(\mu,\ell)+\mu n^*) &\geq Mn^*\frac{\pi^2}{3}\rho^2\left(1+2\rho a-\mathcal{O}\left((\rho R)^{6/5}\right)\right) \\ &= \frac{\pi^2}{3}N\rho^2\left(1+2\rho a-\mathcal{O}\left((\rho R)^{6/5}\right)\right), \end{aligned} \tag{3.46}$$

where the equality follows from the specific choice of $\mu = g'(\rho)$. □

4 Anyons and proof of Theorem 7

In Theorem 5 and below, we discussed the fact that the fermionic ground state energy can be found from Theorem 1 by means of a unitary transformation. It was also mentioned that this concept can be generalized to a version of 1D anyonic symmetry [7, 28, 41]. We will now define our interpretation of such anyons, depending on a statistical parameter $\kappa \in [0,\pi]$ that defines the phase $e^{i\kappa}$ accumulated upon particle exchange. We also include a Lieb–Liniger interaction of strength $2c > 0$, such as in [4, 24, 26].

To start, divide the configuration space into sectors $\Sigma_\sigma := \{x_{\sigma_1} < x_{\sigma_2} < \cdots < x_{\sigma_N}\} \subset \mathbb{R}^N$ indexed by permutations $\sigma = (\sigma_1,\ldots,\sigma_N)$, and the diagonal $\Delta_N := \bigcup_{1\leq i<j\leq N}\{x_i = x_j\}$. Consider the kinetic energy operator on $\mathbb{R}^N \setminus \Delta_N$,

$$H_N = -\sum_{i=1}^N \partial_{x_i}^2, \tag{4.1}$$

with domain

$$\mathcal{D}(H_N) = \Bigg\{ \varphi = \mathrm{e}^{-i\frac{\kappa}{2}\Lambda(x)} f(x) \;\Bigg|\; f \text{ is continuous, symmetric in } x_1,\ldots,x_N, \text{ smooth on each } \Sigma_\sigma, \\ \text{and } (\partial_i-\partial_j)\varphi|_+^{ij} - (\partial_i-\partial_j)\varphi|_-^{ij} = 2c\;\mathrm{e}^{-i\frac{\kappa}{2}\Lambda(x)} f|_0^{ij} \text{ for all } i\neq j \Bigg\}. \tag{4.2}$$

Here, $|_\pm^{ij}$ and $|_0^{ij}$ mean the function should be evaluated for $x_i \to x_j^\pm$ and $x_i = x_j$ respectively, and

$$\Lambda(x) := \sum_{i<j}\epsilon(x_i-x_j) \qquad \text{with} \qquad \epsilon(x) = \begin{cases} 1 & \text{for } x>0 \\ -1 & \text{for } x<0 \\ 0 & \text{for } x=0 \end{cases}. \tag{4.3}$$

The idea is that the (perhaps rather artificial) boundary condition in (4.2) encodes the presence of a delta potential of strength $2c$, just like it would for bosons.

Proposition 27. *Let $0 < \kappa < \pi$. H_N is symmetric with corresponding quadratic form*

$$\mathcal{E}_{\kappa,c}(\varphi) = \sum_{i=1}^{N} \int_{\mathbb{R}^N \setminus \Delta_N} |\partial_{x_i}\varphi(x)|^2 + \frac{2c}{\cos(\kappa/2)} \sum_{i<j} \delta(x_i - x_j)\, |\varphi(x)|^2 \, \mathrm{d}x. \tag{4.4}$$

Proof. Let $\varphi, \vartheta \in \mathcal{D}(H_N)$. Then, by partial integration,

$$\begin{aligned}
\langle \vartheta | H_N \varphi \rangle &= -\sum_{i=1}^{N} \int_{\mathbb{R}^N \setminus \Delta_N} \overline{\vartheta} \partial_{x_i}^2 \varphi \\
&= \sum_{i=1}^{N} \int_{\mathbb{R}^N \setminus \Delta_N} \overline{\partial_{x_i}\vartheta} \partial_{x_i}\varphi - \int_{\mathbb{R}^{N-1} \setminus \Delta_{N-1}} \sum_{i \neq j} \left(\overline{\vartheta} \partial_{x_i}\varphi|_-^{ij} - \overline{\vartheta} \partial_{x_i}\varphi|_+^{ij} \right) \\
&= \sum_{i=1}^{N} \int_{\mathbb{R}^N \setminus \Delta_N} \overline{\partial_{x_i}\vartheta} \partial_{x_i}\varphi + \int_{\mathbb{R}^{N-1} \setminus \Delta_{N-1}} \sum_{i<j} \left(\overline{\vartheta}(\partial_{x_i} - \partial_{x_j})\varphi|_+^{ij} - \overline{\vartheta}(\partial_{x_i} - \partial_{x_j})\varphi|_-^{ij} \right).
\end{aligned} \tag{4.5}$$

Let f, g be the functions such that $\varphi = \mathrm{e}^{-i\frac{\kappa}{2}\Lambda} f$ and $\vartheta = \mathrm{e}^{-i\frac{\kappa}{2}\Lambda} g$. Then,

$$\begin{aligned}
\langle \vartheta | H_N \varphi \rangle &= \sum_{i=1}^{N} \int_{\mathbb{R}^N \setminus \Delta_N} \overline{\partial_{x_i}\vartheta} \partial_{x_i}\varphi + \int_{\mathbb{R}^{N-1} \setminus \Delta_{N-1}} \sum_{i<j} \left(\overline{g}(\partial_{x_i} - \partial_{x_j}) f|_+^{ij} - \overline{g}(\partial_{x_i} - \partial_{x_j}) f|_-^{ij} \right) \\
&= \sum_{i=1}^{N} \int_{\mathbb{R}^N \setminus \Delta_N} \overline{\partial_{x_i}\vartheta} \partial_{x_i}\varphi + \int_{\mathbb{R}^{N-1} \setminus \Delta_{N-1}} 2 \sum_{i<j} \left(\overline{g}(\partial_{x_i} - \partial_{x_j}) f|_+^{ij} \right),
\end{aligned} \tag{4.6}$$

where the last equality follows from the symmetry of f. Note that the boundary condition on $\mathcal{D}(H_N)$ imply

$$(\partial_i - \partial_j)\varphi|_+^{ij} - (\partial_i - \partial_j)\varphi|_-^{ij} = \mathrm{e}^{-i\frac{\kappa}{2}(-1+S)}(\partial_i - \partial_j) f|_+^{ij} - \mathrm{e}^{-i\frac{\kappa}{2}(1+S)}(\partial_i - \partial_j) f|_-^{ij} = 2c\varphi|_0^{ij} = \mathrm{e}^{-i\frac{\kappa}{2}S} 2c f|_0^{ij}, \tag{4.7}$$

where $S := \Lambda - \epsilon(x_i - x_j)$. By symmetry of f, it follows that

$$\begin{aligned}
\mathrm{e}^{-i\frac{\kappa}{2}(-1+S)}(\partial_i - \partial_j) f|_+^{ij} - \mathrm{e}^{-i\frac{\kappa}{2}(1+S)}(\partial_i - \partial_j) f|_-^{ij} &= \mathrm{e}^{-i\frac{\kappa}{2}(-1+S)}(\partial_i - \partial_j) f|_+^{ij} + \mathrm{e}^{-i\frac{\kappa}{2}(1+S)}(\partial_i - \partial_j) f|_+^{ij} \\
&= \mathrm{e}^{-i\frac{\kappa}{2}S} 2\cos(\kappa/2)(\partial_i - \partial_j) f|_+^{ij} \\
&= \mathrm{e}^{-i\frac{\kappa}{2}S} 2c f|_0^{ij},
\end{aligned} \tag{4.8}$$

so that

$$2(\partial_i - \partial_j) f|_+^{ij} = \frac{2c}{\cos(\kappa/2)} f|_0^{ij}. \tag{4.9}$$

Hence, it follows that

$$\langle \vartheta | H_N \varphi \rangle = \sum_{i=1}^{N} \int_{\mathbb{R}^N \setminus \Delta_N} \overline{\partial_{x_i} \vartheta} \partial_{x_i} \varphi(x) + \frac{2c}{\cos(\kappa/2)} \sum_{i<j} \delta(x_i - x_j) \overline{\vartheta(x)} \varphi(x) \, \mathrm{d}^N x. \tag{4.10}$$

Starting from $\langle H_N \vartheta | \phi \rangle$, we can arrive at (4.10) by the same steps, proving that H_N is symmetric. □

Remark 28. *Since $\mathcal{E}_{\kappa,c}$ is non-negative and closable, it follows that H_N has a self-adjoint Friedrichs extension, $\tilde{H}_N$. This is what we regard as the Hamiltonian of the 1D anyon gas with statistical parameter κ and Lieb–Liniger interaction of strength $2c\delta_0$ that is relevant for Theorem 7.*

We are now ready to provide a proof of Theorem 7 along the lines outlined in Section 1.3.

Proof of Theorem 7. Let $\mathcal{E}_c$ denote the bosonic quadratic form with potential $v_c = v + 2c\delta_0$. By Proposition 27 and the observation that the quadratic form is independent of the phase factors, we see that the unitary operator $U_\kappa : f \mapsto \mathrm{e}^{-i\frac{\kappa}{2}\Lambda} f$ provides a unitary equivalence of the bosonic and anyonic set-ups. That is, $U_\kappa \mathcal{D}\left(\mathcal{E}_{0,c/\cos(\kappa/2)}\right) = \mathcal{D}\left(\mathcal{E}_{\kappa,c}\right)$ with $\mathcal{E}_{\kappa,c}(U_\kappa f) = \mathcal{E}_{0,c/\cos(\kappa/2)}(f)$. Hence, the result follows from Theorem 1. □

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Chapter 4

The Ground State Energy of the One-dimensional Dilute Spin–$\frac{1}{2}$ Fermi Gas

In the preprint of Chapter 3, we proved an upper and a lower bound for the ground state energy of a dilute Bose gas in one dimension. It was also shown that, as a corollary, the ground state energy of a one-dimensional dilute spin polarized Fermi gas admitted similar bounds. In this chapter, we seek to analyze instead the full spin–1/2 Fermi gas. Due to an important theorem of Lieb and Mattis, [LM62b], it is known that the ground state of a repulsively interacting spin–1/2 Fermi gas (with an even number of particles), will have vanishing total spin. Therefore, will our bound, in the following, essentially give estimates on the total spin 0 sector of the one-dimensional dilute spin–1/2 Fermi gas.

4.1 The Model

We consider a gas of fermions, each with spin–1/2, interacting through a repulsive pair potential $v \geq 0$. The assumptions on v will be similar to those in Chapter 3, i.e. v has compact support, say in the ball B_{R_0}, and can be decomposed in $v = v_{\text{reg}} + v_{\text{h.c.}}$, where v_{reg} is a finite measure and $v_{\text{h.c.}}$ is a

positive linear combination of hard cores. Formally, we write the Hamiltonian

$$H = -\sum_{i=1}^{N} \partial_i^2 + \sum_{1 \leq i < j \leq N} v(x_i - x_j), \tag{4.1.1}$$

and with a domain contained in the Hilbert space $L^2_{\text{as}}\left(([0,L] \times \{0,1\})^N\right) \cong \left(L^2([0,L]) \otimes \mathbb{C}^2\right)^{\wedge N}$. We recap here the conjecture, from Remark 6 of Chapter 3, about the ground state energy for such a system.

Conjecture 4.1. *Let $v \geq 0$ satisfy the assumption from above, then the ground state energy of the dilute spin–1/2 Fermi gas satisfies*

$$E = N\frac{\pi^2}{3}\rho^2 \left(1 + 2\rho \left(\ln(2) a_e + (1 - \ln(2)) a_o\right) + \mathcal{O}(\rho^2 \max(|a_e|, a_o)^2)\right). \tag{4.1.2}$$

4.2 Upper Bound

In this section, we prove an upper bound for the ground state energy of the model (4.1.1). The upper bound matches, to next-to-leading order, Conjecture 4.1. To prove the desired upper bound, some prerequisites are needed. We have already covered the definition of the scattering length and scattering wave function in Chapter 2, and the free Fermi ground state was found in Chapter 3. For the spin–1/2 gas, we furthermore need knowledge about how to handle the spin degrees of freedom. For this purpose, we give some heuristic arguments based on physical intuition and utilize this intuition in constructing a trial state giving the correct upper bound. The main result of this section is the following theorem.

Theorem 4.2. *Let $v \geq 0$ satisfy the assumption from above, then the ground state energy of the dilute spin–1/2 Fermi gas satisfies*

$$E \leq N\frac{\pi^2}{3}\rho^2 \left(1 + 2\rho \left(\ln(2) a_e + (1 - \ln(2)) a_o\right) + \mathcal{O}\left((\rho R)^{6/5} + N^{-1}\right)\right), \tag{4.2.1}$$

with $R = \max(|a_e|, a_o, R_0)$.

