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PhD thesis

One Dimensional Dilute Quantum Gases and Their Ground State Energies

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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, to set up the mathematical framework, and to 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 1. *A quantum system at 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 quantum system consisting of N particles in a region $\Omega \subseteq \mathbb{R}^d$, possibly with spin degrees of freedom $\{S_i\}_{i\in 1,\dots,N}$. We refer to d as the *dimension* of the system. Such a system is described by having

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

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 turn out that one can restrict the underlying Hilbert space, to have certain symmetries. Considering N indistinguishable particles, we restrict to the physical configuration space to $C_{p,N} = C_N/S_N$, 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 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. *For $d \geq 3$ we have $\pi_1(C_{p,N}) = S_N$, for $d = 2$ we have $\pi_1(C_{p,N}) = B_N$ and for $d = 1$ we have $\pi_1(C_{p,N}) = \{1\}$. In the somewhat special case of $d = 1$, $C_{p,N} = \{x_1 < x_2 < \ldots < x_N\}$. On 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 (see section below) on this space. In section ... we will see examples of different particle statistics in one dimension.*

Remark 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 $\sigma = (\sigma_1, \ldots, \sigma_N) \in \{-S, \ldots, S\}^N$ the configurations spaces $C_{p,N,\sigma} = \{((x_1, \sigma_1), \ldots, (x_N, \sigma_N)) \in (\Omega \times \{-S, \ldots, S\})^N | x_i \neq x_j \text{ if } i \neq j\}$ are path connected and their fundamental groups are isomorphic to the fundamental group in the spinless case independent of σ.*
Alternatively, one can view the wave function as a $(2S+1)^N$-dimensional vector bundle over the physical (spinless) configuration space.

In the remaining part of 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 4. *A quantum system of N spin–S bosons in $\Omega\subseteq\mathbb{R}^d$ at fixed time is a pair*

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

where $\mathcal{H}=L^2_s\left((\Omega\times\{-S,\ldots,S\})^N\right)\cong\vee_{i=1}^N L^2\left(\Omega;\mathbb{C}^{2S+1}\right)$.

Definition 5. *A quantum system of N spin–S fermions in $\Omega\subseteq\mathbb{R}^d$ at fixed time is a pair*

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

where $\mathcal{H}=L^2_a\left((\Omega\times\{-S,\ldots,S\})^N\right)\cong\wedge_{i=1}^N L^2\left(\Omega;\mathbb{C}^{2S+1}\right)$.

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 to $\mathcal{O}$ by the spectral theorem [RS81], the probability of a measurement of $\mathcal{O}$ in state $\Psi\in\mathcal{D}(\mathcal{O})$ having outcome $\lambda\in M\subset\mathbb{R}$ is given by $P\left((\mathcal{O},\Psi)\to\lambda\in M\right)=\int_{\lambda\in M}\langle\Psi,P_\lambda\Psi\rangle$. Furhtermore we defined the expected value of an observable.

Definition 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 to $\mathcal{O}$ by the spectral theorem.

I the previous section we defined a quantum system at a fixed time. However, we are often interested in 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 have set $\hbar = 1$.

Remark 7. *By Stone's theorem (ref Reed and Simon), the existance 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.* Since H is lower bounded, there is a natural notion of lowest energy of H.

Definition 8. *The **ground state energy** of H is defined by*

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

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

Definition 9. *We say that a (normalized) state $\Psi \in \mathcal{D}(H) \subset \mathcal{H}$ is a **ground state** of H if*

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

When studying ground states and ground state energies it is useful to have the following variational characterization.

Remark 10. *It follows from the spectral theorem (ref Reed and Simon) that the ground state energy is given by*

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

Remark 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 12. *Given a Hamiltonian, H, we define the* ***associated energy quadratic form****, $\mathcal{E}_H : \mathcal{D}(\mathcal{E}_{\mathcal{H}}) \to \mathbb{R}$, 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 13. *From the definition of $\mathcal{E}_{\mathcal{H}}$ and from Remark 10 it follows straightforwardly that we have*

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

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

We refer to both (2.2.1) and (2.2.2) as *the variational principle*. We will often in the remaining take (2.2.2) as the vary 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 14 (Ref!!)**.** *Given a densely defined, lower bounded, closable, quadratic form $\mathcal{E} : \mathcal{D}(\mathcal{E}) \to \mathbb{R}$ there exist 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 change between the two equivalent formulations of the dynamics of a quantum system that are 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 seen, 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 remaining of this subsection we will ignore spin, knowing 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

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

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 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

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

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 extensions of the symmetric *formal* Hamiltonian. Now some models of stronger interactions, *e.g.* the hard core interaction, requires 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 15. *For a system of N bosons/fermions in region $\Omega \in \mathbb{R}^d$, we define for $\sigma \in [0, \infty]$* ***the energy quadratic forms***

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

[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

with domain $\mathcal{D}\left(\mathcal{E}_{(v,\sigma)}\right) = \{\Psi \in (C_0^\infty(\Omega^N))_{b/f} | \mathcal{E}_{(v,\sigma)}(\Psi) < \infty\}$. *with* $(C_0^\infty(\Omega^N))_{b/f}$ *meaning the bosonic/fermionic subspace of* $C_0^\infty(\Omega^N)$. $\sigma = \infty$ *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 not be neither densely defined nor closable on $L^2_{s/a}(\Omega^N)$. However, it will both 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 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 17. *There are plenty of allowed potentials, but the notion does depend on the dimension, d. For example is $v = \delta_0$,* i.e. *the delta function potential, 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 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. (Ref!!)*

Remark 18. *For any radial $v \geq 0$ that is measurable $\mathcal{E}_{(v,\sigma)}$ is the quadratic form associated to 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 on $\mathcal{H}_{(v,\sigma)}$. Thus closability of $\mathcal{E}_{(v,\sigma)}$ amount 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* $H_{(v,\sigma)} = -\sum_{i=1}^N \Delta_i + \sum_{1\leq i<j\leq N} v(x_i - x_j)$.

The argument from the previous may be generalized slightly in the case of $d = 1$, in order to show that any σ–finite measure $v\,\mathrm{d}\lambda^N$ is allowed as potential. Notice that we slightly abuse notation and write $v(x_i - x_j)\,\mathrm{d}\lambda^N$ even when v is a singular continuous 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 $\mathrm{d}\mu_{v_{ij}} := v(x_i - x_j)\,\mathrm{d}(x_i - x_j)$ and $\lambda^{N-1}_{(x_i - x_j) = \text{ fixed}}$ to be the measure such that $\mathrm{d}\lambda^N = \mathrm{d}(x_i - x_j) \times \mathrm{d}\lambda^{N-1}_{(x_i - x_j) = \text{ fixed}}$. Uniqueness of the product measure is guaranteed by σ-finiteness of v. We will need the following essential lemma, where we use the notation $\lambda_k^{N-1} := \prod_{i \neq k} \mathrm{d}x_i$

Lemma 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 $f_n^k(t, \overline{x}^k) := f_n(x_1, \dots, x_{k-1}, t, x_{k+1}, \dots, x_N)$ for any $k = 1, \dots, N$, 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 $k = 1, \dots, N$.*

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 $k = 1, \dots, N$ 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 of $g_n^k(\overline{x}^k) := \left\|f_n^k(\cdot, \overline{x}^k)\right\|_{H^1(\Omega)}$. Clearly g_n^k constitute L^2 functions, with norms converging to 0. Hence there exist a subsequence that converges pointwise λ_k^{N-1}–almost everywhere to 0. Then there is a subsequence $f_{n_i}^k$ 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. □

Using this lemma, we may prove the following Proposition

Proposition 20. *Let $d = 1$, then for any σ-finite measure, v, we have that $\mathcal{E}_{(v,\sigma)}$ is the quadratic form associated to a 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 $\mathrm{d}\mu_v = \sum_{1\le i<j\le N} v(x_i - x_j)\,\mathrm{d}\lambda^N$. 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 $(\psi_n)_{n\in\mathbb{N}} \subset L^2\left(\Omega^N, \mathrm{d}\mu_v\right)$ 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 λ^N–almost everywhere to 0. However, since $(\psi_n)_{n\in\mathbb{N}}$ converges to 0 in $H^1(\Omega^N, \mathrm{d}\lambda^N)$, Lemma 19 implies that for $(x_i - x_j)$ fixed $(\psi_n)_{n\in\mathbb{N}}$ converges λ^{N-1}–a.e. to 0. Hence $(\psi_n)_{n\in\mathbb{N}}$ converges pointwise to 0 on λ^{N-1}–almost all lines. Now notice that $\mathrm{d}\mu_v = \sum_{1\leq i<j\leq N} \mathrm{d}\mu_{v_{ij}} \times \mathrm{d}\lambda^{N-1}_{(x_i-x_j)=\text{ fixed}}$. Thus for $\lambda^{N-1}_{(x_i-x_j)=\text{ fixed}}$–almost all lines in Ω^N with $x_i + x_j$ and x_k fixed for all $k \neq i, j$, by passing to a subsequence ψ_n converges pointwise to 0, by Lemma 19. But also on $\lambda^{N-1}_{(x_i-x_j)=\text{ fixed}}$–almost all these lines ψ_n converges $\mu_{v_{ij}}$–almost everywhere to f, and hence $f = 0$ $\mu_{v_{ij}}$–almost everywhere. Thus we conclude that $f = 0$ μ_v–almost everywhere. The lemma now follows from Remark 14. □

Remark 21. *Combining Lemma 20 and Remark 18 we conclude that potentials of the form $v = v_{\sigma\text{–finite}} + v_{abs.cont.}$, where $v_{\sigma\text{–finite}}$ is a σ–finite measure and $v_{abs.cont.}$ is an absolutely continuous measure (w.r.t. Lebesgue measure) are allowed in one dimension, $d = 1$. We will in Chapter.... obtain result about the ground state energy of such systems.*

Remark 22. *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 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 of important throughout the thesis, and 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 makes sense, *i.e.* when it is *allowed*. Let $R_0 > 0$ be such that $\operatorname{supp}(v) \subset B_{R_0}$. Many assumptions on v can be weakened, but these conditions are sufficient for the scope of this thesis. The formal Hamiltonian can be written

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

For now we keep the masses, but we will be mostly interested in the case $m_1 = m_2 = 1/2$. Defining the center of mass coordinate $X = (m_1 x_1 + m_2 x_2)/(m_1 + m_2)$ and the relative coordinate $y = x_1 - x_2$, we see that the kinetic energy may be rewritten

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

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

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

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 nearby? The answer is affirmative, which can be seen

by the following:
Consider the (R-local, relative) energy functional

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

with $R > R_0$. Then we have

Theorem 23 (Theorem A.1 in [LY01]). *Let $R > R_0$ then in the class of functions*

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

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

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

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

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

$$f_0(r) = \begin{cases} 1/\mu(R-a) & \textit{for } d = 1 \\ \pi/[\mu \ln(R/a)] & \textit{for } d = 2 \\ \pi^{n/2} a/[\mu\Gamma(n/2)(1 - aR^{2-n})] & \textit{for } d = 3. \end{cases} \tag{2.3.7}$$

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.
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 mostly interested in different kinds of scattering lengths in dimension $d = 1$, where the masses $m_1 = m_2 = 1/2$. Thus we define the scattering lengths of interest:

Definition 24. *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 25. *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 26. *We did not prove uniqueness of the solutions above. In Definition 24, it follows from Theorem 23 by noting that any solution of (2.3.8) is a minimizer of $\mathcal{E}_R$. In Definition 25 it follows from the fact that by Theorem 23 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 27. *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 28. *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 29. *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 the* v, *does not change the scattering solution from the* $v = 0$ *case, and we have* $f_o(x) = \frac{x}{R}$ *and we conclude* $a_o = 0$.