Constructing a trial state

In constructing a trial state for the dilute Fermi gas, we may restrict to a sector of the form $\{\sigma\} = \{\sigma_1, \sigma_2, \ldots, \sigma_N\} = \{0 < x_{\sigma_1} < x_{\sigma_2} < \ldots < x_{\sigma_N} < L\}$, then the trial state is given by anti-symmetrically extending to other sectors. Of course, this means that certain boundary conditions need to be satisfied at the boundary $\{x_{\sigma_i} = x_{\sigma_{i+1}}\}$ for this extension to be in the relevant domain. This boundary condition is exactly that $\mathrm{P}_t^{i,i+1}\,\Psi|_{\{x_{\sigma_i}=x_{\sigma_{i+1}}\}} = 0$. Here $\mathrm{P}_t^{i,j}$ denotes the spin-projection onto the triplet of particles i and j, and equivalently we will denote the spin-projection onto the singlet of particles i and j by $\mathrm{P}_s^{i,j}$. In terms of spin operators $S = \frac{1}{2}\overline{\sigma}$, with $\overline{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ being the vector of Pauli matrices, we have $\mathrm{P}_s^{i,j} = 1/4 - S_i \cdot S_j$ and $\mathrm{P}_t^{i,j} = 3/4 + S_i \cdot S_j$, where $S_i = I \otimes \ldots \otimes \underbrace{S}_{i^{\text{th}}} \otimes \ldots \otimes I$. We recall from Chapter 3 that the ground state energy (of the Bose gas or spin polarized Fermi gas) may be well approximated in the dilute limit, by a state that resembles a free Fermi state when particles are far apart, and resembles the two-particle scattering solution when a pair is close. With this in mind, we may construct a variational trial state on a sector $\{1, 2, \ldots, N\}$ as follows

$$\Psi_\chi = \begin{cases} \frac{\Psi_F}{\mathcal{R}} \left(\left(\eta\omega_e^{\mathcal{R}} + (1-\eta)\omega_o^{\mathcal{R}}\right) \mathrm{P}_s^{\mathcal{R}} + \omega_o^{\mathcal{R}}\, \mathrm{P}_t^{\mathcal{R}} \right) \chi, & \mathcal{R}(x) < b \\ \Psi_F, & \mathcal{R}(x) \geq b \end{cases}, \tag{4.2.2}$$

where χ is some spin state, $b > R_0$, $\mathcal{R}(x) = \min_{i<j} |x_i - x_j|$, $\omega_{s/o}^{\mathcal{R}}(x) \coloneqq \omega_{s/o}(\mathcal{R}(x)) = b f_{s/o}(\mathcal{R}(x))$ (see Definitions 2.27 and 2.28 with R replaced by b), and for $\mathcal{R}(x) = |x_i - x_j|$, we have $\mathrm{P}_{s/t}^{\mathcal{R}(x)} := \mathrm{P}_{s/t}^{h(i),h(j)}$ with $h(i)$ being the spin-index of the particle with coordinate x_i[1]. Furthermore, η is a continuous and almost everywhere differentiable function with the property $\eta(x) = 0$

[1] When we are on the sector $\{\sigma\}$ and we are defining

$$\Psi\left((x_{\sigma_1}, s_{\sigma_1}), (x_{\sigma_2}, s_{\sigma_2}), \ldots, (x_{\sigma_N}, s_{\sigma_N})\right),$$

we have $h(i) = i$. On the other hand, if we seek to define

$$\Psi\left((x_{\sigma_1}, s_1), (x_{\sigma_2}, s_2), \ldots, (x_{\sigma_N}, s_N)\right),$$

we have $h(i) = \sigma^{-1}(i)$. This is only relevant for considering symmetries different from the fermionic spin-space anti-symmetry, as

$$\Psi\left((x_1, s_1), (x_2, s_2), \ldots, (x_N, s_N)\right) = \mathrm{sgn}(\sigma)\Psi\left((x_{\sigma_1}, s_{\sigma_1}), (x_{\sigma_2}, s_{\sigma_2}), \ldots, (x_{\sigma_N}, s_{\sigma_N})\right),$$

for fermionic wave functions. Hence, in this section, we may as well think of h as $h(i) = i$. A different symmetry is considered below in Section 4.3.

when $\mathcal{R}_2(x) = b$, where $\mathcal{R}_2(x) = \min_{(i,j)\neq(k,l)} \max(|x_i - x_j|, |x_k - x_l|)$ is the distance between the second closest pair. More precisely we define

$$\eta(x) \coloneqq \begin{cases} 0, & \text{if } \mathcal{R}_2(x) \leq b \\ \left(\frac{\mathcal{R}_2(x)}{b} - 1\right), & \text{if } b < \mathcal{R}_2(x) < 2b \\ 1, & \text{if } \mathcal{R}_2(x) \geq 2b. \end{cases} \tag{4.2.3}$$

In this case, we see that $\mathrm{P}_t^{i,j}\,\Psi|_{x_i=x_j} = 0$ due to the boundary condition satisfied by ω_o. We notice that a potential discontinuity could arise from $\mathrm{P}_{s/t}^{\mathcal{R}(x)}$, since these projection are discontinuous at points where $\mathcal{R}_2(x) = \mathcal{R}(x)$. However, since $\mathrm{P}_s^{\mathcal{R}(x)} + \mathrm{P}_t^{\mathcal{R}(x)} = 1$, we see that Ψ is continuous due to the inclusion of η. The extension of Ψ to other sectors $\{\sigma\}$ is then defined by anti-symmetry in the space-spin variables. In this case, due to the symmetry of the Hamiltonian/energy quadratic form, the energy is determined completely by the energy on the sector $\{1, 2, \ldots, N\}$.

As was the case in Chapter 3, the trial state given in (4.2.2) produces an error that grows with the particle number. This is undesirable for proving Theorem 4.2. However, as before, we may construct the full trial state by localizing it to smaller intervals. This is done by splitting the interval $[0, L]$ into smaller intervals $I_m \coloneqq [m(\ell + b), (m+1)\ell + mb]$ $m = 0, 1, 2, \ldots M-1$, where $\ell = L/M - b$. We then consider the trial state given by a product

$$\Psi_{\chi,\text{full}}(x_1, \ldots, x_N) = \prod_{m=0}^{M-1} \Psi_\chi^{I_m}(x_1^m, \ldots, x_{\tilde{N}}^m), \tag{4.2.4}$$

where $\tilde{N} = N/M$ and $x_i^m \coloneqq x_{m\tilde{N}+i}$ and the superscribt I_m in $\Psi_\chi^{I_m}$ means that we take the state Ψ_χ constructed on I_m instead of $[0, L]$. Notice that there are no interactions between boxes since $b > R_0$.

Remark 4.3. *Of course, dividing the particles in this way, might not be possible with desirable integers $\tilde{N}$ and M. However, for a desirable $\tilde{N}$ (not necessarily integer), we may take $M = \left\lceil N/\tilde{N} \right\rceil$, and then the particles in each box will be $\lceil N/M \rceil$ or $\lceil N/M - 1 \rceil$ in such a way that the total number of particles remain N. In this case, the length of a given box may also be chosen, according to the number of particles it contains, to be $\ell_{\lceil N/M \rceil} = \rho^{-1} \lceil N/M \rceil - b$ and $\ell_{\lceil N/M-1 \rceil} = \rho^{-1} \lceil N/M - 1 \rceil - b$. This technical detail produces only errors that are small compared to existing errors in the proof of Theorem 4.2 below, and*

thus for simplicity we ignore it.

We saw in Chapter 3 that the scattering solution, when particles are close, leads to a correction to the free Fermi energy that is of order $2\rho a_{e/o} E_F$. Since $\mathrm{P}_s^{i,j} = 1/4 - S_i \cdot S_j$ and $\mathrm{P}_t^{i,j} = 3/4 + S_i \cdot S_j$, we expect (ignoring the effect of η) that the correction we obtain from the variational state Ψ_χ is of the order

$$2\rho \left((a_o - a_e) \left\langle \chi \left| \frac{1}{N} \sum_i S_i \cdot S_{i+1} \right| \chi \right\rangle + \frac{1}{4} a_e + \frac{3}{4} a_o \right) E_F.$$

The minimizer (in χ) χ_0 is known, and in this case, since $a_o \geq a_e$, it is given by the ground state of the periodic antiferromagnetic Heisenberg chain $\chi_0 = |\mathrm{GS}_{\mathrm{HAF}}\rangle$. This ground state is known explicitly, as it is of Bethe ansatz form [Bet31]. Furthermore, the ground state energy of the antiferromagnetic Heisenberg chain is known to be [Hul38, Mat12] (See lemma 4.11 below)

$$\left\langle \mathrm{GS}_{\mathrm{HAF}} \left| \frac{1}{N} \sum_i S_i \cdot S_{i+1} \right| \mathrm{GS}_{\mathrm{HAF}} \right\rangle = \frac{1}{4} - \ln(2) + \mathcal{O}(1/N). \tag{4.2.5}$$

Hence we find the correction $2\rho \left(\ln(2) a_e + (1 - \ln(2)) a_o \right) E_F$ as desired.

Proof of Theorem 4.2

In this section, we give the rigorous proof of Theorem 4.2. The idea was already sketched in the previous section, and the goal is thus to make the statements in the previous section rigorous. An important, although completely trivial, fact is the following lemma.

Lemma 4.4. *Let η be defined as above, then we have*

$$|\nabla \eta| \leq \frac{\sqrt{2}}{b}, \text{ a.e.} \tag{4.2.6}$$

The quantity of interest in the following will be the energy of the trial state

$$\mathcal{E}(\Psi_\chi) = \int_{[0,L]^N} \sum_{i=1}^N |\partial_i \Psi_\chi|^2 + \sum_{1 \leq i < j \leq N} v_{ij} |\Psi_\chi|^2 . \tag{4.2.7}$$

We will henceforth assume χ to be translation invariant. This assumption is not needed, when we have periodic boundary conditions, see Appendix A. As

was done in Chapter 3, we rewrite this by use of the diamagnetic inequality

$$\begin{aligned}\mathcal{E}(\Psi_\chi) &\leq E_F + \int_B \sum_{i=1}^N |\partial_i \Psi_\chi|^2 + \sum_{1\leq i<j\leq N} v_{ij} |\Psi_\chi|^2 - \sum_{i=1}^N |\partial_i \Psi_F|^2 \\ &= E_F + \binom{N}{2} \int_{B_{12}} \sum_{i=1}^N |\partial_i \Psi_\chi|^2 + \sum_{1\leq i<j\leq N} v_{ij} |\Psi_\chi|^2 - \sum_{i=1}^N |\partial_i \Psi_F|^2 ,\end{aligned} \tag{4.2.8}$$

where $B = \{x \in [0,L]^N | \mathcal{R}(x) < b\}$, and $B_{12} = \{x \in [0,L]^N | \mathcal{R}(x) = |x_1 - x_2| < b\}$. Now due to the presence of η in the trial state, we need to further divide the integration domain. We list here different domains of integration that will be relevant in this section

$$\begin{aligned} B_{12}^{\geq} &= B_{12} \cap \{\mathcal{R}_2(x) \geq 2b\}, \\ B_{12}^{23} &= B_{12} \cap \{\mathcal{R}_2(x) = |x_2 - x_3| < 2b\}, \\ B_{12}^{34} &= B_{12} \cap \{\mathcal{R}_2(x) = |x_3 - x_4| < 2b\}, \\ A_{12} &= \left\{x \in [0,L]^N \;\middle|\; |x_1 - x_2| < b\right\}, \\ A_{12}^{23} &= A_{12} \cap \{|x_2 - x_3| < 2b\}, \\ A_{12}^{34} &= A_{12} \cap \{|x_3 - x_4| < 2b\}. \end{aligned} \tag{4.2.9}$$

In (4.2.8) the last term is dealt with in the same way as in Chapter 3. It is also obvious that we may replace v by v_{reg}, as the trial state vanishes whenever a pair is inside the outermost hard core. Now due to the anti-symmetry, we conclude from (4.2.8)

$$\begin{aligned}\mathcal{E}(\Psi_\chi) \leq E_F &+ \binom{N}{2} \int_{B_{12}^{\geq}} \sum_{i=1}^N |\partial_i \Psi_\chi|^2 + 2(N-2)\binom{N}{2} \int_{B_{12}^{23}} \sum_{i=1}^N |\partial_i \Psi_\chi|^2 \\ &+ \binom{N}{2}\binom{N-2}{2} \int_{B_{12}^{34}} \sum_{i=1}^N |\partial_i \Psi_\chi|^2 \\ &+ \binom{N}{2} \int_{B_{12}} \sum_{1\leq i<j\leq N} (v_{\mathrm{reg}})_{ij} |\Psi_\chi|^2 - \binom{N}{2} \int_{B_{12}} \sum_{i=1}^N |\partial_i \Psi_F|^2 .\end{aligned} \tag{4.2.10}$$

Defining

$$(\Psi_e)_{12} \coloneqq \frac{\Psi_F}{|x_2 - x_1|} \omega_e^{12} \text{ and } (\Psi_o)_{12} \coloneqq \frac{\Psi_F}{|x_2 - x_1|} \omega_o^{12}, \tag{4.2.11}$$

we find by the fact that $B_{12}^{\geq} \subset A_{12}$,

$$\begin{aligned}\int_{B_{12}^{\geq}} |\partial_i \Psi_\chi|^2 \leq & \sum_{\{\sigma\}\in S_{12}} \left(\int_{A_{12}\cap\{\sigma\}} |\partial_i (\Psi_e)_{12}|^2 \right) \left\langle \chi_\sigma \left| \mathrm{P}_s^{1,2} \right| \chi_\sigma \right\rangle \\ & + \sum_{\{\sigma\}\in S_{12}} \left(\int_{A_{12}\cap\{\sigma\}} |\partial_i (\Psi_o)_{12}|^2 \right) \left\langle \chi_\sigma \left| \mathrm{P}_t^{1,2} \right| \chi_\sigma \right\rangle ,\end{aligned} \tag{4.2.12}$$

where $\mathrm{P}_{s/t}^{N,N+1} := \mathrm{P}_{s/t}^{N,1}$ and χ_σ is the spin state χ with spins permuted by $(1,\ldots,N) \mapsto (\sigma_1,\ldots,\sigma_N)$ and

$$S_{12} = \{\text{sectors } \{\sigma\} \mid (\sigma_k, \sigma_{k+1}) = (1,2) \text{ or } (\sigma_k,\sigma_{k+1}) = (2,1) \text{ for some } k\}.$$

Using the translation invariance of χ we see that

$$\left\langle \chi_\sigma \left| \mathrm{P}_{s/t}^{1,2} \right| \chi_\sigma \right\rangle = \frac{1}{N} \sum_{k=1}^{N} \left\langle \chi_\sigma \left| \mathrm{P}_{s/t}^{\sigma_k,\sigma_{k+1}} \right| \chi_\sigma \right\rangle = \frac{1}{N} \sum_{k=1}^{N} \left\langle \chi \left| \mathrm{P}_{s/t}^{k,k+1} \right| \chi \right\rangle$$

is independent of $\sigma \in S_{12}$ and that

$$\begin{aligned}\int_{B_{12}^{\geq}} |\partial_i \Psi_\chi|^2 \leq & \left(\int_{A_{12}} |\partial_i (\Psi_e)_{12}|^2 \right) \frac{1}{N} \sum_{k=1}^{N} \left\langle \chi \left| \mathrm{P}_s^{k,k+1} \right| \chi \right\rangle \\ & + \left(\int_{A_{12}} |\partial_i (\Psi_o)_{12}|^2 \right) \frac{1}{N} \sum_{k=1}^{N} \left\langle \chi \left| \mathrm{P}_t^{k,k+1} \right| \chi \right\rangle ,\end{aligned} \tag{4.2.13}$$

Considering (4.2.10) again, we see from the trivial relation

$$\frac{1}{N} \left(\sum_{k=1}^{N} \left\langle \chi \left| \mathrm{P}_s^{k,k+1} \right| \chi \right\rangle + \sum_{k=1}^{N} \left\langle \chi \left| \mathrm{P}_t^{k,k+1} \right| \chi \right\rangle \right) = 1,$$

and from the fact that $B_{12} \subset A_{12}$ and the observation that $\omega_o \leq \omega_e$ implying

$$|\Psi_\chi|^2 \leq \frac{1}{N} \sum_{k=1}^{N} \left(\left\langle \chi \left| P_s^{k,k+1} \right| \chi \right\rangle |(\Psi_e)_{12}|^2 + \left\langle \chi \left| P_t^{k,k+1} \right| \chi \right\rangle |(\Psi_o)_{12}|^2 \right) \tag{4.2.14}$$

on B_{12} that we have the following upper bound for the energy

$$\begin{aligned}\mathcal{E}(\Psi_\chi) \leq E_F &+ \binom{N}{2}\frac{1}{N}\sum_{k=1}^{N}\left\langle\chi\left|\mathrm{P}_s^{k,k+1}\right|\chi\right\rangle\left(\int_{A_{12}}\sum_{i=1}^{N}\left|\partial_i(\Psi_e)_{12}\right|^2\right.\\ &\left.+\int_{A_{12}}\sum_{1\leq i<j\leq N}(v_{\mathrm{reg}})_{ij}\left|(\Psi_e)_{12}\right|^2-\int_{B_{12}}\sum_{i=1}^{N}\left|\partial_i\Psi_F\right|^2\right)\\ &+\binom{N}{2}\frac{1}{N}\sum_{k=1}^{N}\left\langle\chi\left|\mathrm{P}_t^{k,k+1}\right|\chi\right\rangle\left(\int_{A_{12}}\sum_{i=1}^{N}\left|\partial_i(\Psi_o)_{12}\right|^2\right.\\ &\left.+\int_{A_{12}}\sum_{1\leq i<j\leq N}(v_{\mathrm{reg}})_{ij}\left|(\Psi_o)_{12}\right|^2-\int_{B_{12}}\sum_{i=1}^{N}\left|\partial_i\Psi_F\right|^2\right)\\ &+\binom{N}{2}\binom{N-2}{2}\int_{B_{12}^{34}}\sum_{i=1}^{N}\left|\partial_i\Psi_\chi\right|^2\\ &+2(N-2)\binom{N}{2}\int_{B_{12}^{23}}\sum_{i=1}^{N}\left|\partial_i\Psi_\chi\right|^2.\end{aligned} \tag{4.2.15}$$

We see that this reduces proving an upper bound to a case we have already analyzed in Chapter 3, except for the last two terms, which we then need to estimate. Let us denote the two quantities by

$$\begin{aligned}E_{12}^{34} &:= \binom{N}{2}\binom{N-2}{2}\int_{B_{12}^{34}}\sum_{i=1}^{N}\left|\partial_i\Psi_\chi\right|^2,\\ E_{12}^{23} &:= 2(N-2)\binom{N}{2}\int_{B_{12}^{23}}\sum_{i=1}^{N}\left|\partial_i\Psi_\chi\right|^2.\end{aligned} \tag{4.2.16}$$

The following lemmas, which we prove below, provide estimates of these quantities.

Lemma 4.5. *Let E_{12}^{34} and Ψ_χ be defined as above, then we have the following bound:*

$$E_{12}^{34} \leq \text{ const. } E_F\left(N(\rho b)^4+N^2(\rho b)^6\right). \tag{4.2.17}$$

where E_F denotes the free spin polarized (spinless) Fermi energy.

Lemma 4.6. *Let E_{12}^{23} and Ψ_χ be defined as above, then we have the following bound:*

$$E_{12}^{23} \leq \text{ const. } E_F\left((\rho b)^4+N(\rho b)^6\right). \tag{4.2.18}$$

where E_F denotes the free spin polarized (spinless) Fermi energy.

Using Lemmas 4.5 and 4.6, we deduce, from (4.2.15) the following upper bound on the trial state energy

$$\begin{aligned}\mathcal{E}(\Psi_\chi) \leq E_F &+ \binom{N}{2}\frac{1}{N}\sum_{k=1}^{N}\left\langle \chi \left| \mathrm{P}_s^{k,k+1} \right| \chi \right\rangle \left(\int_{A_{12}} \sum_{i=1}^{N} |\partial_i (\Psi_e)_{12}|^2 \right. \\ &\left. + \int_{A_{12}} \sum_{1\leq i<j\leq N} (v_{\mathrm{reg}})_{ij} \, |(\Psi_e)_{12}|^2 - \int_{B_{12}} \sum_{i=1}^{N} |\partial_i \Psi_F|^2 \right) \\ &+ \binom{N}{2}\frac{1}{N}\sum_{k=1}^{N}\left\langle \chi \left| \mathrm{P}_t^{k,k+1} \right| \chi \right\rangle \left(\int_{A_{12}} \sum_{i=1}^{N} |\partial_i (\Psi_o)_{12}|^2 \right. \\ &\left. + \int_{A_{12}} \sum_{1\leq i<j\leq N} (v_{\mathrm{reg}})_{ij} \, |(\Psi_o)_{12}|^2 - \int_{B_{12}} \sum_{i=1}^{N} |\partial_i \Psi_F|^2 \right) \\ &+ E_F \left(N(\rho b)^4 + N^2 (\rho b)^6 \right).\end{aligned} \tag{4.2.19}$$

Defining the quantities

$$\begin{aligned} E_{1,e} &\coloneqq \binom{N}{2}\left(\int_{A_{12}} \sum_{i=1}^{N} |\partial_i (\Psi_e)_{12}|^2 + \sum_{1\leq i<j\leq N} (v_{\mathrm{reg}})_{ij} \, |(\Psi_e)_{12}|^2 - \sum_{i=1}^{N} |\partial_i \Psi_F|^2 \right), \\ E_{1,o} &\coloneqq \binom{N}{2}\left(\int_{A_{12}} \sum_{i=1}^{N} |\partial_i (\Psi_o)_{12}|^2 + \sum_{1\leq i<j\leq N} (v_{\mathrm{reg}})_{ij} \, |(\Psi_o)_{12}|^2 - \sum_{i=1}^{N} |\partial_i \Psi_F|^2 \right), \end{aligned} \tag{4.2.20}$$

and the quantities from Chapter 3:

$$\begin{aligned} E_2^{(1)} &\coloneqq \binom{N}{2} 2N \int_{A_{12}\cap A_{13}} \sum_{i=1}^{N} |\partial_i \Psi_F|^2 , \\ E_2^{(2)} &\coloneqq \binom{N}{2}\binom{N-2}{2} \int_{A_{12}\cap A_{34}} \sum_{i=1}^{N} |\partial_i \Psi_F|^2 , \end{aligned} \tag{4.2.21}$$

we see by noting $x \in A_{12} \setminus B_{12}$ implies $x \in A_{12} \cap A_{ij}$ for some $\{i,j\} \neq \{1,2\}$

that (4.2.19) implies

$$\begin{aligned}\mathcal{E}(\Psi_\chi) \leq E_F &+ \frac{1}{N}\sum_{k=1}^{N}\left\langle \chi \left| \mathrm{P}_s^{k,k+1} \right| \chi \right\rangle \left(E_{1,e} + E_2^{(1)} + E_2^{(2)}\right) \\ &+ \frac{1}{N}\sum_{k=1}^{N}\left\langle \chi \left| \mathrm{P}_t^{k,k+1} \right| \chi \right\rangle \left(E_{1,o} + E_2^{(1)} + E_2^{(2)}\right) \\ &+ E_F\left(N(\rho b)^4 + N^2(\rho b)^6\right)\end{aligned} \tag{4.2.22}$$

Here $E_{1,e/o}$ corresponds to the quantity E_1 in Chapter 3 with the even/odd wave scattering solution in the trial state. Proving the equivalent bound for the $E_{1,e/o}$ amounts to following the same proof strategy and we have the equivalent lemma:

Lemma 4.7 (Lemma 13 of Chapter 3)**.** *Let $E_{1,e/o}$ be defined as above. For $b > \max(2a_o, R_0)$ we have*

$$\begin{aligned}E_{1,e/o} \leq E_F\Bigg(&2\rho a_{e/o}\frac{b}{b-a_{e/o}} \\ &+ \text{const.}\ \left(N(\rho b)^3\left[1 + \rho b^2\int v_{\mathrm{reg}}\right] + \rho a_{e/o}\frac{\ln(N)}{N}\right)\Bigg).\end{aligned} \tag{4.2.23}$$

We also recall the lemma

Lemma 4.8 (Lemma 14 of Chapter 3)**.**

$$E_2^{(1)} + E_2^{(2)} \leq E_F\left(N(\rho b)^4 + N^2(\rho b)^6\right). \tag{4.2.24}$$

Using Lemmas 4.7 and 4.8 we find the result

Lemma 4.9. *For $N(\rho b)^3 \leq 1$ and $b > \max(2a_o, R_0)$ we have*

$$\begin{aligned}\mathcal{E}(\Psi_\chi) \leq E_F\Bigg(1 + 2\rho&\left[\frac{1}{4}\tilde{a}_e + \frac{3}{4}\tilde{a}_o + (\tilde{a}_o - \tilde{a}_e)\frac{1}{N}\left\langle \chi \left| \sum_{k=1}^{N} S_k \cdot S_{k+1} \right| \chi \right\rangle\right] \\ &+ \ \text{const.}\ \left(N(\rho b)^3\left[1 + \rho b^2\int v_{\mathrm{reg}}\right] + \rho a_o\frac{\ln(N)}{N}\right)\Bigg),\end{aligned} \tag{4.2.25}$$

where $\tilde{a}_{e/o} \coloneqq a_{e/o}\frac{b}{b-a_{e/o}}$.

Proof. This lemma follows directly by combining (4.2.22) with Lemmas 4.7 and 4.8. □

It is then immediately clear that on the right-hand side of (4.2.25), given that $a_o > a_e$, the optimal choice for χ is the ground state of the periodic antiferromagnetic Heisenberg chain, which due to the Marshall-Lieb-Mattis theorem, [LM62a, Mar55], is translation invariant. Of course, if $a_o = a_e$, the choice of χ is irrelevant for the right-hand side of (4.2.25).
We thus conclude that the ground state energy of the antiferromagnetic Heisenberg chain is of importance. Fortunately, this model is exactly solvable, as shown by Bethe [Bet31], and the ground state energy can be found in the thermodynamic limit, as shown by Hulthén [Hul38]:

Lemma 4.10 ([Mat12], Eq. (5.171))**.** *Let* $|\mathrm{GS}_{\mathrm{HAF}}\rangle$ *denote the ground state of the periodic antiferromagnetic Heisenberg chain. Then*

$$\lim_{N\to\infty} \left\langle \mathrm{GS}_{\mathrm{HAF}} \middle| \frac{1}{N}\sum_{k=1}^{N} S_k \cdot S_{k+1} \middle| \mathrm{GS}_{\mathrm{HAF}} \right\rangle = \frac{1}{4} - \ln(2) \tag{4.2.26}$$

This lemma gives the ground state energy of the Heisenberg chain in the thermodynamic limit, however, we need an estimate for the finite chain. This is given by the following lemma:

Lemma 4.11. *Let* $|\mathrm{GS}_{\mathrm{HAF}}\rangle$ *denote the ground state of the periodic antiferromagnetic Heisenberg chain. Then*

$$\left\langle \mathrm{GS}_{\mathrm{HAF}} \middle| \frac{1}{N}\sum_{k=1}^{N} S_k \cdot S_{k+1} \middle| \mathrm{GS}_{\mathrm{HAF}} \right\rangle = \frac{1}{4} - \ln(2) + \mathcal{O}(N^{-1}) \tag{4.2.27}$$

Proof. Denoting the Dirichlet (edge spin down) energy of the spin chain E_D^N with N sites and the periodic energy E_P^N, we have $E_P^N \leq E_D^N$. This follows directly from the variational principle. On the other hand we have the following bound

$$E_D^{N+2} \leq E_P^N + \frac{3}{4}. \tag{4.2.28}$$

To see this, consider a periodic chain of length N in its ground state. Add a spin-down at each edge, making the chain of length $N+2$. The resulting state is now a trial state for the Dirichlet chain of energy at most $E_P^N + \frac{3}{4}$ and (4.2.28) follows. Furthermore, it is not hard to see that for any integer $m \geq 1$

we have $E_D^{mN} \leq E_D^{mN-m+1} \leq mE_D^N$. The first inequality follows simply from the fact that extending a Dirichlet state by Néel ordering (alternating spin) to a larger chain, lowers the energy, hence ground state energy in the larger chain must also be lower. The second inequality follows by constructing a trial state for the Dirichlet chain of length $mN - m + 1$ by gluing m ground states of the Dirichlet chain of length N, such that they share a spin down at the gluing points. Collecting everything we have

$$\frac{1}{mN} E_P^{mN} \leq \frac{1}{mN} E_D^{mN} \leq \frac{1}{N} E_D^N \leq \frac{1}{N} \left(E_P^{N-2} + 3/4 \right). \tag{4.2.29}$$

It is clear that by a trial state argument and by translation invariance, which follows from the Marshall-Lieb-Mattis theorem (uniqueness of the ground state), we have $E_P^N \leq \frac{N}{M} E_P^M + \frac{1}{4}$ for $M > N$, simply take the ground state of chain length M, truncate it at length N, and use that all terms in the Hamiltonian have equal expectation values by translation invariance. Hence we get

$$\frac{1}{mN} E_P^{mN} \leq \frac{N-2}{N} \frac{1}{N-2} \left(E_P^{N-2} + 3/4 \right) \leq \frac{N-2}{N} \left(\frac{1}{M} E_P^M + \frac{1}{N-2} \right) \tag{4.2.30}$$

taking the limits $m \to \infty$ and $M \to \infty$ we have

$$\frac{N}{N-2} e_P - \frac{3}{4N} \leq \frac{1}{N-2} E_P^{N-2} \leq e_P + \frac{1}{4} \frac{1}{N-2}, \tag{4.2.31}$$

where $e_P = \lim_{N\to\infty} \frac{1}{N} E_P^N$. The desired result follows from Lemma 4.10. □