Example 30. *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 Bose Gases

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

Definition 31. *For the d-dimenional* ($d = 1, 2, 3$) *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 32. *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* $\rho \max(||a_e|, a_o|) \ll 1$.

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

In the 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 in known as *Bethe ansatz* or *Bethe's hypothesis* after it was invented by Bethe to solve the one dimensional antiferromagnetic 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 with dynamics given by the Hamiltonian

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

where the left-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 from elliptic regularity, ([Gri11], Theorem 3.2.3.1), the domain is given by

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

The Bethe ansatz then prescribes that we, on a sector $\{1, 2, \ldots, N\}$, seek solution 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 $a(P) \in \mathbb{C}$ suitably chosen coefficients. 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

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

We note that we will 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

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

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 $P := \sum_{i=1}^{N} k_i$ 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 set $(k_i' = k_i + 2\pi n_0/L)_{i\in\{1,\ldots,N\}}$ solves it as well. This corresponds to changing the total momentum by $P' = P + 2\pi n_0 \rho$, with $\rho := N/L$. Thus we may restrict to finding all solutions with $-\pi\rho < P \leq \pi\rho$, 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 $-\pi\rho < P \leq \pi\rho$ 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 ground state

It is clear that within the set of ansatz states, variational ground state must have $n_i = 1$ for all $i = 1, \dots, N-1$. In this case we have by symmetry and uniqueness of the ground state that $k_i = -k_{N-i}$ and since $P = \sum_{i=1}^{N} k_i = Nk_1 + \frac{1}{L}\sum_{j=1}^{N-1}(N-j)\delta_j = 0$ we find $k_1 = -\frac{1}{NL}\sum_{j=1}^{N-1}(N-j)\delta_j = -k_N$.

We may also ask whether the true ground state is attained among these ansatz states. This turn out to be the case, which may be seen by the following result.

Lemma 33. *Let Ψ_V and Ψ_T be the variational (in the Bethe ansatz class) and true ground state of H_{LL}, respectively, then $\Psi_V(x) = e^{i\phi}\Psi_T(x)$, for a constant $\phi \in [0, 2\pi)$.*

Proof. Consider first the limit $c \to \infty$. Here it is easily verified that $\Psi_V = |\Psi_F| = \Psi_T$, where Ψ_F is the free Fermi ground state, *i.e.* a Slater determinant state and that $E_V = E_T = E_F$, where E_F is the free Fermi energy. Now by uniqueness of the bosonic ground state and continuity of the (variational) ground state energy in $1/c$, as well as the fact that Ψ_V is an eigenstate, we conclude that the variational ground state must remain the true ground state, as $1/c$ varies. Were this not the case, would the true ground state Ψ_T at finite $c > 0$ be orthogonal to Ψ_V, and hence they would converge to orthogonal states, contradiction uniqueness in the limit. □

We note that while Lemma 33 holds for the ground state, its proof cannot be generalized to exited states, since there is no unique nth exited 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].

Interestingly, it is possible to study the thermodynamic limit ($N, L \to \infty$ with $N/L = \rho$) of 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)

$$\rho^3 e(\gamma) := \lim_{\substack{N,L\to\infty \\ N/L=\rho}} \frac{1}{L} E_N. \tag{2.5.9}$$

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 by Poisson's summation formula we have

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

The very definition of f implies $\int_{-K}^{K} f(p)\,\mathrm{d}p = \rho$, with ground state energy

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

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

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

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

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

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

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

The first equation is an inhomogeneous Fredholm equation of the second kind which is solved by the Liouville-Neumann series.

Proposition 34. *Let E_c denote the ground state energy of H_{LL} with coupling $c > 0$. Then $\lim_{c\to\infty} E_c = E_F$, where E_F is the free Fermi ground state energy.*

Proof. By going to the quadratic form representation of H_{LL} 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 Ψ_{c_n} is, by possibly passing to a subsequence, weakly convergent 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 $L^2(\Omega^{N-1})$ as $n \to \infty$ for any i, j in order for the potential energy to stay finite. But then the limit Ψ also satisfies $\Psi(x_i = x_j) = 0$ (in $L^2(\Omega^{N-1})$) for any i, j. This follows from the fact that $\delta(x_i - x_j)f(\overline{x^j}) \in H^{-1}(\Omega^N)$ for any $f \in L^2(\Omega^{N-1})$ and from weak H^1 convergence of Ψ_{c_n}. Now we clearly have $E_\Psi < \mathcal{E} < E_F$ by weak lower semi–continuity of the H^1–norm, which contradicts E_F being the ground state energy of the impenetrable boson model. □

Proof in the thermodynamic limit by Bethe ansatz. It follows from (2.5.17) that $\lambda \to \infty$ as $c \to \infty$. Then from (2.5.15) we see that $g = \frac{1}{2\pi}$ so again by (2.5.17) $\lambda = \frac{1}{\pi}\gamma$. Thus by (2.5.16) we have $e(\gamma) = \frac{\pi^2}{3}$, which agrees with the free Fermi ground state energy □

Proposition 35. *Let Ψ_c denote the (normalized) 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 $\Psi_{c_{n_i}} \to \Psi$ 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 $\|\Psi_{c_n}\|_{H^{2m}(\{1,2,\ldots,N\})} \leq C_m \lambda_n^m \|\Psi_{c_n}\|_{L^2(\{1,2,\ldots,N\})} \leq C_m E_F^m$. By Rellich–Kondrachov, there exist for each $m \in \mathbb{N}$ a subsequence $\Psi^m_{c_{n_i}}$ such that $\Psi^m_{c_{n_i}}$ converges in $H^{2m-1}(\{1, 2, \ldots, N\})$. By a diagonal argument we find a subsequence, $\Psi^i_{c_{n_i}}$, which converges in $H^k(\{1, 2, \ldots, N\})$ 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 $C^\infty(\overline{\{1, 2, \ldots, N\}})$. □

Lower bound in the large c limit

From the equations (2.5.15)-(2.5.17), one can obtain an exact lower bound of the ground state energy in the thermodynamic limit, this is done in Chapter 3. However, since this lower bound is shown by the use of the exact solution of the Lieb-Liniger model, it is hard to generalize this lower bound more generic models such as perturbations of the Lieb-Liniger model. In this subsection, we seek to prove a weaker form of this lower bound by a more soft argument. For this purpose we will use Proposition 35 to give an assymptotic (in c) bound in a finite box. The strategy is as follows: Consider the ground state, Ψ_c of the Lieb-Liniger model in a box of size L. We define $\tilde{\Psi}_c : [0, L+(N-1)R]^N \to \mathbb{C}$ to satisfy $\tilde{\Psi}(y_1, \dots, y_N) = \Psi_c(y_1, y_2 - R, y_3 - 2R, \dots, y_N - (N-1)R)$ when $y_{k+1} - kR > y_k$ for all $k = 1, \dots, N$. We denote the set $\{y_{k+1} - kR > y_k$ for all $k = 1, \dots, N\} := \Gamma$. Then $\tilde{\Psi}_c|_\Gamma = \Psi_c$. Now we define $\tilde{\Psi}_c$ on all of $[0, L+(N-1)R]^N$ by extending it to be an eigenfunction of the Laplacian $-\Delta$ with the same eigenvalue as on Γ. Indeed it is an eigenfunction on Γ with eigenvalue E_c. Then we have

$$\int \left|\nabla\tilde{\Psi}_c\right|^2 = E_c \left\|\tilde{\Psi}_c\right\|^2 - \sum_{i<j} \int_{y_i=y_j} \overline{\tilde{\Psi}_c} \nabla_n \tilde{\Psi}_c \tag{2.5.18}$$

where ∇_n denotes the inward normal derivative at the boundary $\{y_i = y_j\}$. Now to give a lower bound, we notice that the extension can be approximated by Taylor expanding from the original boundary, $\partial\Gamma$, into the new region. Heuristically, denote a point on the boundary $x_0 \in \partial\Gamma \setminus \partial\Lambda_{L+(N-1)R}$, we have

$$\tilde{\Psi}_c(y_1 = y_2, y_{i+1} > y_i + R \text{ for all } i \geq 2) = \tilde{\Psi}_c(x_0) - R\nabla_n\tilde{\Psi}_c(x_0) + \frac{1}{2}R^2\nabla_n^2\tilde{\Psi}_c(x_0) + \dots \tag{2.5.19}$$

2.6 The Yang-Gaudin Model

Similarly to the Lieb-Liniger model, the Yang-Gaudin model is exactly solvable, in the sense 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 taken to have any given spatial symmetry.

Labeling the symmetries

To analyze the problem, Yang considers the possible spatial symmetries that may appear problem. Having combined spin-space anti-symmetry, requires that any irreducible representation of S_N determining the spacial 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 are increasing 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 are in the same row. Next anti-symmetrize, in these states, all particle labels that are in the same column. For example:

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

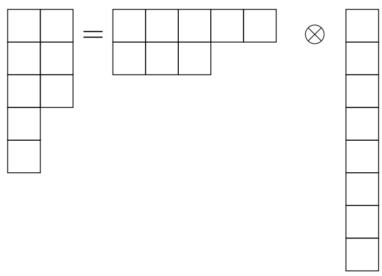
$$\begin{array}{|c|c|}\hline 1 & 3 \\ \hline 2 \\ \cline{1-1}\end{array} = \operatorname{span}\left(|\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\rangle , |\downarrow\uparrow\downarrow\rangle - |\uparrow\downarrow\downarrow\rangle\right), \tag{2.6.3}$$

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

By the before mentioned fact that one cannot anti-symmetrize three spin–1/2, 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

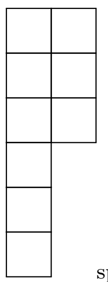
lengths two carry vanishing total spin, because they form a singlet state. On the other hand, all columns of length one are symmetrized with each other. Hence it is well known that they carry maximal total spin. In the subspace labeled by a tableau with M columns of length 2 and $N-2M$ columns of length 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 tableaux, [WJ91]. Recall that for irreducible representations of S_N we have the relation

$$\{\lambda'\} = \{\lambda\} \otimes \mathrm{sgn}$$



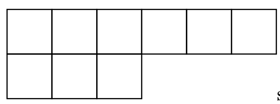
(2.6.5)

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



space

must be defined in the spin subspace



spin .

We notice that this restrict the spacial symmetries that spin–1/2 fermions can posses, 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. 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: One 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 is ψ is symmetric and we recover a Slater determinant if ψ is anti-symmetric.
A crucial observation by Yang is that we have the identities

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

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

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

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, using that $X_{ij} = (1 - P_{ij} x_{ij})/(1 + x_{ij})$, we may consider a spin state, Φ, of total spin $N - 2M$, satisfying the equation

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

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 $N - 2M$, we know that this chain can have components with total spin $N,\ N - 1, \dots N - 2M$. Notice that $P_{ij} = 1 + 2S_i \cdot S_j$ 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 corresponds to eigenvalues of (2.6.1), the theorem of Lieb and Mattis [LM62b] 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.
The Bethe-Yang hypothesis states that

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

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

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

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 find

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

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) 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 $\theta(x) \coloneqq -2\arctan(x/c)$, and where for N even and M odd we have

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

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

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

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

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

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

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 of the Yang-Gaudin model.

Lemma 36. *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 an induction proof: For the induction start, 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 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 36, the second term in (2.6.24) vanish 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 37. *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 through 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 coefficient, 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

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

It follows for any m_0 that

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

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 38. *Let f be the 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 36 with $m \to \infty$ using (2.6.29) and Lemma 37 the result follows. □

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

Proposition 39. *Let e be the 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 38, 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 energy in the dilute limit.