We are now ready to collect everything to give the proof of Theorem 4.2:

Proof of Theorem 4.2. Consider now the full trial state as given in (4.2.4) (See optionally Remark 4.3). Because of the spacing between intervals, I_m, there are no interactions between particles in different intervals. Hence the energy of such a state

$$\mathcal{E}(\Psi_{\chi,\text{full}}) / \left\| \Psi_{\chi,\text{full}} \right\| = M \mathcal{E}(\Psi_\chi^{I_0}) / \left\| \Psi_\chi^{I_0} \right\|. \tag{4.2.32}$$

Combining lemmas 4.9 and 4.11, we find

$$\mathcal{E}(\Psi_{\chi,\text{full}}) \leq N\frac{\pi^2}{3}\tilde{\rho}^2\Bigg(1+2\tilde{\rho}\left[\ln(2)\tilde{a}_e+(1-\ln(2))\tilde{a}_o\right]+\text{const. }\frac{M}{N} \\ +\text{ const. }\left(\frac{N}{M}(\tilde{\rho}b)^3\left[1+\tilde{\rho}b^2\int v_{\text{reg}}\right]+\tilde{\rho}a_o\frac{\ln(N/M)}{N/M}\right)\Bigg), \tag{4.2.33}$$

with $\rho \leq \tilde{\rho} = \frac{N}{L-Mb} \leq \rho\left(1+2\frac{M}{N}\rho b\right)$ for $\frac{M}{N}\rho b \leq 1/2$.
Similarly to the case in Chapter 3, term $\tilde{\rho}a_o\frac{\ln(N/M)}{N/M}$ satisfies

$$\tilde{\rho}a_o\frac{\ln(N/M)}{N/M} \leq \max(\text{const. } M/N, C_\epsilon(\tilde{\rho}a_o)^{2-\epsilon}).$$

It is therefore sub-leading and can be absorbed in other error terms. Thus we will neglect this term.
For $N > (\rho b)^{-3/2}\left(1+\rho b^2\int v_{\mathbf{reg}}\right)^{-1/2}$:
Choosing $M/N = (\rho b)^{3/2}\left(1+\rho b^2\int v_{\text{reg}}\right)^{1/2}$ we find

$$\mathcal{E}(\Psi_{\chi,\text{full}}) \leq N\frac{\pi^2}{3}\rho^2\Bigg(1+2\rho\left[\ln(2)\tilde{a}_e+(1-\ln(2))\tilde{a}_o\right]+ \\ +\text{ const. }(\rho b)^{3/2}\left(1+\rho b^2\int v_{\text{reg}}\right)^{1/2}\Bigg), \tag{4.2.34}$$

For $N < (\rho b)^{-3/2}\left(1+\rho b^2\int v_{\mathbf{reg}}\right)^{-1/2}$:
We see that (4.2.34) follows from choosing $M = 1$.
Furthermore choosing $b = \max(\rho^{-1/5}|a_e|^{4/5}, \rho^{-1/5}a_o^{4/5}, R_0)$ we see that $a_{e/o} \leq \tilde{a}_{e/o} = a_{e/o}\frac{b}{b-a_{e/o}} \leq a_{e/o}\left(1+2(\rho R)^{1/5}\right)$ for $(\rho R)^{1/5} \leq 1/2$ and the desired result follows from the simple estimate on the norm

$$\begin{aligned}\left\|\Psi_\chi^{I_0}\right\| &\geq 1-\int_{A_{12}}\rho^{(2))}(x_1,x_2) \geq 1-\text{ const. }\tilde{N}(\tilde{\rho}b)^3 \\ &\geq 1-\text{ const. }(\rho b)^{3/2} \geq 1-\text{ const. }(\rho R)^{6/5}.\end{aligned} \tag{4.2.35}$$

□

Estimating E_{12}^{34} (proof of lemma 4.5)

Proof of Lemma 4.5. Estimating E_{12}^{34} is a straightforward computation that goes as follows:

Define

$$\xi_{12}^{34} \coloneqq \Big(\big(\eta(|x_3-x_4|)\omega_e^{12}(|x_1-x_2|) + (1-\eta(|x_3-x_4|))\omega_o^{12}(|x_1-x_2|)\big)\,\mathrm{P}_s^{1,2} + \omega_o^{12}(|x_1-x_2|)\,\mathrm{P}_t^{1,2}\Big)\chi_\sigma \tag{4.2.36}$$

on $A_{12}^{34} \cap \{\sigma\}$, for all sectors $\{\sigma\} \in S_{12}^{34}$, with

$$\begin{aligned} S_{12}^{34} \coloneqq \big\{&\text{sectors } \{\sigma\} \mid (1,2) = (\sigma_k, \sigma_{k+1}) \text{ or} \\ &(2,1) = (\sigma_k, \sigma_{k+1}) \text{ for some } k \\ &\text{and } (3,4) = (\sigma_l, \sigma_{l+1}) \text{ or} \\ &(4,3) = (\sigma_l, \sigma_{l+1}) \text{ for some } l\big\}. \end{aligned} \tag{4.2.37}$$

We then see that $\Psi_\chi = \xi_{12}^{34} \frac{\Psi_F}{|x_2-x_1|}$ on B_{12}^{34}: Hence defining

$$\begin{aligned} \big(\xi_{12}^{34}\big)_s &\coloneqq \eta(|x_2-x_3|)\omega_e^{12}(|x_1-x_2|) + (1-\eta(|x_2-x_3|))\omega_o^{12}(|x_1-x_2|), \\ \big(\xi_{12}^{34}\big)_t &\coloneqq \omega_o^{12}(|x_1-x_2|), \end{aligned} \tag{4.2.38}$$

we find using $B_{12}^{34} \subset A_{12}^{34}$

$$\begin{aligned} E_{12}^{34} =& \binom{N}{2} 2(N-2) \int_{B_{12}^{34}} \sum_{i=1}^{N} \left| \partial_i \left(\xi_{12}^{34} \frac{\Psi_F}{|x_2-x_1|} \right) \right|^2 \\ \leq& \binom{N}{2} 2(N-1) \sum_{a\in\{s,t\}} \sum_{\{\sigma\}\in S_{12}^{34}} \left\langle \chi_\sigma \left| \mathrm{P}_a^{12} \right| \chi_\sigma \right\rangle \\ &\times \left[\int_{A_{12}^{34}\cap\{\sigma\}} \sum_{i=1}^{N} \left| \partial_i \left(\big(\xi_{12}^{34}\big)_a \frac{\Psi_F}{|x_2-x_1|} \right) \right|^2 \right]. \end{aligned} \tag{4.2.39}$$

One may use that $\left\langle \chi_\sigma \left| \mathrm{P}_a^{12} \right| \chi_\sigma \right\rangle$ is independent of σ, however, since we are not interested in finding the optimal constant in Lemma 4.5 we instead use the cruder bound, $\left\langle \chi_\sigma \left| \mathrm{P}_a^{12} \right| \chi_\sigma \right\rangle \leq 1$, to find

$$\begin{aligned} E_{12}^{34} \leq& \binom{N}{2} 2(N-1) \sum_{a\in\{s,t\}} \Bigg[\int_{A_{12}^{34}} \sum_{i=1}^{4} \left| \partial_i \left(\big(\xi_{12}^{34}\big)_a \frac{\Psi_F}{|x_2-x_1|} \right) \right|^2 \\ &+ \int_{A_{12}^{34}} \sum_{i=5}^{N} \overline{\big(\xi_{12}^{34}\big)_a \frac{\Psi_F}{|x_2-x_1|}} \left(\xi_{12}^{34} \frac{(-\partial_i^2 \Psi_F)}{|x_2-x_1|} \right) \Bigg]. \end{aligned} \tag{4.2.40}$$

where we used integration by parts and $\bigsqcup_{\{\sigma\}\in S_{12}^{34}} \left(A_{12}^{34} \cap \{\sigma\}\right) \subset A_{12}^{34}$, with

$\bigsqcup$ meaning disjoint union. Using that Ψ_F is an eigenfunction of $(-\Delta)$, with eigenvalue E_F we further find

$$\begin{aligned} E_{12}^{34} \leq & \binom{N}{2} 2(N-2) \sum_{a\in\{s,t\}} \Bigg[\int_{A_{12}^{34}} \sum_{i=1}^{4} \left| \partial_i \left(\left(\xi_{12}^{34}\right)_a \frac{\Psi_F}{|x_2-x_1|} \right) \right|^2 \\ & - \int_{A_{12}^{34}} \sum_{i=1}^{4} \overline{\left(\xi_{12}^{34}\right)_a \frac{\Psi_F}{|x_2-x_1|}} \left(\left(\xi_{12}^{34}\right)_a \frac{(-\partial_i^2 \Psi_F)}{|x_2-x_1|} \right) \\ & + E_F \int_{A_{12}^{34}} \left| \left(\xi_{12}^{34}\right)_a \frac{\Psi_F}{|x_2-x_1|} \right| \Bigg]. \end{aligned} \tag{4.2.41}$$

Thus, using $\left|\left(\xi_{12}^{34}\right)_a\right|^2 \leq b^2$ and restricting to $b \geq 2a_o \geq 2a_e$, we find

$$\begin{aligned} E_{12}^{34} \leq & 4 \sum_{a\in\{s,t\}} \int_{A_{12}^{34}} \Bigg(\sum_{i=1}^{4} \partial_{y_i} \partial_{x_i} \frac{\overline{\left(\xi_{12}^{34}\right)_a (y)}}{|y_2-y_1|} \frac{\left(\xi_{12}^{34}\right)_a (x)}{|x_2-x_1|} \gamma^{(4)}(y_1,y_2,y_3,y_4;x_1,x_2,x_3,x_4) \Big|_{y=x} \\ & + \left| \frac{\left(\xi_{12}^{34}\right)_a (x)}{|x_2-x_1|} \right|^2 \left| \sum_{i=1}^{4} \partial_{y_i}^2 \gamma^{(4)}(y_1,y_2,y_3,y_4;x_1,x_2,x_3,x_4) \Big|_{y=x} \right| \\ & + E_F \left| \frac{\left(\xi_{12}^{34}\right)_a (x)}{|x_2-x_1|} \right|^2 \rho^{(4)}(x_1,x_2,x_3,x_4) \Bigg) \\ \leq & \text{ const. } E_F \left(N (\rho b)^4 + N^2 (\rho b)^6 \right) \end{aligned} \tag{4.2.42}$$

where we used the following bounds

$$\begin{aligned} \partial_{y_i} \partial_{x_i} \frac{\gamma^{(4)}(y_1,y_2,y_3,y_4;x_1,x_2,x_3,x_4)}{|x_2-x_1|\,|y_2-y_1|} \Big|_{y=x} & \leq \text{const.} \rho^8, \\ \partial_{y_i} \frac{\gamma^{(4)}(y_1,y_2,y_3,y_4;x_1,x_2,x_3,x_4)}{|x_2-x_1|\,|y_2-y_1|} \Big|_{y=x} & \leq \text{const.} \rho^8 |x_3-x_4|, \\ \frac{\gamma^{(4)}(y_1,y_2,y_3,y_4;x_1,x_2,x_3,x_4)}{|x_2-x_1|\,|y_2-y_1|} \Big|_{y=x} & \leq \text{const.} \rho^8 |x_3-x_4|^2, \\ \left| \sum_{i=1}^{4} \partial_{y_i}^2 \gamma^{(4)}(y_1,y_2,y_3,y_4;x_1,x_2,x_3,x_4) \Big|_{y=x} \right| & \leq \text{const.} \rho^{10} |x_1-x_2|^2 |x_3-x_4|^2, \end{aligned} \tag{4.2.43}$$

and

$$\rho^{(4)}(x_1,x_2,x_3,x_4) \leq \text{const.} \rho^8 |x_1-x_2|^2 |x_3-x_4|^2, \tag{4.2.44}$$

which all follows from Taylor expansion of the free Fermi reduced density (matrices). Furthermore, we used the bounds

$$\sqrt{\left|\partial_i \left(\xi_{12}^{34}\right)_a\right|^2} \leq b \max\left(\frac{\sqrt{2}}{b}, \frac{1}{b-a_o}\right) \leq 2, \qquad \sqrt{\left|\left(\xi_{12}^{34}\right)_a\right|^2} \leq b \tag{4.2.45}$$

which follows from properties of the scattering solution, monotonicity of its derivative, and Lemma 4.4. □

Estimating E_{12}^{23} (proof of Lemma 4.6)

Proof of Lemma 4.6. Estimating E_{12}^{23} is, similarly to the estimation of E_{12}^{34}, a straightforward computation. We retrace the steps of the previous calculation, suitably modified for E_{12}^{23}, in the following:
Defining

$$\begin{aligned}\xi_{12}^{23} \coloneqq \Big(\big(\eta(|x_2-x_3|)\omega_e^{12}(|x_1-x_2|) + (1-\eta(|x_2-x_3|))\omega_o^{12}(|x_1-x_2|)\big)\, \mathrm{P}_s^{1,2} \\ +\omega_o^{12}(|x_1-x_2|)\, \mathrm{P}_t^{1,2}\Big)\chi_\sigma\end{aligned} \tag{4.2.46}$$

on $A_{12}^{23} \cap \{\sigma\}$, for all sectors $\{\sigma\} \in S_{12}^{23}$, with

$$\begin{aligned}S_{12}^{23} \coloneqq \big\{\text{sectors } \{\sigma\} \mid (1,2,3) = (\sigma_k, \sigma_{k+1}, \sigma_{k+2}) \text{ or} \\ (3,2,1) = (\sigma_k, \sigma_{k+1}, \sigma_{k+2}) \text{ for some } k\big\}\end{aligned} \tag{4.2.47}$$

. We then see that $\Psi_\chi = \xi_{12}^{23} \frac{\Psi_F}{|x_2-x_1|}$ on B_{12}^{23}: Hence defining

$$\begin{aligned}\left(\xi_{12}^{23}\right)_s &\coloneqq \eta(|x_2-x_3|)\omega_e^{12}(|x_1-x_2|) + (1-\eta(|x_2-x_3|))\omega_o^{12}(|x_1-x_2|), \\ \left(\xi_{12}^{23}\right)_t &\coloneqq \omega_o^{12}(|x_1-x_2|),\end{aligned} \tag{4.2.48}$$

we find using $B_{12}^{23} \subset A_{12}^{23}$

$$\begin{aligned}E_{12}^{23} =& \binom{N}{2} 2(N-2) \int_{B_{12}^{23}} \sum_{i=1}^{N} \left|\partial_i \left(\xi_{12}^{23} \frac{\Psi_F}{|x_2-x_1|}\right)\right|^2 \\ \leq& \binom{N}{2} 2(N-1) \sum_{a\in\{s,t\}} \sum_{\{\sigma\}\in S_{12}^{23}} \left\langle \chi_\sigma \left|\mathrm{P}_a^{12}\right| \chi_\sigma \right\rangle \\ &\times \left[\int_{A_{12}^{23}\cap\{\sigma\}} \sum_{i=1}^{N} \left|\partial_i \left(\left(\xi_{12}^{23}\right)_a \frac{\Psi_F}{|x_2-x_1|}\right)\right|^2\right].\end{aligned} \tag{4.2.49}$$

One may use that $\left\langle \chi_\sigma \left| \mathrm{P}_a^{12} \right| \chi_\sigma \right\rangle$ is independent of σ, however, since we are not interested in finding the optimal constant in Lemma 4.6 we instead use the cruder bound, $\left\langle \chi_\sigma \left| \mathrm{P}_a^{12} \right| \chi_\sigma \right\rangle \leq 1$, to find

$$\begin{aligned} E_{12}^{23} \leq & \binom{N}{2} 2(N-1) \sum_{a\in\{s,t\}} \left[\int_{A_{12}^{23}} \sum_{i=1}^{3} \left| \partial_i \left(\left(\xi_{12}^{23}\right)_a \frac{\Psi_F}{|x_2-x_1|} \right) \right|^2 \right. \\ & \left. + \int_{A_{12}^{23}} \sum_{i=4}^{N} \overline{\left(\xi_{12}^{23}\right)_a \frac{\Psi_F}{|x_2-x_1|}} \left(\xi_{12}^{23} \frac{(-\partial_i^2 \Psi_F)}{|x_2-x_1|} \right) \right]. \end{aligned} \tag{4.2.50}$$

where we used integration by parts and $\bigsqcup_{\{\sigma\}\in S_{12}^{23}} \left(A_{12}^{23} \cap \{\sigma\} \right) \subset A_{12}^{23}$. Using that Ψ_F is an eigenfunction of $(-\Delta)$, with eigenvalue E_F we further find

$$\begin{aligned} E_{12}^{23} \leq & \binom{N}{2} 2(N-2) \sum_{a\in\{s,t\}} \left[\int_{A_{12}^{23}} \sum_{i=1}^{3} \left| \partial_i \left(\left(\xi_{12}^{23}\right)_a \frac{\Psi_F}{|x_2-x_1|} \right) \right|^2 \right. \\ & - \int_{A_{12}^{23}} \sum_{i=1}^{3} \overline{\left(\xi_{12}^{23}\right)_a \frac{\Psi_F}{|x_2-x_1|}} \left(\left(\xi_{12}^{23}\right)_a \frac{(-\partial_i^2 \Psi_F)}{|x_2-x_1|} \right) \\ & \left. + E_F \int_{A_{12}^{23}} \left| \left(\xi_{12}^{23}\right)_a \frac{\Psi_F}{|x_2-x_1|} \right| \right]. \end{aligned} \tag{4.2.51}$$

Thus, using $\left|\left(\xi_{12}^{23}\right)_a\right|^2 \leq b^2$ and restricting to $b \geq 2a_o \geq 2a_e$, we find

$$\begin{aligned} E_{12}^{23} \leq & 4 \sum_{a\in\{s,t\}} \int_{A_{12}^{23}} \left(\sum_{i=1}^{3} \partial_{y_i} \partial_{x_i} \frac{\overline{\left(\xi_{12}^{23}\right)_a (y)}}{|y_2-y_1|} \frac{\left(\xi_{12}^{23}\right)_a (x)}{|x_2-x_1|} \gamma^{(3)}(y_1,y_2,y_3;x_1,x_2,x_3) \right|_{y=x} \right. \\ & + \left| \frac{\left(\xi_{12}^{23}\right)_a (x)}{|x_2-x_1|} \right|^2 \left| \sum_{i=1}^{3} \partial_{y_i}^2 \gamma^{(3)}(y_1,y_2,y_3;x_1,x_2,x_3) \right|_{y=x} \Bigg| \\ & \left. + E_F \left| \frac{\left(\xi_{12}^{23}\right)_a (x)}{|x_2-x_1|} \right|^2 \rho^{(3)}(x_1,x_2,x_3) \right) \\ \leq & \text{ const. } E_F \left((\rho b)^4 + N (\rho b)^6 \right) \end{aligned} \tag{4.2.52}$$

where we used the following bounds

$$\begin{aligned}
\partial_{y_i}\partial_{x_i}\frac{\gamma^{(3)}(y_1,y_2,y_3;x_1,x_2,x_3)}{|x_2-x_1|\,|y_2-y_1|}\bigg|_{y=x} &\leq \text{const.}\rho^7,\\
\partial_{y_i}\frac{\gamma^{(3)}(y_1,y_2,y_3;x_1,x_2,x_3)}{|x_2-x_1|\,|y_2-y_1|}\bigg|_{y=x} &\leq \text{const.}\rho^7\,|x_2-x_3|\,,\\
\frac{\gamma^{(3)}(y_1,y_2,y_3;x_1,x_2,x_3)}{|x_2-x_1|\,|y_2-y_1|}\bigg|_{y=x} &\leq \text{const.}\rho^7\,|x_2-x_3|^2\,,\\
\left|\sum_{i=1}^{3}\partial_{y_i}^2\gamma^{(3)}(y_1,y_2,y_3;x_1,x_2,x_3)\bigg|_{y=x}\right| &\leq \text{const.}\rho^{11}\,|x_1-x_2|^2\,|x_2-x_3|^2\,|x_1-x_3|^2\,,
\end{aligned} \tag{4.2.53}$$

and

$$\rho^{(3)}(x_1,x_2,x_3) \leq \text{const.}\rho^9\,|x_1-x_2|^2\,|x_2-x_3|^2\,|x_1-x_3|^2\,, \tag{4.2.54}$$

which all follows from Taylor expansion of the free Fermi reduced density (matrices) and Wick's theorem, as in Chapter 3. Furthermore, we used the bounds

$$\sqrt{\left|\partial_i\left(\xi_{12}^{23}\right)_a\right|^2} \leq b\max\left(\frac{\sqrt{2}}{b},\frac{1}{b-a_o}\right) \leq 2, \qquad \sqrt{\left|\left(\xi_{12}^{23}\right)_a\right|^2} \leq b \tag{4.2.55}$$

which follows from properties of the scattering solution, monotonicity of its derivative, and Lemma 4.4. □

4.3 Extending the Upper Bound to Other Symmetries and Spin-Dependent Potentials

We present here corollaries that follow directly, *mutatis mutandis*, from the proof of Theorem 4.2. We also apply one of the results to a model where the new upper bound improves the up to now best-known result.

Spin-1/2 Bosons

Going through the proof of Theorem 4.2 (and the lemmas used), we obtain an immediate corollary. Changing spin-space anti-symmetry to spin-space symmetry, we obtain the equivalent result for bosons. The change of symmetry

interchanges the even and odd condition in the singlet and triplet, hence constructing the trial state (4.2.2), we must interchange P_s and P_t. Thus we get

$$\Psi_\chi = \begin{cases} \frac{\Psi_F}{\mathcal{R}} \left(\left(\eta \omega_e^{\mathcal{R}} + (1-\eta)\omega_o^{\mathcal{R}} \right) \mathrm{P}_t^{\mathcal{R}} + \omega_o^{\mathcal{R}} \mathrm{P}_s^{\mathcal{R}} \right) \chi, & \mathcal{R}(x) < b \\ \Psi_F, & \mathcal{R}(x) \geq b \end{cases}. \tag{4.3.1}$$

The proof is unchanged except for the choice of χ. In this case, since $a_o \geq a_e$ and the roles of a_o and a_e are exchanged, the optimal choice for χ is a spin polarized state. Hence we get the following corollary:

Corollary 4.12 (Bosonic version of Theorem 4.2)**.** *Let v satisfy the assumption from above, then the ground state energy of the dilute spin–1/2 Bose gas satisfies*

$$E \leq N \frac{\pi^2}{3} \rho^2 \left(1 + 2\rho a_e + \mathcal{O}\left((\rho R)^{6/5} + N^{-1} \right) \right) \tag{4.3.2}$$

Here $R = \max(|a_e|, R_0)$.

Spin-Dependent Potentials

Interestingly, the proof of Theorem 4.2 we gave in the last section, allows for a slight generalization to potentials that are of the form

$$v(x_i - x_j) = v_e(x_i - x_j)\, \mathrm{P}_s^{i,j} + v_o(x_i - x_j)\, \mathrm{P}_t^{i,j} \tag{4.3.3}$$

with $v_{e/o} = v_{e/o,\mathrm{h.c.}} + v_{e/o,\mathrm{reg}}$ each satisfying the assumptions on v. In this case the $E_{1,e/o}$ becomes

$$\begin{aligned} E_{1,e} &\coloneqq \binom{N}{2} \left(\int_{A_{12}} \sum_{i=1}^{N} |\partial_i (\Psi_e)_{12}|^2 + \sum_{1 \leq i < j \leq N} (v_{e,\mathrm{reg}})_{ij} \, |(\Psi_e)_{12}|^2 - \sum_{i=1}^{N} |\partial_i \Psi_F|^2 \right), \\ E_{1,o} &\coloneqq \binom{N}{2} \left(\int_{A_{12}} \sum_{i=1}^{N} |\partial_i (\Psi_o)_{12}|^2 + \sum_{1 \leq i < j \leq N} (v_{o,\mathrm{reg}})_{ij} \, |(\Psi_o)_{12}|^2 - \sum_{i=1}^{N} |\partial_i \Psi_F|^2 \right), \end{aligned} \tag{4.3.4}$$

Consequently, Theorem 4.2 still holds, with a_e the even-wave scattering length of v_e and a_o the odd wave scattering length of v_o. We summarize this observation in the following corollary

Corollary 4.13 (Spin-dependent version of Theorem 4.2)**.** *Let $v = v_e \, \mathrm{P}_s + v_o \, \mathrm{P}_t$ be repulsive ($v \geq 0$) satisfy the assumption from above, then the ground state energy of the dilute spin–1/2 Fermi gas satisfies*

$$E \leq N \frac{\pi^2}{3} \rho^2 \left(1 + 2\rho \left(\ln(2) a_e + (1 - \ln(2)) a_o \right) + \mathcal{O}\left((\rho R)^{6/5} + N^{-1} \right) \right), \tag{4.3.5}$$

if $a_o \geq a_e$ and

$$E \leq N \frac{\pi^2}{3} \rho^2 \left(1 + 2\rho a_o + \mathcal{O}\left((\rho R)^{6/5} + N^{-1} \right) \right), \tag{4.3.6}$$

if $a_o \leq a_e$.
Here $R = \max(|a_e|, a_o, R_0)$. Furthermore, a_e denotes the even-wave scattering length of v_e and a_o the odd wave scattering length of v_o.

Proof. Repeat the proof of Theorem 4.2 but change $\omega_{e/o}$ to even/odd wave scattering solutions of $v_{e/o}$. Notice that it is no longer clear that $a_o \geq a_e$ and hence the choice of χ is the periodic antiferromagnetic Heisenberg chain when $a_o \geq a_e$ and a spin polarized state when $a_e > a_o$, both of which are translation invariant. Furthermore, (4.2.14) is no longer clear, as $\omega_e \geq \omega_o$ might not be satisfied. Instead, one may notice that (4.2.14) is actually an equality on $B_{12}^{\geq}$, and use that

$$\begin{aligned}
&\binom{N}{2} \int_{B_{12} \setminus B_{12}^{\geq}} \sum_{1 \leq i < j \leq N} v_e(x_i - x_j) \left| \mathrm{P}_s^{i,j} \, \Psi_\chi \right|^2 + v_o(x_i - x_j) \left| \mathrm{P}_t^{i,j} \, \Psi_\chi \right|^2 \\
&\leq \binom{N}{2} \int_{B_{12} \setminus B_{12}^{\geq}} \sum_{1 \leq i < j \leq N} \left(v_e(x_i - x_j) + v_o(x_i - x_j) \right) |\Psi_\chi|^2 \\
&\leq \text{const. } b^2 \int_{A_{12} \cap A_{23}} v(x_1 - x_2) \frac{1}{(x_1 - x_2)^2} \rho^{(3)}(x_1, x_2, x_3) \\
&+ \text{const. } b^2 \int_{A_{12} \cap A_{34}} v(x_1 - x_2) \frac{1}{(x_1 - x_2)^2} \rho^{(4)}(x_1, x_2, x_3, x_4) \\
&+ \text{const. } b^2 \int_{A_{12} \cap A_{23} \cap A_{45}} v(x_4 - x_5) \frac{1}{(x_1 - x_2)^2} \rho^{(5)}(x_1, x_2, x_3, x_4, x_5) \\
&+ \text{const. } b^2 \int_{A_{12} \cap A_{34} \cap A_{56}} v(x_5 - x_6) \frac{1}{(x_1 - x_2)^2} \rho^{(6)}(x_1, x_2, x_3, x_4, x_5, x_6) \\
&\leq \text{const. } E_0 \left(N(\rho b)^3 + N^2 (\rho b)^6 \right) \rho b^2 \left(\int v \right).
\end{aligned}$$

which can be absorbed in other errors. Alternatively, one use a trial state of

the form

$$\Psi_\chi = \begin{cases} \frac{\Psi_F}{\mathcal{R}} \left(f_1 \, \mathrm{P}_s^{\mathcal{R}} + f_2 \, \mathrm{P}_t^{\mathcal{R}} \right) \chi, & \mathcal{R}(x) < b \\ \Psi_F, & \mathcal{R}(x) \geq b \end{cases}, \tag{4.3.7}$$

with $f_1 = \min\left(\omega_e, \left(\eta\omega_e^{\mathcal{R}} + (1-\eta)\omega_o^{\mathcal{R}}\right)\right)$ and $f_2 = \min\left(\omega_o, \left(\eta\omega_o^{\mathcal{R}} + (1-\eta)\omega_e^{\mathcal{R}}\right)\right)$. In this case (4.2.14) is valid and the trial state is unchanged in $B_{12}^{\geq}$. With this trial state, the proofs of Lemmas 4.5 and 4.6 are proved in the same way as before. □