Chapter 3

The ground state energy of the one dimensional dilute Bose gas (paper)

This chapter contains a revised edition of the preprint [ARS22]. In order to be transparent about this being a collaboration with my co-authors Robin Reuvers and Jan Philip Solovej and to emphasize that this work stands on is own, the title page with abstract and authors is included. Furthermore, the labeling of equations, theorems, lemma, and references is kept seperate from the rest of the thesis.

Repetitions from the preceeding chapters of this thesis might occur, and repitions of the content in this preprint may also occur in the following chapters. When refering to 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 [29] 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 [26] 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 [30] proved that the leading term in this expansion holds for a very general class of potentials v, and the same generality was proved for the second-order term [3, 13, 14, 48].

The situation is similar in 2D. The leading order in the energy expansion for $\rho a^2 \ll 1$ derived by Schick [42] was proved rigorously by Lieb and Yngvason [35]. A second-order term has also been derived and is equally predicted to be general [1, 12, 37], 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.

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 as well now.

The first is the famous Lieb–Liniger model [32]. 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 [32], 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 ([32]; see, for example, [20, 24]),

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

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, 16]

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

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 and translation-invariant 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 $0 \leq x_1 \leq x_2 \leq R_0$.[1] We will consider the N-body Hamiltonian

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

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

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

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

[1] Note we allow $0 \leq x_1 = x_2 \leq R_0$, 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 $|x| = x_1$.

8 in Section 2, and a matching lower bound in the form of Proposition 16 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* $N\pi^2/3\rho^2$*, as first understood by Girardeau [16] (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 that 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 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 is also possible, 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 [29].

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 supp*$(v) \subset [-R_0, R_0]$*). Let* $R > R_0$*. For*

[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).

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 (this 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, 30, 35], 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). Successful 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 $\rho|a| \to 0$. Here, we can rely on Girardeau's solution [16] of the $c/\rho \to \infty$ case of the Lieb–Liniger model. In this limit, the bosons are impenetrable, since the delta function in (1.4) enforces a zero boundary condition whenever two bosons meet. 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]

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

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

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

[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.

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 good 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 (small) 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

$$\begin{cases} f_0(x)\sin(\pi b/L) & |x| \leq b \\ \sin(\pi(x_i - x_j)/L) & |x| > b \end{cases} \tag{1.17}$$

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 also need a way to extract the leading order free Fermi term in the energy, and 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

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

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, and to obtain the symmetric delta potential for any neighbouring pairs of bosons. Then—crucially—we throw away the regions where $|x_{i+1} - x_i| \leq R$ (this is inspired by a similar step in [34]). That should produce 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 $4/(R - a)$. 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

[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. This is discussed further in Section 1.5.

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

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

Crucially, we can show a priori that 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 of v, obtained from Lemma 4 by imposing the antisymmetric boundary condition $f(R)=-f(-R)=1$.

Theorem 5 (spinless fermions)**.** *Consider a Fermi gas with repulsive interaction $v=v_{reg}+v_{h.c.}$ as defined before Theorem 1. 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_o and ρR_0 sufficiently small, the ground state energy can be expanded as*

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

where $a_o\geq 0$ is the odd wave scattering length of v.

This theorem follows from Theorem 1 by using Girardeau's insight [16] 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 $0\leq x_1\leq\dots\leq x_N\leq L$, 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 [31]. For each of these sectors, an explicit solution in terms of the Bethe ansatz exists [15, 47]. In certain cases, these can be expanded in the limit* c/ρ *[21], 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 [17, 21]*

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

Both the Lieb–Liniger exact solution and the expansions can be generalized to higher spins (or Young diagrams) [22, 45]. 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* $a_e = a$ *and the odd-wave scattering length* a_o *of the potential will play a role. In the Lieb–Liniger example* (1.21)*,* $a_o = 0$*, since the delta interaction does not affect antisymmetric wave functions. However, for hard-core fermions of diameter* a*,* $a_o = a_e = a$*, and the energy should be* (1.8) *since the spin symmetry plays no role. These two examples suggest that the correct formula is*

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

We will discuss this expansion in a future publication.

This approach followed to obtain Theorem 5 can actually be taken further. What if, starting from some wave function on a sector $0 \le x_1 < \cdots < x_N \le L$, we want to add anyonic phases $e^{i\kappa}$ with $0 \le \kappa \le \pi$ whenever two particles are interchanged? It turns out this can be made to work, going back to, amongst others, [25, 27] (see [7, 40] 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 [40], 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, 23]. 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 $\kappa \in [0, \pi]$ with repulsive interaction $v = v_{\text{reg}} + v_{\text{h.c.}} + 2c\delta_0$, where $v_{\text{h.c.}}$ is defined before Theorem 1, and v_{reg} is a finite measure with $v_{\text{reg}}(\{0\}) = 0$. 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 a 1D equivalent was seemingly never studied. On the other hand, given the existence of the Lieb–Liniger model, this is perhaps not surprising at all. Not only can

[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.

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 [33, 34, 39, 44]. 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 $-\mathcal{O}(N^2)$ [32, 36], so 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 [18, 19, 38, 43]. As mentioned, the Lieb–Liniger model is very relevant to such set-ups [33, 34, 39, 44], but only in certain parameter regimes. In these references, the confinement length $l_\perp$ in the trapping 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 $l_\perp \gg a$ is sometimes referred to as weak confinement [5].

There should also be a 'strong confinement' regime $l_\perp \ll a$, 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 hold (3D), and are expected to hold (2D), for a wide class of potentials. As motivated in the introduction, the same might be true in the 1D expansion (1.7).

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 are very different. 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 diverges like $1/\sqrt{k}$ for small k [28, 46]. 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 Theorem 1

Proposition 8 (Upper bound 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 $|\Psi_F^{\mathrm{per}}|$ 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.

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*

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

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 is supported in $B_b(0)$ and $\Psi_\omega = |\Psi_F|$ except in the region $B = \{x \in \mathbb{R}^N | \mathcal{R}(x) < b\}$, we may rewrite this, using the diamagnetic inequality, as

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

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 exchange of particles, and the diamagnetic inequality, we find

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

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

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

We may, by an inclusion-exclusion argument, estimate

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

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

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

2.1.1 1-body reduced density matrix

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

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

Of course, Wick's theorem can be used to compute any n-body reduced density matrix.

2.1.2 Taylor's theorem

For later use, we define the one particle reduced density matrix $\gamma^{(1)}(x,y)$, as well as the translation invariant part $\tilde{\gamma}^{(1)}(x,y)$

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

where $D_n(x) = \frac{1}{2\pi}\sum_{k=-n}^n \mathrm{e}^{ikx} = \frac{\sin((n+1/2)x)}{2\pi\sin(x/2)}$ is the Dirichlet kernel. One obvious consequence is that $\left|\partial_x^{k_1}\partial_y^{k_2}\gamma^{(1)}(x,y)\right| \leq \frac{1}{\pi}(2N)^{k_1+k_2+1}\left(\frac{\pi}{L}\right)^{k_1+k_2+1} = \pi^{k_1+k_2}(2\rho)^{k_1+k_2+1}$. This bound will allow us to Taylor expand any $\gamma^{(k)}$, as all derivatives are uniformly bounded by a constant times some power of ρ. In fact the relevant power of ρ can be directly obtained from dimensional analysis.

2.1.3 Useful bounds on various reduced density matrices of Ψ_F

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

$$\rho^{(2)}(x_1,x_2)=\left(\frac{\pi^2}{3}\rho^4+f(x_2)\right)(x_1-x_2)^2+\mathcal{O}(\rho^6(x_1-x_2)^4), \tag{2.18}$$

with $\int |f(x_2)|\,\mathrm{d}x_2 \leq$ const. $\rho^3\ln(N)$.

Proof. Note that by translation invariance it holds that

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

Furthermore, we have $\gamma^{(1)}(x_1,x_2)-\rho^{(1)}((x_1+x_2)/2)=\tilde{\gamma}^{(1)}(x_1,x_2)-(\rho+1/(2L))$. Now, by Wick's theorem,

$$\rho^{(2)}(x_1,x_2)=\rho^{(1)}(x_1)\rho^{(1)}(x_2)-\gamma^{(1)}(x_1,x_2)\gamma^{(1)}(x_2,x_1). \tag{2.19}$$

Using that $\gamma^{(1)}$ is symmetric, and that

$$\begin{aligned}\rho^{(1)}(x_1)=\rho^{(1)}((x_1+x_2)/2)+\rho^{(1)\prime}((x_1+x_2)/2)\frac{x_1-x_2}{2}\\ +\frac{1}{2}\rho^{(1)\prime\prime}((x_1+x_2)/2)\left(\frac{x_1-x_2}{2}\right)^2+\mathcal{O}(\rho^4(x_1-x_2)^3),\end{aligned} \tag{2.20}$$

$$\begin{aligned}\rho^{(1)}(x_2)=\rho^{(1)}((x_1+x_2)/2)+\rho^{(1)\prime}((x_1+x_2)/2)\frac{x_2-x_1}{2}\\ +\frac{1}{2}\rho^{(1)\prime\prime}((x_1+x_2)/2)\left(\frac{x_1-x_2}{2}\right)^2+\mathcal{O}(\rho^4(x_1-x_2)^3),\end{aligned} \tag{2.21}$$

where both expressions can be expanded further if needed, we see that

$$\begin{aligned}\rho^{(2)}(x_1,x_2)=\rho^{(1)}((x_1+x_2)/2)^2-\gamma^{(1)}(x_1,x_2)^2-\left[\rho^{(1)\prime}((x_1+x_2)/2)\right]^2\left(\frac{x_1-x_2}{2}\right)^2\\ +\rho^{(1)}((x_1+x_2)/2)\rho^{(1)\prime\prime}((x_1+x_2)/2)\left(\frac{x_1-x_2}{2}\right)^2+\mathcal{O}(\rho^6(x_1-x_2)^4).\end{aligned} \tag{2.22}$$

Notice that terms of order $\mathcal{O}(\rho^5(x_1-x_2)^3)$ must cancel due to symmetry. Now use the fact that $0\leq\rho^{(1)}\leq 2\rho$, and $\rho^{(1)\prime}:[0,L]\to\mathbb{R}$, and $\int_{[0,L]}\left|\rho^{(1)\prime\prime}\right|\leq$ const. $\rho^2\ln(N)$, and finally that $\int_{[0,L]}\left|\rho^{(1)\prime}\right|\leq$ const. $\rho\ln(N)$, which follows from the bound on Dirichlet's kernel $\left\|D_N^{(k)}\right\|_{L^1([0,2\pi])} \leq \text{const. } N^k \ln(N)$, to conclude that

$$\rho^{(2)}(x_1,x_2) = \rho^{(1)}((x_1+x_2)/2)^2 - \gamma^{(1)}(x_1,x_2)^2 + g_1(x_1+x_2)(x_1-x_2)^2 + \mathcal{O}(\rho^6(x_1-x_2)^4), \tag{2.23}$$

for some function g_1 satisfying $\int_{[0,L]} |g_1| \leq \text{const. } \rho^3 \ln(N)$. Furthermore, notice that

$$\begin{aligned}
&\rho^{(1)}((x_1+x_2)/2)^2 - \gamma^{(1)}(x_1,x_2)^2 \\
&\quad = (\rho^{(1)}((x_1+x_2)/2) - \gamma^{(1)}(x_1,x_2))(\rho^{(1)}((x_1+x_2)/2) + \gamma^{(1)}(x_1,x_2)) \\
&\quad = \left[\rho + 1/(2L) - \tilde{\gamma}^{(1)}(x_1,x_2)\right]\left[-\rho - 1/(2L) + \tilde{\gamma}^{(1)}(x_1,x_2) + 2\rho^{(1)}((x_1+x_2)/2)\right] \\
&\quad = -\left[\rho + 1/(2L) - \tilde{\gamma}^{(1)}(x_1,x_2)\right]^2 + 2\left[\rho + 1/(2L) - \tilde{\gamma}^{(1)}(x_1,x_2)\right]\rho^{(1)}((x_1+x_2)/2) \\
&\quad = 2\left(\frac{\pi^2}{6}(\rho+1/(2L))^3(x_1-x_2)^2 + \mathcal{O}(\rho^5(x_1-x_2)^4)\right)\left(\rho + \frac{1}{2L} - \frac{\pi}{L}D_N((x_1+x_2)/(2L))\right) \\
&\quad = \frac{\pi^2}{3}\rho^4(x_1-x_2)^2 + g_2(x_1-x_2)(x_1-x_2)^2 + \mathcal{O}(\rho^6(x_1-x_2)^4),
\end{aligned} \tag{2.24}$$

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 $\int_{[0,L]} g_2 \leq \text{const. } \rho^3 \ln(N)$. Thus, we conclude that

$$\rho^{(2)}(x_1,x_2) = \left(\frac{\pi^2}{3}\rho^4 + f(x_2)\right)(x_1-x_2)^2 + \mathcal{O}(\rho^6(x_1-x_2)^4), \tag{2.25}$$

with $f = g_1 + g_2$ satisfying $\int_{[0,L]} |f| \leq \text{const. } \rho^3 \ln(N)$. □

Lemma 12. *We have the following bounds.*

$$\begin{aligned}
\rho^{(3)}(x_1,x_2,x_3) &\leq \text{const. } \rho^9(x_1-x_2)^2(x_2-x_3)^2(x_1-x_3)^2 \\
\rho^{(4)}(x_1,x_2,x_3,x_4) &\leq \text{const. } \rho^8(x_1-x_2)^2(x_3-x_4)^2 \\
\left|\sum_{i=1}^2 \partial_{y_i}^2\gamma^{(2)}(x_1,x_2,y_1,y_2)|_{y=x}\right| &\leq \text{const. } \rho^6(x_1-x_2)^2 \\
\left|\partial_{y_1}^2\left(\frac{\gamma^{(2)}(x_1,x_2,y_1,y_2)}{y_1-y_2}\right)\right|_{y=x}\Bigg| &\leq \text{const. } \rho^6\,|x_1-x_2| \\
\left|\sum_{i=1}^2(-1)^{i-1}\partial_{y_i}\left(\frac{\gamma^{(2)}(x_1,x_2,y_1,y_2)}{y_1-y_2}\right)\right|_{y=x}\Bigg| &\leq \text{const. } \rho^6(x_1-x_2)^2
\end{aligned} \tag{2.26}$$

Proof. The bounds follows straightforwardly from Taylor's theorem and the symmetries of the left-hand sides. As an example, 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). Since we previously argued that all derivatives of $\gamma^{(n)}$ are bounded by a constant times ρ^k for some $k \in \mathbb{N}$, we can clearly Taylor-expand $\gamma^{(2)}$. Taylor-expanding x_1 around x_2 and similarly y_1 around y_2, we see by the anti-symmetry that $\sum_{i=1}^{2} \partial_{y_i}^2 \gamma^{(2)}(x_1, x_2, y_1, y_2) \leq \text{const. } \rho^6 (x_1 - x_2)(y_1 - y_2)$, where the power of ρ can be found by simple dimensional analysis. $\square$

Lemma 13. *We have the following bounds.*

$$\begin{aligned} \sum_{i=1}^{3} \left(\partial_{x_i} \partial_{y_i} \gamma^{(3)}(x_1, x_2, x_3; y_1, y_2, y_3) \right) \Big|_{y=x} &\leq \text{const. } \rho^9 (x_2 - x_3)^2 (x_1 - x_2)^2, \\ \left| \sum_{i=1}^{3} \left(\partial_{y_i}^2 \gamma^{(3)}(x_1, x_2, x_3; y_1, y_2, y_3) \right) \Big|_{y=x} \right| &\leq \text{const. } \rho^9 (x_1 - x_2)^2 (x_2 - x_3)^2, \\ \left| \left[\partial_y \gamma^{(4)}(x_1, x_2, x_3, x_4; y, x_2, x_3, x_4) \Big|_{y=x_1} \right]_{x_1=x_2-b}^{x_1=x_2+b} \right| &\leq \text{const. } \rho^8 b (x_3 - x_4)^2 \end{aligned} \tag{2.27}$$

Proof. The proof follows straightforwardly from Taylor's theorem and the symmetries of the left-hand sides. $\square$

2.2 Estimating E_1

Recall the definition

$$E_1 := \binom{N}{2} \int_{A_{12}} \sum_{i=1}^{N} |\partial_i \Psi_{12}|^2 + \sum_{1 \leq i < j \leq N} (v_{\text{reg}})_{ij} |\Psi_{12}|^2 - \sum_{i=1}^{N} |\partial_i \Psi_F|^2 . \tag{2.28}$$

We prove the following bound.

Lemma 14.

$$E_1 \leq E_0 \left(2\rho a \frac{b}{b-a} + \text{const. } N(\rho b)^3 \left[1 + \rho b^2 \int v_{\text{reg}} \right] \right). \tag{2.29}$$

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

$E_1^{(3)} + E_1^{(4)}$. First, we have

$$\begin{aligned} E_1^{(1)} &= 2\binom{N}{2} \int_{A_{12}} |\partial_1 \Psi_{12}|^2 \\ &= 2\binom{N}{2} \int_{A_{12}} \overline{\Psi_{12}} \left(-\partial_1^2 \Psi_{12}\right) + 2\binom{N}{2} \int \left[\overline{\Psi_{12}} \partial_1 \Psi_{12}\right]_{x_1=x_2-b}^{x_1=x_2+b} \mathrm{d}x_2 \ldots \mathrm{d}x_N, \end{aligned} \tag{2.30}$$

The boundary term can be calculated explicitly, and we find

$$\begin{aligned} 2\binom{N}{2} \int \left[\overline{\Psi_{12}} \partial_1 \Psi_{12}\right]_{x_1=x_2-b}^{x_1=x_2+b} \mathrm{d}x_2 \ldots \mathrm{d}x_N = \int \left[\frac{\omega(x_1-x_2)}{|x_1-x_2|} \partial_{x_1} \left(\frac{\omega(x_1-x_2)}{|x_1-x_2|} \right) \rho^{(2)}(x_1,x_2) \right]_{x_2-b}^{x_2+b} \mathrm{d}x_2 \\ + \int \left[\left(\frac{\omega(x_1-x_2)}{|x_1-x_2|} \right)^2 \partial_{x_1} \left(\gamma^{(2)}(x_1,x_2;y,x_2) \right) \Big|_{y=x_1} \right]_{x_2-b}^{x_2+b} \mathrm{d}x_2 \end{aligned} \tag{2.31}$$

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

$$\partial_{x_1} \left(\frac{\omega(x_1-x_2)}{|x_1-x_2|} \right) \Big|_{x=x_2 \pm b} = \pm \frac{\frac{b}{b-a} - 1}{b} = \pm \frac{a}{b(b-a)}. \tag{2.32}$$

Using Lemma 11, we find

$$\int \left[\frac{\omega(x_1-x_2)}{|x_1-x_2|} \partial_{x_1} \left(\frac{\omega(x_1-x_2)}{|x_1-x_2|} \right) \rho^{(2)}(x_1,x_2) \right]_{x_2-b}^{x_2+b} \mathrm{d}x_2 \leq 2a \frac{b}{b-a} N \frac{\pi^2}{3} \rho^3 \left(1 + \text{const. } \frac{\ln(N)}{N} \right). \tag{2.33}$$

Furthermore, we denote

$$\begin{aligned} &\int \left[\left(\frac{\omega(x_1-x_2)}{|x_1-x_2|} \right)^2 \partial_{x_1} \left(\gamma^{(2)}(x_1,x_2;y,x_2) \right) \Big|_{y=x_1} \right]_{x_2-b}^{x_2+b} \mathrm{d}x_2 \\ &= \int \left[\partial_{x_1} \left(\gamma^{(2)}(x_1,x_2;y,x_2) \right) \Big|_{y=x_1} \right]_{x_2-b}^{x_2+b} \mathrm{d}x_2 =: \kappa_1. \end{aligned} \tag{2.34}$$

Thus, we have

$$E_1^{(1)} = \frac{\pi^2}{3} N \rho^3 (2a) \frac{b}{b-a} + \kappa_1 + 2\binom{N}{2} \int_{A_{12}} \overline{\Psi_{12}} (-\partial_1^2 \Psi_{12}). \tag{2.35}$$

Another contribution to E_1 is

$$
\begin{aligned}
E_1^{(2)} &= -\binom{N}{2}\int_{A_{12}}\left(2\left|\partial_1\Psi_F\right|^2+\sum_{i=3}^{N}\left|\partial_i\Psi_F\right|^2\right)\\
&= -\binom{N}{2}\int_{A_{12}}\sum_{i=1}^{N}\overline{\Psi_F}(-\partial_i^2\Psi_F)-2\binom{N}{2}\int\left[\overline{\Psi_F}\partial_1\Psi_F\right]_{x_1=x_2-b}^{x_1=x_2+b}\\
&= -E_0\binom{N}{2}\int_{A_{12}}\left|\Psi_F\right|^2-\underbrace{\int\left[\partial_y\gamma^{(2)}(x_1,x_2;y,x_2)|_{y=x_1}\right]_{x_2-b}^{x_2+b}\mathrm{d}x_2}_{\kappa_1},
\end{aligned}
\tag{2.36}
$$

and using Lemma 11, we find

$$
E_1^{(2)} = -\text{const. } E_0N\rho^3b^3-\kappa_1. \tag{2.37}
$$

The last contributions are
$E_1^{(3)} = \binom{N}{2}\int_{A_{12}}\sum_{1\le i<j\le N}(v_{\text{reg}})_{ij}\left|\Psi_{12}\right|^2 = \binom{N}{2}\int_{A_{12}}v_{12}\left|\Psi_{12}\right|^2+2\binom{N}{2}\int_{A_{12}}\sum_{2\le i<j}^{N}(v_{\text{reg}})_{ij}\left|\Psi_{12}\right|^2$
and
$E_1^{(4)} = \int_{A_{12}}\sum_{i=3}^{N}\left|\partial_i\Psi_{12}\right|^2$. First, notice that

$$
\begin{aligned}
&\binom{N}{2}\int_{A_{12}}\sum_{2\le i<j}^{N}(v_{\text{reg}})_{ij}\left|\Psi_{12}\right|^2\\
&\quad\le \text{const. } b^2\left(\int_{\{|x_1-x_2|<b\}\cap\text{supp}((v_{\text{reg}})_{34})}v_{\text{reg}}(|x_3-x_4|)\frac{1}{(x_1-x_2)^2}\rho^{(4)}(x_1,x_2,x_3,x_4)\right.\\
&\qquad\left.+\int_{\{|x_1-x_2|<b\}\cap\text{supp}((v_{\text{reg}})_{23})}v_{\text{reg}}(|x_2-x_3|)\frac{1}{(x_1-x_2)^2}\rho^{(3)}(x_1,x_2,x_3)\right).
\end{aligned}
\tag{2.38}
$$