An interesting application of a version of Corollary 4.13 given below in Corollary 4.14 is the Lieb-Liniger-Heisenberg model introduced by Girardeau in [Gir06]. In his paper, an upper bound is given by a trial state argument in the case $c > c'$. Girardeau finds

$$E_{LLH} \leq E_{LL}(\ln(2)c' + (1 - \ln(2))c), \tag{4.3.8}$$

where $E_{LL}(\cdot)$ is the ground state energy of the Lieb-Liniger model as a function of the coupling strength. The Lieb-Liniger-Heisenberg model is defined with the formal Hamiltonian

$$H_{LLH} = -\sum_i \partial_i^2 + 2\sum_{i<j} \left(c' \, \tilde{\mathrm{P}}_s^{i,j} + c \, \tilde{\mathrm{P}}_t^{i,j} \right) \delta(x_i - x_j), \tag{4.3.9}$$

where the spin projectors, $\tilde{\mathrm{P}}_{s/t}$ are defined on the sector $\{\sigma\}$ to be

$$\tilde{\mathrm{P}}_{s/t}^{ij} = \mathrm{P}_{s/t}^{\sigma^{-1}(i)\sigma^{-1}(j)},$$

with $\sigma^{-1}(i)$ defined such that $\sigma_{\sigma^{-1}(i)} = i$, and the domain of (4.3.9) is taken to be wave functions that are *symmetric in the spatial coordinates*. This means that under combined spin-space coordinate exchange $(x_i, \sigma_i) \leftrightarrow (x_j, \sigma_j)$ the (i,j)-singlet part of the wave function is anti-symmetric and (i,j)-triplet part is symmetric. For spatially symmetric systems, we require in general potentials to of the form

$$v_s(x_i - x_j) \, \tilde{\mathrm{P}}_s^{ij} + v_t(x_i - x_j) \, \tilde{\mathrm{P}}_t^{ij}, \tag{4.3.10}$$

with $v_{s/t}$ satisfying the same conditions as $v_{e/o}$ above. This is to ensure that

the total energy is determined by the energy on any ordered sector[2]. This of course implies that Corollary 4.13 is not directly useful in this case. However, Going through the proof of Theorem 4.2, we see that we may as well get the following corollary.

Corollary 4.14 (Spatially symmetric, spin-dependent version of Theorem 4.2)**.** *Let $v = v_s \tilde{\mathrm{P}}_s + v_t \tilde{\mathrm{P}}_t \geq 0$ satisfy the assumption from above, then the ground state energy of the dilute spin–1/2 spatially symmetric gas satisfies*

$$E \leq N\frac{\pi^2}{3}\rho^2\left(1 + 2\rho\left(\ln(2)a_s + (1-\ln(2))a_t\right) + \mathcal{O}\left((\rho R)^{6/5} + N^{-1}\right)\right), \tag{4.3.11}$$

if $a_t \geq a_s$ and

$$E \leq N\frac{\pi^2}{3}\rho^2\left(1 + 2\rho a_t + \mathcal{O}\left((\rho R)^{6/5} + N^{-1}\right)\right), \tag{4.3.12}$$

if $a_t \leq a_s$.
Here $R = \max(|a_s|, |a_t|, R_0)$. Furthermore, a_s denotes the even wave scattering length of v_s and a_t the even wave scattering length of v_t.

Proof. Repeat the proof of Theorem 4.2, with the same modifications as in Corollary 4.13 (including lemmas used) but change $\omega_{e/o}$ to the even wave scattering solution of $v_{s/t}$ and extend the trial state to all sectors, $\{\sigma\}$, by spatial symmetry instead of spin-space anti-symmetry. The choice of χ is the periodic antiferromagnetic Heisenberg chain when $a_t \geq a_s$ and a spin polarized state when $a_s \geq a_t$. Whenever anti-symmetry was used in the proof of Theorem 4.2 the same step may be justified by spatial symmetry. To see this, we note that (4.2.10) can be derived by use of only spatial symmetry.

[2]This is case for potentials of the form (4.3.10) since for spatially a symmetric function we have on the sector $\{\sigma\}$

$$\int_{\{\sigma\}} v(x_i - x_j) \sum_{(s_1,\ldots,s_N)} \left|\tilde{\mathrm{P}}^{i,j}_{s/t}\psi((x_1,s_1),(x_2,s_2),\ldots(x_N,s_N))\right|^2 =$$
$$\int_{\{\sigma\}} v(x_i - x_j) \sum_{(s_1,\ldots,s_N)} \left|\mathrm{P}^{i,j}_{s/t}\,\psi((x_{\sigma_1},s_{\sigma_1}),(x_{\sigma_2},s_{\sigma_2}),\ldots,(x_{\sigma_N},s_{\sigma_N}))\right|^2 =$$
$$\int_{\{1,2,\ldots,N\}} v(x_{\sigma^{-1}(i)} - x_{\sigma^{-1}(j)}) \sum_{(s_1,\ldots,s_N)} \left|\mathrm{P}^{\sigma^{-1}(i),\sigma^{-1}(j)}_{s/t}\,\psi((x_1,s_1),(x_2,s_2),\ldots(x_N,s_N))\right|^2,$$

where we used spatial symmetry and relabeled the spin indices by $i \to \sigma^{-1}(i)$ in the first equality. We then relabeled the particle coordinates $x_i \to x_{\sigma_i}$ and the spin indices $i \to \sigma_i$ in the second equality.

However, in (4.2.12) we find instead

$$\int_{B_{12}^{\geq}} |\partial_i \Psi_\chi|^2 \leq \sum_{\{\sigma\}\in S_{12}} \left(\int_{A_{12}\cap\{\sigma\}} |\partial_i (\Psi_e)_{12}|^2 \right) \left\langle \chi \left| \mathrm{P}_s^{\sigma^{-1}(1),\sigma^{-1}(2)} \right| \chi \right\rangle + \sum_{\{\sigma\}\in S_{12}} \left(\int_{A_{12}\cap\{\sigma\}} |\partial_i (\Psi_o)_{12}|^2 \right) \left\langle \chi \left| \mathrm{P}_t^{\sigma^{-1}(1),\sigma^{-1}(2)} \right| \chi \right\rangle . \tag{4.3.13}$$

This is a consequence of the fact that the spins are not permuted when defining the trial state using the spatial symmetry (see Footnote 1 above in Section 4.2). A similar modification is made in the proofs of Lemmas 4.5 and 4.6. From this point, the proof proceeds as before by noticing that

$$\left\langle \chi \left| \mathrm{P}_{s/t}^{\sigma^{-1}(1),\sigma^{-1}(2)} \right| \chi \right\rangle = \frac{1}{N} \sum_{k=1}^{N} \left\langle \chi \left| \mathrm{P}_{s/t}^{k,k+1} \right| \chi \right\rangle$$

is independent of $\sigma \in S_{12}$ because of translation invariance of χ. □

We see that the upper bound given by Corollary 4.14 (up to a small error in the dilute limit) is

$$E_{LLH} \leq E_{LL} \left(\left(\frac{\ln(2)}{c'} + \frac{1-\ln(2)}{c} \right)^{-1} \right), \tag{4.3.14}$$

when $c > c'$. By the weighted harmonic-arithmetic mean inequality it is clear that our bound improves (4.3.8). The two bounds agree in the limit $\frac{c-c'}{c'} \to 0$. However, (4.3.8) gives just the free Fermi energy on the right-hand side when $c \to \infty$, whereas our bound reduces to the correct Yang-Gaudin energy, to leading order, in this limit.

Remark 4.15. *In the settings of Corollaries 4.13 and 4.14 we will refer to the regimes where $a_o \leq a_e$ or $a_t \leq a_s$ as the* ferromagnetic phase *and the regimes where $a_o \geq a_e$ or $a_t \geq a_s$ as the* antiferromagnetic phase.

4.4 Lower Bound

In this section, we will further motivate the Conjecture 4.1, however, a complete proof of a lower bound matching the upper bound in Theorem 4.2 is still missing. One may try to apply the same technique as was used in Chapter 3,

however, we will see that there are obstacles in this strategy.

Solvable Cases

To begin with, we may analyze the solvable models at hand. We will see that these are in agreement with Conjecture 4.1.

The hard core model: The first solvable case is the hard core model, with $v = \infty \mathbb{1}_{[-a,a]}$, with $a_e = a_o = a$ by Example 2.34. In this case, we have

$$E = E_F\left(L \to \frac{1}{1-\rho a}L\right) = N\frac{\pi^2}{3}\rho^2\left(1-\rho a\right)^{-2} + \mathcal{O}(\rho^2), \tag{4.4.1}$$

with $E_F\left(L \to \frac{1}{1-\rho a}L\right)$ denoting the spin polarized free Fermi energy in a box of length $\frac{1}{1-\rho a}L$. Of course since since $a_e = a_o = a$ in this case we have

$$E = N\frac{\pi^2}{3}\rho^2\left(1-\ln(2)\rho a_e - (1-\ln(2))\rho a_o\right)^{-2} + \mathcal{O}(\rho^2), \tag{4.4.2}$$

which match Conjecture 4.1.

The Yang-Gaudin model: This model was studied in Section 2.6. In this case, we have $a_e = -2/c$ and $a_o = 0$ by Example 2.33 Of course the upper bound from Theorem 4.2 applies. Furthermore, we found in Proposition 2.48 the bound

$$e = \text{“}\lim_{\substack{N,L\to\infty \\ N/L=\rho}} E/L\text{”} \geq \frac{\pi^2}{3}\rho^3\left[\left(1-\ln(2)\rho a_e\right)^{-2}\right]. \tag{4.4.3}$$

Here “” is used to emphasize that e is strictly speaking not known to be the true ground state energy (see Subsection 2.6). Hence we conclude $e = \frac{\pi^2}{3}\rho^3\left(1+2\ln(2)\rho a_e + \mathcal{O}(\rho\left|a_e\right|)^{6/5}\right)$, which is in agreement with Conjecture 4.1.

The General Case

In the case of a general potential, v, where the resulting model is not solvable, we might attempt to mimic the proof from the bosonic/spin polarized case in Chapter 3. We will here follow this strategy. We note first that Lemmas 19 and 20 of Chapter 3 do not depend on any symmetry of the wave function.

Dyson's lemma (Lemma 21 of Chapter 3) is modified slightly in the following way: Let $H^1_{\text{even/odd}}$ denote even/odd H^1 functions, then we have the following lemma.

Lemma 4.16 (Dyson's lemma spin–1/2 fermions)**.** *Let $R > R_0 = \text{range}(v)$ and $\varphi \in \left(H^1_{\text{even}}(\mathbb{R}) \otimes \mathrm{P}_s\left(\left(\mathbb{C}^2\right)^2\right)\right) \oplus \left(H^1_{\text{odd}}(\mathbb{R}) \otimes \mathrm{P}_t\left(\left(\mathbb{C}^2\right)^2\right)\right)$, then for any interval $\mathcal{I} \ni 0$*

$$\int_{\mathcal{I}} |\partial\varphi|^2 + \frac{1}{2} v\,|\varphi|^2 \geq \int_{\mathcal{I}} \overline{\varphi}\left(\frac{1}{R-a_e}\,\mathrm{P}_s + \frac{1}{R-a_o}\,\mathrm{P}_t\right)(\delta_R + \delta_{-R})\,\varphi, \quad (4.4.4)$$

where a is the s-wave scattering length.

Proof. The lemma follows straightforwardly from the Definitions 2.27 and 2.28. □

Thus we may prove the equivalent of Lemma 22 of Chapter 3: In the following Ψ denotes the spin–1/2 fermionic (Neumann) ground state of

$$H = -\sum_{i=1}^{N} \partial_i^2 + \sum_{1\leq i<j\leq N} v(x_i - x_j). \quad (4.4.5)$$

We shall also define the continuous function $\psi \in \left(L^2([0, L-(N-1)R]) \otimes \mathbb{C}^2\right)^{\otimes N}$, with $R \geq \max\left(R_0, 2\,|a_e|\,, 2a_o\right)$, such that for $0 \leq x_1 \leq \cdots \leq x_N \leq L-(N-1)R$

$$\psi(x_1, x_2, \ldots, x_N) := \Psi(x_1, R + x_2, \ldots, (n-1)R + x_N), \quad (4.4.6)$$

and extended by spatial symmetry.

Lemma 4.17. *Let $R > \max\left(R_0, 2\,|a|\right)$ and $\epsilon \in [0,1]$. For ψ defined in* (4.4.6)*,*

$$\begin{aligned}\int \sum_i |\partial_i \Psi|^2 + \sum_{i\neq j} \frac{1}{2} v_{ij}\,|\Psi|^2 \geq E^N_{LLH}\left(N, \tilde{L}, \frac{2\epsilon}{R-a_e}, \frac{2\epsilon}{R-a_o}\right)\langle\psi|\psi\rangle \\ + \frac{(1-\epsilon)}{R^2}\text{const.}\ (1 - \langle\psi|\psi\rangle).\end{aligned} \quad (4.4.7)$$

where $\tilde{L} := L - (n-1)R$, the superscript "N" denotes Neumann boundary condition, and $E_{LLH}(N, L, c', c)$ is the ground state energy of the Lieb-Liniger-Heisenberg model in (4.3.9)*.*

Proof. We mimic the proof of Chapter 3 ([ARS22]): Splitting the energy functional into two parts, and using Lemma 20 from Chapter 3[3] on one term and Lemma 4.16 on the other, we find

$$\begin{aligned}\int \sum_i |\partial_i \Psi|^2 + \sum_{i\neq j} \frac{1}{2} v_{ij} |\Psi|^2 \geq \\ \int \sum_i |\partial_i \Psi|^2 \mathbb{1}_{\mathfrak{r}_i(x)>R} + \overline{\Psi}\epsilon \sum_i \delta(\mathfrak{r}_i(x) - R) \left(\frac{1}{R-a_e} \mathrm{P}_s^{i,j_i} + \frac{1}{R-a_o} \mathrm{P}_t^{i,j_i} \right) \Psi \\ + (1-\epsilon) \left(\sum_{i<j} \int_{D_{ij}} |\partial_i \Psi|^2 + \int \sum_{i<j} v_{ij} |\Psi|^2 \right),\end{aligned} \tag{4.4.8}$$

where $\mathfrak{r}_i(x) = \min_{j\neq i}(|x_i - x_j|)$, $j_i := j$ with $\mathfrak{r}_i(x) = |x_i - x_j|$, is unique a.e., and the nearest neighbor delta interaction can be written $\delta(\mathfrak{r}_i(x) - R) = \left(\sum_{j\neq i} [\delta(x_i - x_j - R) + \delta(x_i - x_j + R)] \right) \mathbb{1}_{\mathfrak{r}_i(\mathfrak{x})\geq R}$. The nearest-neighbor interaction is obtained from Lemma 4.16 in the following manner: For each term in the sum $\sum_i$, fix all particles $x_j \neq x_i$, then divide the integration domain in x_i into Voronoi cells around all remaining particles, and integrate over all Voronoi cells individually.