By Lemma 12,

$$
\begin{aligned}
&\binom{N}{2}\int_{A_{12}}\sum_{2\le i<j}^{N}(v_{\text{reg}})_{ij}\left|\Psi_{12}\right|^2\\
&\quad\le \text{const. }\left(N^2(\rho b)^3\rho^3\int x^2v_{\text{reg}}(x)\,\mathrm{d}x+N(\rho b)^3\rho^5\int x^4v_{\text{reg}}(x)\,\mathrm{d}x+N(\rho b)^4\rho^4\int x^3v_{\text{reg}}(x)\,\mathrm{d}x\right.\\
&\qquad\left.+N(\rho b)^5\rho^3\int x^2v_{\text{reg}}(x)\,\mathrm{d}x\right)\\
&\quad\le \text{const. } N^2(\rho b)^5\rho\int v_{\text{reg}} = \text{const. } E_0N(\rho b)^3\left(\rho b^2\int v_{\text{reg}}\right),
\end{aligned}
\tag{2.39}
$$

and so

$$
\begin{aligned}
E_1 &= E_1^{(1)} + E_1^{(2)} + E_1^{(3)} + E_1^{(4)} \\
&\leq \frac{2\pi^2}{3} N\rho^3 a \frac{b}{b-a} + 2\binom{N}{2} \int_{A_{12}} \left(\overline{\Psi_{12}}(-\partial_1^2)\Psi_{12} + \frac{1}{2}\sum_{i=3}^{N} |\partial_i \Psi_{12}|^2 + \frac{1}{2} v_{12} |\Psi_{12}|^2 \right) \\
&\qquad + E_0 N(\rho b)^3 \text{const.} \left(1 + \rho b^2 \int v_{\text{reg}}\right).
\end{aligned} \tag{2.40}
$$

Using the two-body scattering equation from Lemma 4, this implies

$$
\begin{aligned}
E_1 \leq {} & \frac{2\pi^2}{3} N\rho^3 a \frac{b}{b-a} + 2\binom{N}{2} \int_{A_{12}} \frac{\overline{\Psi_F}}{(x_1-x_2)} \omega^2 (-\partial_1^2) \frac{\Psi_F}{(x_1-x_2)} \\
& + 2\binom{N}{2} \int_{A_{12}} \frac{\overline{\Psi_F}}{(x_1-x_2)} \omega(\partial_1 \omega)\partial_1 \frac{\Psi_F}{(x_1-x_2)} \\
& + \binom{N}{2} \int_{A_{12}} \sum_{i=3}^{N} \frac{\overline{\Psi_F}}{(x_1-x_2)} \frac{\omega^2}{(x_1-x_2)} (-\partial_i^2)\Psi_F \\
& + \text{const. } E_0 N(\rho b)^3 \left(1 + \rho b^2 \int v_{\text{reg}}\right).
\end{aligned} \tag{2.41}
$$

Furthermore, we have

$$
\begin{aligned}
&\binom{N}{2} \int_{A_{12}} \sum_{i=3}^{N} \overline{\Psi_{12}} \frac{\omega}{(x_1-x_2)} (-\partial_i^2)\Psi_F \\
&\quad = E_0 \binom{N}{2} \int_{A_{12}} \left| \frac{\omega}{(x_1-x_2)} \Psi_F \right|^2 - 2\binom{N}{2} \int_{A_{12}} \overline{\Psi_{12}} \frac{\omega}{(x_1-x_2)} (-\partial_1^2)\Psi_F.
\end{aligned} \tag{2.42}
$$

By Lemma 11, it follows that

$$
\binom{N}{2} \int_{A_{12}} \left| \frac{\omega}{(x_1-x_2)} \Psi_F \right|^2 \leq b^2 \int_{\{|x_1-x_2|<b\}} \frac{\rho^{(2)}(x_1,x_2)}{|x_1-x_2|^2} \,\mathrm{d}x_1\,\mathrm{d}x_2 \leq \text{const. } b^2\rho^4 L b = \text{const. } N\rho^3 b^3 \tag{2.43}
$$

and by Lemma 12, it follows that

$$
\begin{aligned}
2\binom{N}{2} \int_{A_{12}} \overline{\Psi_{12}} \frac{\omega}{(x_1-x_2)} (-\partial_1^2)\Psi_F &= \frac{1}{2}\sum_{i=1}^{2} \int_{A_{12}} \left| \frac{\omega}{x_1-x_2} \right|^2 \left[\partial_{y_i}^2 \gamma^{(2)}(x_1,x_2,y_1,y_2)\right]\Big|_{y=x} \\
&\leq \text{const. } N\rho^2(\rho b)^3,
\end{aligned} \tag{2.44}
$$

so that we find

$$\binom{N}{2}\int_{A_{12}}\sum_{i=3}^{N}\overline{\Psi_{12}}\frac{\omega}{(x_1-x_2)}(-\partial_i^2)\Psi_F \le \text{const. } E_0 N(\rho b)^3. \tag{2.45}$$

Finally, again by Lemma 12, we have

$$\begin{aligned} 2\binom{N}{2}\int_{A_{12}}\overline{\Psi_{12}}\omega(-\partial_1^2)\frac{\Psi_F}{(x_1-x_2)} &= \int_{A_{12}}\left|\frac{\omega^2}{x_1-x_2}\right|\left[\partial_{y_1}^2\left(\frac{\gamma^{(2)}(x_1,x_2,y_1,y_2)}{(y_1-y_2)}\right)\right]\Big|_{y=x} \\ &\le \text{const. } N\rho^2(\rho b)^3, \end{aligned} \tag{2.46}$$

and by using $\partial^2\omega = \frac{1}{2}v\omega \ge 0$ which implies $0 \le \omega'(x) \le \omega'(b) = \frac{b}{b-a}$ for $|x| < b$, we find that

$$\begin{aligned} 2\binom{N}{2}\int_{A_{12}}\overline{\Psi_{12}}(\partial_1\omega)\partial_1\left(\frac{\Psi_F}{(x_1-x_2)}\right) &\le \frac{1}{2}\sum_{i=1}^{2}\int_{A_{12}}\left|\frac{\omega}{x_1-x_2}\right|(-1)^{i-1}\omega'(x_1-x_2)\partial_{y_i}\left(\frac{\gamma^{(2)}(x_1,x_2,y_1,y_2)}{y_1-y_2}\right) \\ &\le \text{const. } \frac{b}{b-a}N\rho^2(\rho b)^3. \end{aligned} \tag{2.47}$$

Combining everything, we get the desired result.

□

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

Recall that

$$\begin{aligned} E_2^{(1)} &= \binom{N}{2}2N\int_{A_{12}\cap A_{13}}\sum_{i=1}^{N}|\partial_i\Psi_F|^2, \\ E_2^{(2)} &= \binom{N}{2}\binom{N-2}{2}\int_{A_{12}\cap A_{34}}\sum_{i=1}^{N}|\partial_i\Psi_F|^2. \end{aligned} \tag{2.48}$$

We now prove the following bound.

Lemma 15.

$$E_2^{(1)} + E_2^{(2)} \le E_0\left(N(\rho b)^4 + N^2(\rho b)^6\right). \tag{2.49}$$

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

$$
\begin{aligned}
E_2^{(1)} &= \binom{N}{2} 2N \int_{A_{12}\cap A_{23}} \sum_{i=1}^{N} |\partial_i \Psi_F|^2 \\
&= \binom{N}{2} 2N \left(2 \int_{A_{12}\cap A_{23}} |\partial_1 \Psi_F|^2 + \int_{A_{12}\cap A_{23}} |\partial_2 \Psi_F|^2 \right) + \binom{N}{2} 2N \int_{A_{12}\cap A_{23}} \sum_{i=4}^{N} |\partial_i \Psi_F|^2 .
\end{aligned} \tag{2.50}
$$

For the second term, we can perform partial integration directly to obtain

$$
\begin{aligned}
&\binom{N}{2} 2N \int_{A_{12}\cap A_{23}} \sum_{i=4}^{N} |\partial_i \Psi_F|^2 = \binom{N}{2} 2N \int_{A_{12}\cap A_{23}} \sum_{i=4}^{N} \overline{\Psi_F}(-\partial_i^2 \Psi_F) \\
&\quad \leq E_0 N^3 \int_{A_{12}\cap A_{23}} |\Psi_F|^2 - N^3 \int_{A_{12}\cap A_{23}} \sum_{i=1}^{3} \overline{\Psi_F}(-\partial_i^2 \Psi_F) \\
&\quad \leq 2E_0 \int_{[0,L]} \int_{[x_2-b,x_2+b]} \int_{[x_2-b,x_2+b]} \rho^{(3)}(x_1,x_2,x_3)\, \mathrm{d}x_3\, \mathrm{d}x_1\, \mathrm{d}x_2 - N^3 \int_{A_{12}\cap A_{23}} \sum_{i=1}^{3} \overline{\Psi_F}(-\partial_i^2 \Psi
\end{aligned} \tag{2.51}
$$

Using Lemma 12, we find

$$
2E_0 \int_{[0,L]} \int_{[x_2-b,x_2+b]} \int_{[x_2-b,x_2+b]} \rho^{(3)}(x_1,x_2,x_3)\, \mathrm{d}x_3\, \mathrm{d}x_1\, \mathrm{d}x_2 \leq N E_0 (\rho b)^6. \tag{2.52}
$$

Furthermore, we find by Lemma 13 that

$$
\binom{N}{2} 2N \int_{A_{12}\cap A_{23}} \sum_{i=1}^{3} \left(|\partial_i \Psi_F|^2 - \overline{\Psi_F}(-\partial_i^2 \Psi_F) \right) \leq \text{const. } \rho^9 L b^6 = \text{const. } E_0 (b\rho)^6. \tag{2.53}
$$

Collecting everything, we find

$$
E_2^{(1)} \leq \text{const. } N E_0 (\rho b)^6. \tag{2.54}
$$

To estimate $E_2^{(2)}$, we use integration by parts to obtain

$$
\begin{aligned}
E_2^{(2)} &= \binom{N}{2}\binom{N-2}{2}\int_{A_{12}\cap A_{34}}\left(4\left|\partial_1\Psi_F\right|^2+\sum_{i=5}^{N}\left|\partial_i\Psi_F\right|^2\right)\\
&= \binom{N}{2}\binom{N-2}{2}\left(4\int_{|x_3-x_4|<b}\left[\overline{\Psi_F}\partial_1\Psi_F\right]_{x_1=x_2-b}^{x_1=x_2+b}+\int_{A_{12}\cap A_{34}}\sum_{i=1}^{N}\overline{\Psi_F}(-\partial_i^2\Psi_F)\right)\\
&= 4\int_{x_2\in[0,L]}\int_{|x_3-x_4|<b}\left[\partial_{y_1}\gamma^{(4)}(x_1,x_2,x_3,x_4;y_1,x_2,x_3,x_4)\Big|_{y_1=x_1}\right]_{x_1=x_2-b}^{x_1=x_2+b}\\
&\quad + E_0\int_{A_{12}\cap A_{34}}\rho^{(4)}(x_1,\ldots,x_4).
\end{aligned}
\tag{2.55}
$$

By Lemma 13, we get

$$
4\int_{x_2\in[0,L]}\int_{|x_3-x_4|<b}\left[\partial_{y_1}\gamma^{(4)}(x_1,x_2,x_3,x_4;y_1,x_2,x_3,x_4)\Big|_{y_1=x_1}\right]_{x_1=x_2-b}^{x_1=x_2+b}=\text{const. }E_0N(\rho b)^4.
\tag{2.56}
$$

Furthermore, by Lemma 13 again, it follows that

$$
E_0\int_{A_{12}\cap A_{34}}\rho^{(4)}(x_1,\ldots,x_4)\leq\text{const. }E_0N^2(\rho b)^6.
\tag{2.57}
$$