With the use of Lemma 20 of Chapter 3 with $R > 2|a_e|$ in the last term, and by realizing that the first two terms can be obtained by using ψ as a trial state in the Lieb-Liniger-Heisenberg model [4]

, we obtain

$$\begin{aligned}\int \sum_i |\partial_i \Psi|^2 + \sum_{i\neq j} \frac{1}{2} v_{ij} |\Psi|^2 \geq E_{LLH}^N \left(N, \tilde{L}, \frac{2\epsilon}{R-a_e}, \frac{2\epsilon}{R-a_o} \right) \langle \psi | \psi \rangle \\ + \frac{(1-\epsilon)}{R^2} \text{const. } (1 - \langle \psi | \psi \rangle),\end{aligned}$$

which is the desired result. □

[3] In this case Lemma 20 from Chapter 3 is valid with a replaced by a_e.

[4] To see this, notice that on $\{\sigma\}$ we have

$$\begin{aligned}&= \sum_{(s_1,\ldots,s_N)} \left| \mathrm{P}_{s/t}^{i,j} \Psi((x_{\sigma_1}, s_{\sigma_1}), (R + x_{\sigma_2}, s_{\sigma_2}), \ldots, ((N-1)R + x_{\sigma_N}, s_{\sigma_N})) \right|^2 \\ &= \sum_{(s_1,\ldots,s_N)} \left| \mathrm{P}_{s/t}^{i,j} \psi((x_{\sigma_1}, s_{\sigma_1}), (x_{\sigma_2}, s_{\sigma_2}), \ldots, (x_{\sigma_N}, s_{\sigma_N})) \right|^2 \\ &= \sum_{(s_1,\ldots,s_N)} \left| \tilde{\mathrm{P}}_{s/t}^{i,j} \psi((x_1, s_1), (x_2, s_2), \ldots, (x_N, s_N)) \right|^2\end{aligned}$$

We may also prove the equivalent of Lemma 23 of Chapter 3, by using that $E_{LLH}(N,\tilde{L},c',c) \geq E_{LL}(N.\tilde{L},c')$ when $c > c'$.

Lemma 4.18. *For $n(\rho R)^2 \leq \frac{3}{16\pi^2}\frac{1}{8}$, $\rho R \leq \frac{1}{2}$ and $R > 2\max(|a_e|, a_o, R_0)$ we have*

$$\langle\psi|\psi\rangle \geq 1 - \text{const.}\ \left(n(\rho R)^3 + n^{1/3}(\rho R)^2\right). \tag{4.4.9}$$

Proof. We mimic the proof of Lemma 23 in Chapter 3 ([ARS22]): From the known upper bound, i.e. Theorem 4.2, and by Lemma 4.17 with $\epsilon = 1/2$, it follows that

$$\begin{aligned} &N\frac{\pi^2}{3}\rho^2\left(1 + 2\rho\left(\ln(2)a_e + (1-\ln(2)a_o)\right) + \text{const.}\ (\rho R)^{6/5}\right) \\ &\geq E^N_{LLH}\left(N,\tilde{L},\frac{1}{R-a_e},\frac{1}{R-a_o}\right)\langle\psi|\psi\rangle + \frac{1}{16R^2}(1-\langle\psi|\psi\rangle). \end{aligned} \tag{4.4.10}$$

Subtracting $E^N_{LLH}\left(N,\tilde{L},\frac{1}{R-a_e},\frac{1}{R-a_o}\right)$ on both sides, and using

$$E_{LLH}(N,\tilde{L},c',c) \geq E_{LL}(N.\tilde{L},c'),$$

and Lemma 17 of Chapter 3 on the left-hand side, we find

$$\begin{aligned} &n\frac{\pi^2}{3}\Bigg(\rho^2\left(1 + 2\rho\left(\ln(2)a_e + (1-\ln(2)a_o)\right) + \text{const.}\ (\rho R)^{6/5}\right) \\ &\qquad\qquad - \tilde{\rho}^2\left(1 - 4\tilde{\rho}(R-a_e) - \text{const.}\ n^{-2/3}\right)\Bigg) \\ &\geq \left(\frac{1}{16R^2} - E^N_{LLH}\left(N,\tilde{L},\frac{1}{R-a_e},\frac{1}{R-a_o}\right)\right)(1-\langle\psi|\psi\rangle), \end{aligned} \tag{4.4.11}$$

with $\tilde{\rho} = n/\tilde{\ell} = \rho/(1-(\rho-1/\ell)R)$.
Using the upper bound $E^N_{LLH}\left(N,\tilde{L},\frac{1}{R-a_e},\frac{1}{R-a_o}\right) \leq n\frac{\pi^2}{3}\tilde{\rho}^2$ on the right-hand side, as well as $2\rho \geq \tilde{\rho} \geq \rho(1+\rho R)$, we find

$$\text{const.}\ n\rho^2R^2\left(\rho R + (\rho R)^{6/5} + n^{-2/3}\right) \geq \left(\frac{1}{16} - R^2 n\frac{4\pi^2}{3}\rho^2\right)(1-\langle\psi|\psi\rangle). \tag{4.4.12}$$

It follows that we have

$$\langle\psi|\psi\rangle \geq 1 - \text{const.}\ \left(n(\rho R)^3 + n^{1/3}(\rho R)^2\right). \tag{4.4.13}$$

□

We continue the generalizations from Chapter 3 and prove the following equivalent of Proposition 24 of Chapter 3:

Proposition 4.19. *For $n(\rho R)^2 \leq \frac{3}{16\pi^2}\frac{1}{8}$, $\rho R \leq \frac{1}{2}$ and $R > 2\max(|a_e|, a_o, R_0)$ we have*

$$E^N(N,L) \geq E^N_{LLH}\left(N, \tilde{L}, \frac{2}{R-a_e}, \frac{2}{R-a_o}\right) \times \left(1 - \text{const.}\left(n(\rho R)^3 + n^{1/3}(\rho R)^2\right)\right). \tag{4.4.14}$$

Proof. This follow by using Lemma 4.17 with $\epsilon = 1$ and 4.18. □

We now see that this is where the strategy of Chapter 3 is obstructed. The obstruction lies with the Lieb-Liniger-Heisenberg model not being Yang-Baxter solvable, meaning that the Bethe ansatz approach no longer gives exact solutions for the eigenvalue problem, as the Yang-Baxter equation is no longer satisfied. This being said, there is still hope that one might obtain a tight lower bound for the ground state energy of the Lieb-Linger-Heisenberg model in the dilute limit. We may even conjecture such a lower bound:

Conjecture 4.20. *Let E_{LLH} denote the ground state energy of the Lieb-Liniger-Heisenberg model* (4.3.9)*. Then we have*

$$E_{LLH} \geq N\frac{\pi^2}{3}\rho^2\left(1 - 4\rho\left(\frac{\ln(2)}{c'} + \frac{1-\ln(2)}{c}\right)\right). \tag{4.4.15}$$

We that this conjecture is in line with both the Lieb-Liniger scenario, $c = c'$, and the Yang-Gaudin scenario, $c = \infty$. The validity of Conjecture 4.20, would give us the desired lower bound in Proposition 4.19. In the following subsection, we will give some heuristics for such a lower bound.

The Lieb-Liniger-Heisenberg Ground State Energy: Heuristics

In this subsection, we give only heuristic arguments for a lower bound of the Lieb-Liniger-Heisenberg (LLH) ground state energy, E_{LLH}. We do not claim the arguments given to be rigorous. For simplicity, we restrict to having periodic boundary conditions.

Degenerate perturbation theory

The first natural approach to estimating E_{LLH}, is to do first-order perturbation theory. To do this let is rewrite the LLH Hamiltonian (4.3.9) on the sector $\{1, 2, \ldots, N\}$ as follows

$$H = -\sum_{i=1}^{N} \partial_i^2 + 2 \sum_{1 \leq i \leq N} \left(\frac{c' + 3c}{4} + (c - c') S_i \cdot S_{i+1} \right) \delta(x_i - x_{i+1}), \quad (4.4.16)$$

with $c > c'$. We restrict to the regime $c, c' \gg \rho$, $\frac{c-c'}{c'} \ll 1$, i.e. the perturbative dilute regime. We consider $H_0 = -\sum_{i=1}^{N} \partial_i^2 + 2 \sum_{1 \leq i \leq N} \frac{c'+3c}{4} \delta(x_i - x_{i+1})$ the "unperturbed" Hamiltonian, which is a Lieb-Liniger (LL) model with coupling $\tilde{c} = \frac{c'+3c}{4}$. This model is of course, due to the presence of spin, degenerate (with finite multiplicity). The Perturbation is then

$$H' = 2 \sum_{1 \leq i \leq N} \left((c - c') S_i \cdot S_{i+1} \right) \delta(x_i - x_{i+1}).$$

We restrict to analyzing the problem on the sector $\{1, 2, \ldots, N\}$, since all other sectors are related by symmetry. In this case first-order (finitely degenerate) perturbation theory, [RS78], dictates that the perturbed eigenvalue is approximated by

$$E_{LLH} \approx E_{LL}(\tilde{c}) + \inf_{\chi \in \text{spin states}} \left\langle \Psi_{LL}^{\tilde{c}} \chi \left| H' \right| \Psi_{LL}^{\tilde{c}} \chi \right\rangle, \quad (4.4.17)$$

with $\Psi_{LL}^{\tilde{c}}$ begin the LL ground state at coupling $\tilde{c}$. For the Lieb-Liniger model, we have by the Feynman-Hellmann theorem and translation invariance

$$\left\langle \Psi_{LL}^{\tilde{c}} \left| \delta(x_i - x_{i+1}) \right| \Psi_{LL}^{\tilde{c}} \right\rangle = \frac{1}{N} \frac{\partial}{\partial \tilde{c}} E_{LL}(\tilde{c}). \quad (4.4.18)$$

Therefore, it follows that we have

$$E_{LLH} \approx E_{LL}(\tilde{c}) + \frac{c - c'}{N} \frac{\partial}{\partial \tilde{c}} E_{LL}(\tilde{c}) \inf_{\chi \in \text{spin states}} \left\langle \chi \left| \sum_{i=1}^{N} S_i \cdot S_{i+1} \right| \chi \right\rangle \quad (4.4.19)$$

and by Lemma 4.11, we find

$$\begin{aligned} E_{LLH} &\approx E_{LL}(\tilde{c}) + (c-c')\frac{\partial}{\partial \tilde{c}} E_{LL}(\tilde{c}) \left(\frac{1}{4} - \ln(2)\right) \\ &\approx N\frac{\pi^2}{3}\rho^2 \left(1 - \frac{4\rho}{\tilde{c}}\left[1 - \left(\frac{1}{4} - \ln(2)\right)\frac{c-c'}{\tilde{c}}\right]\right) \\ &\approx N\frac{\pi^2}{3}\rho^2 \left(1 - \frac{4\rho}{\tilde{c}^2}\left[\frac{1}{4}c' + \frac{3}{4}c - \left(\frac{1}{4} - \ln(2)\right)(c-c')\right]\right) \\ &\approx N\frac{\pi^2}{3}\rho^2 \left(1 - \frac{4\rho}{\tilde{c}^2}\left[\left(\frac{1}{2} - \ln(2)\right)c' + \left(\frac{1}{2} + \ln(2)\right)c\right]\right) \end{aligned} \tag{4.4.20}$$

Now by Taylor expanding in c' around c we find

$$E_{LLH} \approx N\frac{\pi^2}{3}\rho^2 \left(1 - 4\rho\left(\frac{\ln(2)c'}{c^2} + \frac{1-\ln(2)}{c}\right)\right) \tag{4.4.21}$$

which agrees with Conjecture 4.20.