□

2.4 Constructing the trial state for arbitrary N

Together, Lemmas 10, 14 and 15 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 $\Psi_{\text{full}}=\prod_{i=1}^{M}\Psi_{\omega,\ell}(x_1^i,\ldots,x_{\tilde N}^i)$, where $(x_1^i,\ldots,x_{\tilde N}^i)$ are the particles in box i and ℓ is the length of each box. Of course, $\cup_{i=1}^{M}\{x_1^i,\ldots,x_{\tilde N}^i\}=\{x_1,\ldots,x_N\}$ and $\{x_1^i,\ldots,x_{\tilde N}^i\}\cap\{x_1^j,\ldots,x_{\tilde N}^j\}=\emptyset$ for $i\neq j$, such that $M\tilde N=N$. The boxes are of length $\ell=L/M-b$, 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

$$E \leq Me_0\left(1+2\tilde\rho a\frac{b}{b-a}+\text{const. }\tilde N(b\tilde\rho)^3\left(1+\rho b^2\int v_{\text{reg}}\right)\right)/\left\|\Psi_\omega\right\|^2, \tag{2.58}$$

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 $bM/L \leq 1/2$. Clearly, we have $\left\|\Psi_\omega\right\|^2 \geq 1-\int_B\left|\Psi_F\right|^2 \geq 1-\int_{|x_1-x_2|<b}\rho^{(2)}(x_1,x_2) \geq 1-\text{const. }\tilde N(\rho b)^3$, where the last inequality follows from Lemma 11. Thus, choosing M such that $bM/L \ll 1$, we have

$$E \leq N\frac{\pi^2}{3}\rho^2\frac{\left(1+\frac{2\rho ab}{b-a}+\text{const. }\frac{M}{N}+\text{const. }2\rho abM/L+\text{const. }\tilde N(b\rho)^3\left(1+\rho b^2\int v_{\text{reg}}\right)\right)}{1-\tilde N(\tilde\rho b)^3}. \tag{2.59}$$

First assume that $N \geq (\rho b)^{-3/2}\left(1+\rho b^2\int v_{\text{reg}}\right)^{1/2}$. 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

$$\text{const. }\left[(1+2\rho^2ab^2/(b-a))x+x^{-1}(b\rho)^3\left(1+\rho b^2\int v_{\text{reg}}\right)\right], \tag{2.60}$$

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 $x = M/N = \frac{(b\rho)^{3/2}\left(1+\rho b^2\int v_{\text{reg}}\right)^{1/2}}{1+2\rho^2ab} \simeq (b\rho)^{3/2}\left(1+\rho b^2\int v_{\text{reg}}\right)^{1/2}$, which gives the error

$$\text{const. }(b\rho)^{3/2}\left(1+\rho b^2\int v_{\text{reg}}\right)^{1/2}. \tag{2.61}$$

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

$$\frac{b}{b-a} \leq 1+2a/b \leq 1+2(\rho\left|a\right|)^{1/5}. \tag{2.62}$$

Notice that

$$(\rho b)^{3/2} = \max\left((\rho\left|a\right|)^{6/5},(\rho R_0)^{3/2}\right) \leq (\rho\left|a\right|)^{6/5}+(\rho R_0)^{3/2}. \tag{2.63}$$

Now, for $N < (\rho b)^{-3/2}\left(1+\rho b^2\int v_{\text{reg}}\right)^{1/2}$, the result follows from (2.58). □

3 Lower bound Theorem 1

Proposition 16 (Lower bound 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 25 and Corollary 26 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 16.

3.1 Lieb-Liniger model: preparatory facts

The thermodynamic ground state energy of the Lieb-Liniger model is determined by the system of equations [32]

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

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

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

This allows for a rigorous lower bound.

Lemma 17 (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 $g \leq \frac{1}{2\pi}+2\frac{1}{\lambda}\int_{-1}^{1} g(x)\,\mathrm{d}x$. On the other hand, (3.4) shows that $e(\gamma) = \frac{\int_{-1}^{1} g(x)x^2\,\mathrm{d}x}{\left(\int_{-1}^{1} g(x)\,\mathrm{d}x\right)^3}$. We denote $\int_{-1}^{1} g(x)\,\mathrm{d}x = M$, notice that $g \leq \frac{1}{2\pi}\left(1+\frac{2M}{\lambda}\right) = \frac{1}{2\pi}\left(1+\frac{2}{\gamma}\right)$, and 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. $\square$

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

Lemma 18 (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.

Lemma 19 (Robinson [41])**.** *For simplicity, we will consider the Lieb-Liniger model on $[-L/2, L/2]$ in this subsection, and use the notation $\Lambda_s := [-s/2, s/2]$. Let v be symmetric and decreasing (that is, $v \circ \mathfrak{c} \geq v$ for any contraction $\mathfrak{c}$). For any $b > 0$,*

$$E^D_{\Lambda_{L+2b}} \leq E^N_{\Lambda_L} + \frac{2n}{b^2}. \tag{3.7}$$

Proof. The idea of the proof is given on page 66 of [41], 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 [41]. Also, we clearly have $Vf \in \mathcal{D}(\mathcal{E}^{D}_{\Lambda_{L+2b}})$. Let ψ be the ground state of $\mathcal{E}^{N}_{\Lambda_L}$, 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 [41]. 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

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

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.

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

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 $|s_1 y_1 - s_2 y_2| \geq |y_1 - y_2|$ 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

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

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

Proof of Lemma 18. Lemma 19 implies that for any $b > 0$

$$E_{LL}^N(n,\ell,c) \geq E_{LL}^D(n,\ell+b,c) - \text{const. } \frac{n}{b^2}. \tag{3.11}$$

Since the range of the interaction in the Lieb-Liniger model is zero, we see that $e_{LL}^D(2^m n, 2^m\ell, c) := \frac{1}{2^m\ell}E_{LL}^D(2^m n, 2^m\ell, c)$ 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 $E_{LL}^D(2^m n, 2^m\ell) \leq 2E_{LL}^D(2^{m-1}n, 2^{m-1}\ell)$. Since we also have $e_{LL}^D(2^m n, 2^m\ell, c) \geq e_{LL}(2^m n, 2^m\ell, c) \to e_{LL}(n/\ell, c)$ as $m\to\infty$ [32], we see that

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

Here, $\rho = n/\ell$, and the second inequality follows from Lemma 17. Optimizing in b, we find

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

□

3.2 Lower bound for small particle numbers n

In this subsection, we work our way towards Proposition 25 and Corollary 26, 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

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

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

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

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

$$|\phi(x)| \le \int_0^x |\phi'(t)|\,\mathrm{d}t. \tag{3.16}$$

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

We can estimate the norm loss in the following way

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

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 21. *For ψ be defined in* (3.14),

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

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

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

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

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

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. Now, rewriting and (3.17) give the result. $\square$

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 23. First, we state a direct adaptation of Lemma 4, more suited to our purpose here.

Lemma 22 (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 s-wave scattering length.

Lemma 23. *Let $R > \max(R_0, 2|a|)$ and $\epsilon \in [0,1]$. For ψ defined in* (3.14),

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

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

Proof. Splitting the energy functional in two parts, and using Lemma 21 on one term and Lemma 22 on the other (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 $\delta(\mathfrak{r}_i(x)-R) = \left(\sum_{j\neq i}\left[\delta(x_i - x_j - R) + \delta(x_i - x_j + R)\right]\right)\mathbb{1}_{\mathfrak{r}_i(\mathfrak{r})\geq R}$. The nearest-neighbor interaction is obtained from Lemma 22 by dividing the integration domain into Voronoi cells, and restricting to the cell around particle i.

With use of Lemma 21 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

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

□

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 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*

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

Proof. From the known upper bound, *i.e.* Proposition 8, and by Lemma 23 with $\epsilon = 1/2$, it follows that

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

Subtracting $E^N_{LL}\left(n, \tilde{\ell}, \frac{1}{R-a} \right)$ on both sides, and using Lemma 18 on the left-hand side, we find

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

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 left-hand side, as well as $2\rho \geq \tilde{\rho} \geq \rho(1 + \rho R)$, we find

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

It follows that we have

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

□

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

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

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

Proposition 25. *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 23 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 18 and 24,

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

□

Corollary 26. *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 26 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 μ.

Lemma 27. *Let $\Xi \geq 4$ be fixed. 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 $\rho R \leq 1$ 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 26, we have

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

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

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

□

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

Proof of Proposition 16. For the case $N < \tau(\rho R)^{-9/5}$, the result follows from Proposition 25.
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,

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

with $\ell = L/M$ and $M \in \mathbb{N}_+$. Now, let $\Xi = 4$ 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 $\mu = \frac{\mathrm{d}}{\mathrm{d}\rho}(\frac{\pi^2}{3}\rho^3(1+2\rho a)))$. By Lemma 27,

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

It is known from Proposition 25 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 $\Xi\rho a \geq -\frac{1}{4}$ (the case of $\Xi\rho a < -\frac{1}{4}$ is trivial, by choosing a sufficiently large constant in the error term). Hence,

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

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, 27, 40]. 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, 23, 25].

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

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

Here, $|_{\pm,0}^{ij}$ means the function should be evaluated at $x_i = x_j|_{\pm,0}$. Also,

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

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. The following proposition holds.

Proposition 28. *Let $0 < k < \pi$. H_N is symmetric with corresponding quadratic form*

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

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

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

Let $f, g \in C_0^\infty(\mathbb{R}^N)$ 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,

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

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

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

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

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

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 29. *Since $\mathcal{E}_{\kappa,c} \geq 0$, 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 28 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, $U_\kappa\mathcal{D}\left(\mathcal{E}_{c/\cos(\kappa/2)}\right) = \mathcal{D}\left(\mathcal{E}_{\kappa,c}\right)$ with $\mathcal{E}_{\kappa,c}(U_\kappa f) = \mathcal{E}_{c/\cos(\kappa/2)}(f)$. 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 paper 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 analyse 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. Thus we will focus 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 Chapter 3, about the ground state energy for such a system.

Conjecture 40. *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 match, to next to leading order, Conjecture 40. In order 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...., 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 heuristics 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 41. *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 $\{\sigma\}=\{\sigma_1,\sigma_2,\dots,\sigma_N\}=\{0<x_{\sigma_1}<x_{\sigma_2}<\ldots<x_{\sigma_N}<L\}$, then the full trial state is given by anti-symmetrically extending to other sectors. Of course this means that certain boundary conditions needs to be satisfied at the boundary $\{x_{\sigma_i}=x_{\sigma_{i+1}}\}$ in order 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 $\mathrm{P}_s^{i,j}$. 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 state trial state on a sector $\{1,2,\dots,N\}$ 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, $b>R_0$, $\omega_{s/o}^{\mathcal{R}}(x):=\omega_{s/o}(\mathcal{R}(x))$, and $\mathrm{P}_{s/t}^{\mathcal{R}(x)}:=\mathrm{P}_{s/t}^{i,j}$ when $\mathcal{R}(x)=|x_i-x_j|$, and η is a continuous and almost everywhere differentiable function with the property $\eta(x)=0$ 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

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

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 symmetry of the Hamiltonian/energy form, the energy is determined completely by the energy on the sector $\{1,2,\dots,N\}$.

As was the case in Chapter 3, the trial state given in (4.2.2) produces error that grow with the particle number. This is undesirable for proving Theorem 41. However, as before, we may construct the full trial state by localizing to smaller intervals. This is done by splitting the interval $[0,L]$ into smaller intervals $I_m:=[m(\ell+b),(m+1)\ell+mb]$ $m=0,1,2,\dots M-1$, 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 $x_i^m := x_{m\tilde{N}+i}$ 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 $b > R_0$.

We saw in Chapter 3 that the scattering solution, when particles are close, leads to correction to the free Fermi energy that are 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

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

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 is known, 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 49 below)

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

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 41

In this section, we give the formal proof of Theorem 41. 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, though completely trivial fact is the following lemma.