Lower bound by adding space Consider the two particle case. By translation invariance we expect the ground state to depend only on the distance between the two particles, $x_1 - x_2$, and by spatial symmetry, we may further restrict to $|x_1 - x_2|$. Now we may define new coordinates on the sector $\{1,2\}$ given by $y_1 = x_1$, $y_2 = x_2 + \mathfrak{r}$. Let $\Psi(|x_1 - x_2|)$ denote the LLH ground state, then we may define the extended state $\tilde{\Psi}(|y_1 - y_2|) = \Psi(|y_1 - y_2 + \mathfrak{r}|)$, when $y_2 > y_1 + \mathfrak{r}$, and extended to the whole $[0, L + \mathfrak{r}]$ by $\mathrm{P}_t\,\tilde{\Psi}(r) = \mathrm{P}_t\,\Psi(0)\left(1 - \frac{c}{2}r\right)$ and $\mathrm{P}_s\,\tilde{\Psi}(r) = \mathrm{P}_s\,\Psi(0)\left(1 - \frac{c'}{2}r\right)$ for $r < \mathfrak{r}$. Notice that we defined Ψ such that we have the boundary conditions $2\,\mathrm{P}_t\,\Psi'(0_+) = (\partial_2 - \partial_1)\,\mathrm{P}_t\,\Psi|_{x_2 = x_{1+}} = c\,\mathrm{P}_t\,\Psi(0)$ and $2\,\mathrm{P}_s\,\Psi'(0_+) = (\partial_2 - \partial_1)\,\mathrm{P}_s\,\Psi|_{x_2 = x_{1+}} = c'\,\mathrm{P}_s\,\Psi(0)$. With this definition, we see that

$$2\int_0^{L+\mathfrak{r}} \left|\mathrm{P}_t\,\tilde{\Psi}'(r)\right|^2 \mathrm{d}r + \tilde{c}\left|\mathrm{P}_t\,\tilde{\Psi}(0)\right|^2 = 2\int_0^{L} \left|\mathrm{P}_t\,\Psi'(r)\right|^2 \mathrm{d}r + c\left|\mathrm{P}_t\,\Psi(0)\right|^2 \tag{4.4.22}$$

If $\frac{1}{2}c^2\mathfrak{r}\left|\Psi(0)\right|^2 + \tilde{c}\left|\Psi(0)\right|^2\left(1 - \frac{c}{2}\mathfrak{r}\right)^2 = c\left|\Psi(0)\right|^2$, that is $\tilde{c} = \frac{c}{1-\frac{c}{2}\mathfrak{r}}$. And similarly, we find

$$2\int_0^{L+\mathfrak{r}} \left|\mathrm{P}_s\,\tilde{\Psi}'(r)\right|^2 \mathrm{d}r + \tilde{c}'\left|\mathrm{P}_s\,\tilde{\Psi}(0)\right|^2 = 2\int_0^{L} \left|\mathrm{P}_s\,\Psi'(r)\right|^2 \mathrm{d}r + c'\left|\mathrm{P}_s\,\Psi(0)\right|^2 \tag{4.4.23}$$

if $\tilde{c}' = \frac{c'}{1-\frac{c'}{2}\mathfrak{r}}$. Now of course we have $\left\|\tilde{\Psi}\right\| > \|\Psi\|$, so by using $\tilde{\Psi}$ as a trial state for $H_{LLH}^{\tilde{c}',\tilde{c}}$, i.e. the LLH model with couplings $\tilde{c}'$ and $\tilde{c}$, we find

$E_{LLH}(2,L,c',c) \geq E_{LLH}(2,L+\mathfrak{r},\tilde{c}',\tilde{c}) = E_{LLH}\left(2,L+\mathfrak{r},\frac{2}{\frac{2}{c'}-\mathfrak{r}},\frac{2}{\frac{2}{c}-\mathfrak{r}}\right)$. We may choose $\mathfrak{r}=\frac{2}{c}$, in which case we find

$$\begin{aligned} E_{LLH}(2,L,c',c) &\geq E_{LLH}\left(2,L+\frac{2}{c},\left(\frac{1}{c'}-\frac{1}{c}\right)^{-1},\infty\right) \\ &= E_{YG}\left(2,L+\frac{2}{c},\left(\frac{1}{c'}-\frac{1}{c}\right)^{-1}\right) \\ &\geq 2\frac{\pi^2}{3}\rho^2\left(1-2\rho\left[\ln(2)\left(\frac{1}{c'}-\frac{1}{c}\right)+\frac{1}{c}\right]\right) \end{aligned} \tag{4.4.24}$$

where we used Proposition 2.48, and recall that the last inequality strictly speaking is conjecture (see Subsection 2.6).

4.5 Lower Bound for Other Symmetries

Recall the Corollaries 4.12, 4.13, and 4.14. For these, we may in some cases prove a lower bound. This is always the case for the bosonic case, and exactly the case when $a_o \leq a_e$ in the spin-dependent fermionic case, and when $a_t \leq a_s$ in the spin dependent spatially symmetric case. Hence we have

Theorem 4.21. *Consider a spin–1/2 Bose gas with repulsive interaction $v = v_{\text{reg.}} + v_{\text{h.c.}}$ as defined above. Then there exists a constant $C_L > 0$ such that the ground state energy $E^N(N,L)$ satisfies*

$$E^N(N,L) \geq N\frac{\pi^2}{3}\rho^2\left(1+2\rho a_e - C_L\left((\rho R)^{6/5}+N^{-2/3}\right)\right). \tag{4.5.1}$$

$R = \max(|a_e|, R_0)$

Proof. This follows simply from the fact that the spin–1/2 bosonic ground state energy is greater than or equal to the spinless bosonic ground state energy and hence from Proposition 15 in Chapter 3. □

Theorem 4.22. *Consider a spin–1/2 Fermi gas with repulsive interaction $v = v_e\,\mathrm{P}_s + v_o\,\mathrm{P}_t$. Assume furthermore that $a_o \leq a_e$. Then there exists a constant $C_L > 0$ such that the ground state energy $E^N(N,L)$ satisfies*

$$E^N(N,L) \geq N\frac{\pi^2}{3}\rho^2\left(1+2\rho a_o - C_L\left((\rho R)^{6/5}+N^{-2/3}\right)\right). \tag{4.5.2}$$

Here $R = \max(|a_e|, a_o, R_0)$

Proof. This follows from Proposition 4.19 (the proof hold regardless of the more general potential), and from the fact that for $a_o \leq a_e$, we have

$$E^N_{LLH}\left(N, \tilde{L}, \frac{2}{R-a_e}, \frac{2}{R-a_o}\right) \geq E^N_{LL}\left(N, \tilde{L}, \frac{2}{R-a_o}\right)$$

. The remainder of the proof is identical to the proof of Chapter 3 from Proposition 24 of Chapter 3 and down. □

Theorem 4.23. *Consider a spin–*1/2 *spatially symmetric gas with repulsive interaction* $v = v_s \tilde{\mathrm{P}}_s + v_t \tilde{\mathrm{P}}_t$. *Assume furthermore that* $a_t \leq a_s$. *Then there exists a constant* $C_L > 0$ *such that the ground state energy* $E^N(N, L)$ *satisfies*

$$E^N(N, L) \geq N\frac{\pi^2}{3}\rho^2\left(1 + 2\rho a_t - C_L\left((\rho R)^{6/5} + N^{-2/3}\right)\right). \tag{4.5.3}$$

Here $R = \max(|a_s|, |a_t|, R_0)$

Proof. This follows from Proposition 4.19 (the proof hold regardless of the more general potential and different symmetry), and from the fact that for $a_t \leq a_s$, we have

$$E^N_{LLH}\left(N, \tilde{L}, \frac{2}{R-a_s}, \frac{2}{R-a_t}\right) \geq E^N_{LL}\left(N, \tilde{L}, \frac{2}{R-a_t}\right)$$

. The remainder of the proof is identical to the proof of Chapter 3 from Proposition 24 of Chapter 3 and down. □

We see that combining these results with the Corollaries 4.12, 4.13, and 4.14 we obtain ground state energy expansions to next-to-leading order in the diluteness parameter in all these cases.

Chapter 5

Conclusion and Outlook

In this chapter, we summarize both the findings of this thesis and questions that are left open.

5.1 Conclusion

In Chapter 2, we started by reviewing basic many-body quantum mechanics. Here we defined relevant systems and quantities. We also proved results on the generality of the potentials that would be *allowed* for the energy quadratic form to be associated with a unique self-adjoint Hamiltonian. In particular, we showed that in one dimension potentials of the form $v = v_{\sigma\text{–finite}} + v_{\text{meas.}} + c\delta_0$ with $c \in \{0, \infty\}$, were allowed. We then proceeded by reviewing the *scattering length* and known results on *dilute* quantum systems in dimensions two and three. We also revisited the bosonic and fermionic one-dimensional point interacting models, i.e. the Lieb-Liniger model and the Yang-Gaudin model. For the Yang-Gaudin model, we proved a lower bound on the thermodynamic ground state (within the Yang-Bethe ansatz states).

Chapter 3 consisted of a preprint written in collaboration with Robin Reuvers and Jan Philip Solovej. Here we proved matching upper and lower bounds on the ground state energy of the one-dimensional dilute Bose gas, resulting in a next-to-leading order ground state energy expansion. As a corollary, we found a ground state energy expansion for spinless or equivalently spin polarized (spin-aligned) fermions as well. Finally, as another corollary, we found the ground state energy expansion for a one-dimensional dilute gas of anyons. Interestingly, the expansions we found in one dimension exhibit

universality, as is the case in dimensions two and three. However, in one dimension, the error must depend on the range of the potential, as the scattering length may vanish. The one-dimensional expansion also suggests that no Bose-Einstein condensate is formed. This is evident in the proof, where the formation of a Bose-Einstein condensate is absent both in the low-energy trial state and in the lower-bounding Lieb-Liniger model. The ground state energy expansion also appears to resemble a perturbed Fermi sea, rather than a perturbed condensate, as the leading order term is equal to the free Fermi energy.

In Chapter 4, we generalized some of the results obtained in Chapter 3 to the spin–1/2 Fermi gas, and to other symmetries or spin-dependent potentials. Most noteworthy, we proved an upper bound, which we conjectured to be tight based on the solvable models at hand. This upper bound exhibits the same universality as was found for the Bose or spin polarized Fermi gases. Perhaps even more interestingly, the upper bound seemed connected with magnetism in terms of the Heisenberg chain. For spin–1/2 fermions, with $a_o \geq a_e$, we found that the energy of the variational trial state was related to the antiferromagnetic (Heisenberg chain) energy of the spin part on an ordered sector. Thus the optimal spin part of the variational trial state on a sector was shown to be the antiferromagnetic Heisenberg ground state. Phrased differently, the energy of the variational trial state was shown to be determined by an effective Heisenberg chain model. For other symmetries or spin-dependent potentials, both the ferro- and antiferromagnetic Heisenberg chains were shown to be effective models for the energy of the variational trial state.
We then proceeded in Chapter 4 by motivating a matching lower bound for the ground state energy of the spin–1/2 fermions. We generalized in this case certain results from Chapter 3. However, the lower bounding model in these generalizations was shown to be the Lieb-Liniger-Heisenberg model. We stated a conjecture about the ground state energy of this model in the antiferromagnetic phase that, if proven true, implies a rigorous lower bound on the one-dimensional dilute spin–1/2 Fermi gas. This conjecture was further motivated by heuristic arguments, but never proven. Finally, we noted that for certain different symmetries of the domain and properties of the interaction potential or certain spin-dependent interaction potentials, the lower bounding (ferromagnetic) Lieb-Liniger-Heisenberg model admits a tight lower bound by a Lieb-Liniger model. This reduced the completion of the lower bound proof

to the case of Chapter 3. Hence for these symmetries and potentials, and spin-dependent potentials, we obtained a lower bound, matching the upper bound already found previously.

5.2 Outlook and Open Problems

In the making of this thesis, we have encountered some problems which are, at the time of writing, still left open. We give an overview of these problems here:

- The first problem, which, to the best of our knowledge, seems to have been left open in the literature, is proving that the ground state of the Yang-Gaudin model is among the Yang-Bethe ansatz states. Furthermore, a proof of the existence of solutions to the equations (2.6.19)–(2.6.22) seems also to be absent. Solving this problem appears to be a key ingredient in giving a rigorous proof of Conjecture 4.20 and thus, this may be a step in the direction of proving Conjecture 4.1.

- The proof of Conjecture 4.1. We have already identified a possible strategy by proving Conjecture 4.20. However, one may also consider following entirely different strategies.

- Conjecture 4.20, was heuristically motivated but ultimately left open. Given a solution to the first open problem above, we showed in Chapter 4 that the conjecture, in the case of two particles, can be proved by adding space and reducing the model to a Yang-Gaudin model. This may be a strategy for more than two particles as well, if one can suitably generalize the methods. It may also be possible to prove the conjecture in certain regimes of the couplings c', c by making degenerate perturbation theory rigorous.

Some of the content in this thesis also open up the possibility of pursuing new results in the future. We list some of these in the following:

- Finding the next order term in the ground state energy expansion. Although we obtain ground state energy expansions to next-to-leading order (first order in the diluteness parameter) in the bosonic case, the solvable models seem to suggest that the expansion may be valid even to second order in the diluteness parameter.

- Giving an approximate momentum distribution of the ground states of dilute quantum gases in one dimension. In Chapter 3 it was briefly touched upon in (1.24) and (1.25) of Chapter 3 that the momentum distributions of these ground states are predicted to exhibit some universality as well.

- Making rigorous the effective Heisenberg chain model for spin-1/2 fermions (and the other symmetries and spin-dependent potential analyzed in Chapter 4). In the upper bound proof, this effective model was evident. Similarly, such effective models are predicted for point interacting models in one dimension in recent physics literature [YC16, VPV$^+$15].

- Generalizing the results of Chapter 4 to higher spin. For higher spin, the upper bound from Chapter 4 seems to have a straightforward generalization. However, we have no intuition for whether this bound is still tight. To answer this, one may start by lower bounding the Yang-Gaudin ground state energy for higher spin models.

Appendix A

Upper Bound with Periodic Boundary Conditions

If we, in the upper bound for spin–1/2 fermions, consider the case with periodic boundary conditions in the box, one may actually, without the assumption of translation invariance on χ, show that the antiferromagnetic Heisenberg ground state, is the optimal spin state in the trial state. Starting from (4.2.12), where no properties of χ have been used, we find, using translation invariance of $(\Psi_{e/o})_{12}$,

$$\begin{aligned}\int_{B_{12}^{\geq}} |\partial_i \Psi_\chi|^2 \leq & \left(\int_{A_{12}\cap\{1,2,\ldots,N\}} |\partial_i (\Psi_e)_{12}|^2 \right) \sum_{\{\sigma\}\in S_{12}} \left\langle \chi_\sigma \left| \mathrm{P}_s^{1,2} \right| \chi_\sigma \right\rangle \\ & + \left(\int_{A_{12}\cap\{1,2,\ldots,N\}} |\partial_i (\Psi_o)_{12}|^2 \right) \sum_{\{\sigma\}\in S_{12}} \left\langle \chi_\sigma \left| \mathrm{P}_t^{1,2} \right| \chi_\sigma \right\rangle \\ = & 2(N-2)! \left(\int_{A_{12}\cap\{1,2,\ldots,N\}} |\partial_i (\Psi_e)_{12}|^2 \right) \sum_{k=1}^{N} \left\langle \chi \left| \mathrm{P}_s^{k,k+1} \right| \chi \right\rangle \\ & + 2(N-2)! \left(\int_{A_{12}\cap\{1,2,\ldots,N\}} |\partial_i (\Psi_o)_{12}|^2 \right) \sum_{k=1}^{N} \left\langle \chi \left| \mathrm{P}_t^{k,k+1} \right| \chi \right\rangle . \end{aligned} \tag{A.0.1}$$

Using now that

$$2(N-2)!N \int_{A_{12}\cap\{\ldots,1,2,\ldots\}} \left| \partial_i (\Psi_{e/o})_{12} \right|^2 \leq \int_{A_{12}} \left| \partial_i (\Psi_{e/o})_{12} \right|^2 , \tag{A.0.2}$$

equation (4.2.13) follows. But from (4.2.13) it is clear that the antiferromagnetic Heisenberg ground state is optimal. Thus we circumvented the use of translation invariance of χ.

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