Lemma 42. *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

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

We will henceforth assume χ to be translation invariant. In fact, 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

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

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

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

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)

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

Defining

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

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 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 $|\Psi_\chi|^2\leq\left|\left(\tilde{\Psi}_\chi\right)_{12}\right|^2$ on B_{12} that we have the following upper bound for the energy

$$\begin{aligned}\mathcal{E}(\Psi_\chi)\leq E_F&+\binom{N}{2}\frac{1}{N}\sum_{k=1}^{N}\left\langle\chi\left|\mathrm{P}_s^{k,k+1}\right|\chi\right\rangle\left(\int_{A_{12}}\sum_{i=1}^{N}|\partial_i(\Psi_e)_{12}|^2\right.\\&\left.+\int_{A_{12}}\sum_{1\leq i<j\leq N}(v_{\mathrm{reg}})_{ij}\,|(\Psi_e)_{12}|^2-\int_{B_{12}}\sum_{i=1}^{N}|\partial_i\Psi_F|^2\right)\\&+\binom{N}{2}\frac{1}{N}\sum_{k=1}^{N}\left\langle\chi\left|\mathrm{P}_t^{k,k+1}\right|\chi\right\rangle\left(\int_{A_{12}}\sum_{i=1}^{N}|\partial_i(\Psi_o)_{12}|^2\right.\\&\left.+\int_{A_{12}}\sum_{1\leq i<j\leq N}(v_{\mathrm{reg}})_{ij}\,|(\Psi_o)_{12}|^2-\int_{B_{12}}\sum_{i=1}^{N}|\partial_i\Psi_F|^2\right)\\&+\binom{N}{2}\binom{N-2}{2}\int_{B_{12}^{34}}\sum_{i=1}^{N}|\partial_i\Psi_\chi|^2\\&+2(N-2)\binom{N}{2}\int_{B_{12}^{23}}\sum_{i=1}^{N}|\partial_i\Psi_\chi|^2.\end{aligned}\tag{4.2.14}$$

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

$$\begin{aligned}E_{12}^{34}&:=\binom{N}{2}\binom{N-2}{2}\int_{B_{12}^{34}}\sum_{i=1}^{N}|\partial_i\Psi_\chi|^2,\\E_{12}^{23}&:=2(N-2)\binom{N}{2}\int_{B_{12}^{23}}\sum_{i=1}^{N}|\partial_i\Psi_\chi|^2.\end{aligned}\tag{4.2.15}$$

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

Lemma 43. *Let E_{12}^{34} and Ψ_χ be defined as above, then we have the following* *bound:*

$$E_{12}^{34} \leq \text{ const. } E_F \left(N \left(\rho b \right)^4 + N^2 \left(\rho b \right)^6 \right). \tag{4.2.16}$$

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

Lemma 44. *Let E_{12}^{23} and Ψ_χ be defined as above, then we have the following bound:*

$$E_{12}^{23} \leq \text{ const. } E_F \left(\left(\rho b \right)^4 + N \left(\rho b \right)^6 \right). \tag{4.2.17}$$

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

Using Lemmas 43 and 44, we deduce, from (4.2.14) the following bound upper bound on the trial state energy

$$\begin{aligned} \mathcal{E}(\Psi_\chi) \leq E_F &+ \binom{N}{2} \frac{1}{N} \sum_{k=1}^{N} \left\langle \chi \middle| \mathrm{P}_s^{k,k+1} \middle| \chi \right\rangle \left(\int_{A_{12}} \sum_{i=1}^{N} \left| \partial_i (\Psi_e)_{12} \right|^2 \right. \\ &+ \left. \int_{A_{12}} \sum_{1 \leq i < j \leq N} (v_{\text{reg}})_{ij} \left| (\Psi_e)_{12} \right|^2 - \int_{B_{12}} \sum_{i=1}^{N} \left| \partial_i \Psi_F \right|^2 \right) \\ &+ \binom{N}{2} \frac{1}{N} \sum_{k=1}^{N} \left\langle \chi \middle| \mathrm{P}_t^{k,k+1} \middle| \chi \right\rangle \left(\int_{A_{12}} \sum_{i=1}^{N} \left| \partial_i (\Psi_o)_{12} \right|^2 \right. \\ &+ \left. \int_{A_{12}} \sum_{1 \leq i < j \leq N} (v_{\text{reg}})_{ij} \left| (\Psi_o)_{12} \right|^2 - \int_{B_{12}} \sum_{i=1}^{N} \left| \partial_i \Psi_F \right|^2 \right) \\ &+ E_F \left(N (\rho b)^4 + N^2 (\rho b)^6 \right). \end{aligned} \tag{4.2.18}$$

Defining the quantities

$$\begin{aligned} E_{1,e} &:= \binom{N}{2} \left(\int_{A_{12}} \sum_{i=1}^{N} \left| \partial_i (\Psi_e)_{12} \right|^2 + \sum_{1 \leq i < j \leq N} (v_{\text{reg}})_{ij} \left| (\Psi_e)_{12} \right|^2 - \sum_{i=1}^{N} \left| \partial_i \Psi_F \right|^2 \right), \\ E_{1,o} &:= \binom{N}{2} \left(\int_{A_{12}} \sum_{i=1}^{N} \left| \partial_i (\Psi_o)_{12} \right|^2 + \sum_{1 \leq i < j \leq N} (v_{\text{reg}})_{ij} \left| (\Psi_o)_{12} \right|^2 - \sum_{i=1}^{N} \left| \partial_i \Psi_F \right|^2 \right), \end{aligned} \tag{4.2.19}$$

and the quantities from Chapter 3:

$$\begin{aligned} E_2^{(1)} &:= \binom{N}{2} 2N \int_{A_{12} \cap A_{13}} \sum_{i=1}^{N} \left| \partial_i \Psi_F \right|^2, \\ E_2^{(2)} &:= \binom{N}{2} \binom{N-2}{2} \int_{A_{12} \cap A_{34}} \sum_{i=1}^{N} \left| \partial_i \Psi_F \right|^2, \end{aligned} \tag{4.2.20}$$

we see from an inclusion/exclusion argument identical to the one in Chapter 3 that

$$\begin{aligned}\mathcal{E}(\Psi_\chi) \leq E_F &+ \frac{1}{N}\sum_{k=1}^{N}\left\langle \chi \middle| \mathrm{P}_s^{k,k+1} \middle| \chi \right\rangle \left(E_{1,e} + E_2^{(1)} + E_2^{(2)}\right) \\ &+ \frac{1}{N}\sum_{k=1}^{N}\left\langle \chi \middle| \mathrm{P}_t^{k,k+1} \middle| \chi \right\rangle \left(E_{1,o} + E_2^{(1)} + E_2^{(2)}\right) \\ &+ E_F\left(N(\rho b)^4 + N^2(\rho b)^6\right)\end{aligned} \tag{4.2.21}$$

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

Lemma 45 (Lemma 14 of Chapter 3)**.** *Let $E_{1,e/o}$ be defined as above. For $N(\rho b)^3 \leq 1$ we have*

$$E_{1,e/o} \leq E_F\left(2\rho a_{e/o}\frac{b}{b-a_{e/o}} + \text{const. } N(\rho b)^3\left[1 + \rho b^2\int v_{\text{reg}}\right]\right). \tag{4.2.22}$$

We also recall the lemma

Lemma 46 (Lemma 15 of Chapter 3)**.**

$$E_2^{(1)} + E_2^{(2)} \leq E_F\left(N(\rho b)^4 + N^2(\rho b)^6\right). \tag{4.2.23}$$

Using Lemmas 45 and 46 we find the result

Lemma 47. *For $N(\rho b)^3 \leq 1$ and $b > 2a_o$ we have*

$$\begin{aligned}\mathcal{E}(\Psi_\chi) \leq E_F\Bigg(1 + 2\rho&\left[\frac{1}{4}\tilde{a}_e + \frac{3}{4}\tilde{a}_o + (\tilde{a}_o - \tilde{a}_e)\frac{1}{N}\left\langle \chi \middle| \sum_{k=1}^{N} S_k \cdot S_{k+1} \middle| \chi \right\rangle\right] \\ &+ \text{ const. } N(\rho b)^3\left(1 + \rho b^2\int v_{\text{reg}}\right)\Bigg),\end{aligned} \tag{4.2.24}$$

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

Proof. This lemma follows directly by combining (4.2.21) with Lemmas 45 and 46. □

It is then immediately clear that on the right-hand side of (4.2.24), 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 (4.2.24).

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

$$\lim_{N\to\infty}\left\langle \mathrm{GS}_{\mathrm{HAF}}\left|\frac{1}{N}\sum_{k=1}^{N} S_k\cdot S_{k+1}\right|\mathrm{GS}_{\mathrm{HAF}}\right\rangle = \frac{1}{4}-\ln(2) \tag{4.2.25}$$

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

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

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

$$E_D^{N+2} \leq E_P^N + \frac{3}{4}. \tag{4.2.27}$$

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 (4.2.27) 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

$$\frac{1}{mN}E_P^{mN} \leq \frac{1}{mN}E_D^{mN} \leq \frac{1}{N}E_D^N \leq \frac{1}{N}\left(E_P^{N-2}+3/4\right). \tag{4.2.28}$$

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 $E_P^N \leq \frac{N}{M+1}E_P^M + \frac{1}{4}$ for $M > N$, simply take the ground state of chain length M and truncate it at length N. Hence we get

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

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

$$\frac{N}{N-2}e_P - \frac{3}{4N} \leq \frac{1}{N-2}E_P^{N-2} \leq e_P + \frac{1}{4}\frac{1}{N-2}, \tag{4.2.30}$$

where $e_P = \lim\limits_{N\to\infty}\frac{1}{N}E_P^N$. The desired result the follows from Lemma 48. □

We are now ready to collect everything to give the proof of Theorem 41:

Proof of Theorem 41. Consider now the full trial state as given in (4.2.4). Because of the spacing between intervals, I_m, there no interacting between particles in different intervals. Hence the energy of such a state

$$\mathcal{E}(\Psi_{\chi,\text{full}})/\left\|\Psi_{\chi,\text{full}}\right\| = M\mathcal{E}(\Psi_\chi^{I_0})/\left\|\Psi_\chi^{I_0}\right\|. \tag{4.2.31}$$

Combining lemmas 47 and 49, we find

$$\begin{aligned}\mathcal{E}(\Psi_{\chi,\text{full}}) \leq N\frac{\pi^2}{3}\tilde{\rho}^2\Bigg(&1+2\tilde{\rho}\left[\ln(2)\tilde{a}_e+(1-\ln(2))\tilde{a}_o\right]+\frac{M}{N}\\ &+\ \text{const.}\ \frac{N}{M}(\tilde{\rho}b)^3\left(1+\tilde{\rho}b^2\int v_{\text{reg}}\right)\Bigg),\end{aligned} \tag{4.2.32}$$

with $\rho \leq \tilde{\rho} = \frac{N}{L-Mb} \leq \rho\left(1+2\frac{M}{N}\rho b\right)$ for $\frac{M}{N}\rho b \leq 1/2$. Choosing $M/N =$

$(\rho b)^{3/2}\left(1+\rho b^2\int v_{\mathrm{reg}}\right)^{1/2}$ we find

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

Furthermore choosing $b=\max(\rho^{-1/5}\left|a_e\right|^{4/5}, \rho^{-1/5}a_o^{4/5}, R_0)$ 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

$$\begin{aligned}\left\|\Psi_\chi^{I_0}\right\| &\geq 1-\int_{A_{12}}\rho^{(2))}(x_1,x_2) \geq 1- \text{ const. } \tilde{N}(\tilde{\rho}b)^3 \\ &\geq 1- \text{ const. } (\rho b)^{3/2} \geq 1- \text{ const. } (\rho R)^{6/5}.\end{aligned} \tag{4.2.34}$$

□

Estimating E_{12}^{34} (proof of lemma 43)

Proof of Lemma 43. Estimating E_{12}^{34} is a straightforward computation that goes as follows:
Define

$$\xi_{12}^{34} := \Big(\left(\eta(|x_3-x_4|)\omega_e^{12}(|x_1-x_2|)+(1-\eta(|x_3-x_4|))\omega_o^{12}(|x_1-x_2|)\right)\mathrm{P}_s^{1,2} + \omega_o^{12}(|x_1-x_2|)\,\mathrm{P}_t^{1,2}\Big)\chi_\sigma \tag{4.2.35}$$

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

$$\begin{aligned}S_{12}^{34} := \big\{\text{sectors } \{\sigma\} \mid\ & (1,2)=(\sigma_k,\sigma_{k+1}) \text{ or} \\ & (2,1)=(\sigma_k,\sigma_{k+1}) \text{ for some } k \\ & \text{and } (3,4)=(\sigma_l,\sigma_{l+1}) \text{ or} \\ & (4,3)=(\sigma_l,\sigma_{l+1}) \text{ for some } l\big\}.\end{aligned} \tag{4.2.36}$$

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

$$\begin{aligned}&\left(\xi^{34}_{12}\right)_s := \eta(|x_2-x_3|)\omega_e^{12}(|x_1-x_2|) + (1-\eta(|x_2-x_3|))\omega_o^{12}(|x_1-x_2|),\\ &\left(\xi^{34}_{12}\right)_t := \omega_o^{12}(|x_1-x_2|),\end{aligned} \tag{4.2.37}$$

we find using $B^{34}_{12} \subset A^{34}_{12}$

$$\begin{aligned}E^{34}_{12} =& \binom{N}{2} 2(N-2)\int_{B^{34}_{12}}\sum_{i=1}^{N}\left|\partial_i\left(\xi^{34}_{12}\frac{\Psi_F}{|x_2-x_1|}\right)\right|^2\\ \leq& \binom{N}{2}2(N-1)\sum_{a\in\{s,t\}}\sum_{\{\sigma\}\in S^{34}_{12}}\left\langle\chi_\sigma\left|\mathrm{P}^{12}_a\right|\chi_\sigma\right\rangle\\ &\times\left[\int_{A^{34}_{12}\cap\{\sigma\}}\sum_{i=1}^{N}\left|\partial_i\left(\left(\xi^{34}_{12}\right)_a\frac{\Psi_F}{|x_2-x_1|}\right)\right|^2\right].\end{aligned} \tag{4.2.38}$$

One may use that $\left\langle\chi_\sigma\left|\mathrm{P}^{12}_a\right|\chi_\sigma\right\rangle$ is independent of σ, however, since we are not interested in finding the optimal constant in Lemma 43 we instead use the more crude bound, $\left\langle\chi_\sigma\left|\mathrm{P}^{12}_a\right|\chi_\sigma\right\rangle \leq 1$, to find

$$\begin{aligned}E^{34}_{12} \leq& \binom{N}{2}2(N-1)\sum_{a\in\{s,t\}}\left[\int_{A^{34}_{12}}\sum_{i=1}^{4}\left|\partial_i\left(\left(\xi^{34}_{12}\right)_a\frac{\Psi_F}{|x_2-x_1|}\right)\right|^2\right.\\ &\left.+\int_{A^{34}_{12}}\sum_{i=5}^{N}\overline{\left(\xi^{34}_{12}\right)_a\frac{\Psi_F}{|x_2-x_1|}}\left(\xi^{34}_{12}\frac{(-\partial_i^2\Psi_F)}{|x_2-x_1|}\right)\right].\end{aligned} \tag{4.2.39}$$

where we used integration by parts and $\bigsqcup_{\{\sigma\}\in S^{34}_{12}}\left(A^{34}_{12}\cap\{\sigma\}\right) \subset A^{34}_{12}$. Using that Ψ_F is an eigenfunction of $(-\Delta)$, with eigenvalue E_F we further find

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

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

$$\begin{aligned}
E_{12}^{34} \leq & 4 \sum_{a\in\{s,t\}} \int_{A_{12}^{34}} \left(\sum_{i=1}^{4} \partial_{y_i}\partial_{x_i} \frac{\overline{\left(\xi_{12}^{34}\right)_a(y)}}{|y_2-y_1|} \frac{\left(\xi_{12}^{34}\right)_a(x)}{|x_2-x_1|} \gamma^{(4)}(y_1,y_2,y_3,y_4;x_1,x_2,x_3,x_4)\Big|_{y=x} \right. \\
& + \left| \frac{\left(\xi_{12}^{34}\right)_a(x)}{|x_2-x_1|} \right|^2 \left| \sum_{i=1}^{4} \partial_{y_i}^2 \gamma^{(4)}(y_1,y_2,y_3,y_4;x_1,x_2,x_3,x_4)\Big|_{y=x} \right| \\
& \left. + E_F \left| \frac{\left(\xi_{12}^{34}\right)_a(x)}{|x_2-x_1|} \right|^2 \rho^{(4)}(x_1,x_2,x_3,x_4) \right) \\
\leq & \text{ const. } E_F \left(N(\rho b)^4 + N^2 (\rho b)^6 \right)
\end{aligned} \tag{4.2.41}$$

where we used the following bounds

$$\begin{aligned}
\partial_{y_i}\partial_{x_i} \frac{\gamma^{(4)}(y_1,y_2,y_3,y_4;x_1,x_2,x_3,x_4)}{|x_2-x_1|\,|y_2-y_1|}\Bigg|_{y=x} & \leq \text{const.}\rho^8, \\
\partial_{y_i} \frac{\gamma^{(4)}(y_1,y_2,y_3,y_4;x_1,x_2,x_3,x_4)}{|x_2-x_1|\,|y_2-y_1|}\Bigg|_{y=x} & \leq \text{const.}\rho^8 |x_3-x_4|, \\
\frac{\gamma^{(4)}(y_1,y_2,y_3,y_4;x_1,x_2,x_3,x_4)}{|x_2-x_1|\,|y_2-y_1|}\Bigg|_{y=x} & \leq \text{const.}\rho^8 |x_3-x_4|^2, \\
\left| \sum_{i=1}^{4} \partial_{y_i}^2 \gamma^{(4)}(y_1,y_2,y_3,y_4;x_1,x_2,x_3,x_4)\Big|_{y=x} \right| & \leq \text{const.}\rho^{10} |x_1-x_2|^2 |x_3-x_4|^2,
\end{aligned} \tag{4.2.42}$$

and

$$\rho^{(4)}(x_1,x_2,x_3,x_4) \leq \text{const.}\rho^8 |x_1-x_2|^2 |x_3-x_4|^2, \tag{4.2.43}$$

which all follows from Taylor expansion of the free Fermi reduced density (matrices). Furthermore, we used the bounds

$$\sqrt{\left|\partial_i \left(\xi_{12}^{34}\right)_a\right|^2} \leq b \max\left(\frac{\sqrt{2}}{b}, \frac{1}{b-a_o} \right) \leq 2, \qquad \sqrt{\left|\left(\xi_{12}^{34}\right)_a\right|^2} \leq b \tag{4.2.44}$$

which follows from properties of the scattering solution, monotonicity of its derivative, and Lemma 42. □

Estimating E_{12}^{23} (proof of Lemma 44)

Proof of Lemma 44. 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

$$\xi_{12}^{23} := \Big(\big(\eta(|x_2 - x_3|)\omega_e^{12}(|x_1 - x_2|) + (1 - \eta(|x_2 - x_3|))\omega_o^{12}(|x_1 - x_2|)\big) \operatorname{P}_s^{1,2} + \omega_o^{12}(|x_1 - x_2|) \operatorname{P}_t^{1,2} \Big) \chi_\sigma \tag{4.2.45}$$

on $A_{12}^{23} \cap \{\sigma\}$, for all sectors $\{\sigma\} \in S_{12}^{23}$, with

$$S_{12}^{23} := \big\{ \text{sectors } \{\sigma\} \mid (1,2,3) = (\sigma_k, \sigma_{k+1}, \sigma_{k+2}) \text{ or } (3,2,1) = (\sigma_k, \sigma_{k+1}, \sigma_{k+2}) \text{ for some } k \big\} \tag{4.2.46}$$

. We then see that $\Psi_\chi = \xi_{12}^{23} \frac{\Psi_F}{|x_2 - x_1|}$ on B_{12}^{23}: Hence defining

$$\begin{aligned} \left(\xi_{12}^{23}\right)_s &:= \eta(|x_2 - x_3|)\omega_e^{12}(|x_1 - x_2|) + (1 - \eta(|x_2 - x_3|))\omega_o^{12}(|x_1 - x_2|), \\ \left(\xi_{12}^{23}\right)_t &:= \omega_o^{12}(|x_1 - x_2|), \end{aligned} \tag{4.2.47}$$

we find using $B_{12}^{23} \subset A_{12}^{23}$

$$\begin{aligned} E_{12}^{23} = & \binom{N}{2} 2(N-2) \int_{B_{12}^{23}} \sum_{i=1}^{N} \left| \partial_i \left(\xi_{12}^{23} \frac{\Psi_F}{|x_2 - x_1|} \right) \right|^2 \\ \leq & \binom{N}{2} 2(N-1) \sum_{a \in \{s,t\}} \sum_{\{\sigma\} \in S_{12}^{23}} \left\langle \chi_\sigma \left| \operatorname{P}_a^{12} \right| \chi_\sigma \right\rangle \\ & \times \left[\int_{A_{12}^{23} \cap \{\sigma\}} \sum_{i=1}^{N} \left| \partial_i \left(\left(\xi_{12}^{23}\right)_a \frac{\Psi_F}{|x_2 - x_1|} \right) \right|^2 \right]. \end{aligned} \tag{4.2.48}$$

One may use that $\left\langle \chi_\sigma \left| \operatorname{P}_a^{12} \right| \chi_\sigma \right\rangle$ is independent of σ, however, since we are not interested in finding the optimal constant in Lemma 44 we instead use the more crude bound, $\left\langle \chi_\sigma \left| \mathrm{P}_a^{12} \right| \chi_\sigma \right\rangle \leq 1$, to find

$$\begin{aligned}E_{12}^{23} \leq & \binom{N}{2} 2(N-1) \sum_{a\in\{s,t\}} \left[\int_{A_{12}^{23}} \sum_{i=1}^{3} \left| \partial_i \left(\left(\xi_{12}^{23}\right)_a \frac{\Psi_F}{|x_2-x_1|} \right) \right|^2 \right. \\ & \left. + \int_{A_{12}^{23}} \sum_{i=4}^{N} \overline{\left(\xi_{12}^{23}\right)_a \frac{\Psi_F}{|x_2-x_1|}} \left(\xi_{12}^{23} \frac{(-\partial_i^2 \Psi_F)}{|x_2-x_1|} \right) \right].\end{aligned} \tag{4.2.49}$$

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

$$\begin{aligned}E_{12}^{23} \leq & \binom{N}{2} 2(N-2) \sum_{a\in\{s,t\}} \left[\int_{A_{12}^{23}} \sum_{i=1}^{3} \left| \partial_i \left(\left(\xi_{12}^{23}\right)_a \frac{\Psi_F}{|x_2-x_1|} \right) \right|^2 \right. \\ & - \int_{A_{12}^{23}} \sum_{i=1}^{3} \overline{\left(\xi_{12}^{23}\right)_a \frac{\Psi_F}{|x_2-x_1|}} \left(\left(\xi_{12}^{23}\right)_a \frac{(-\partial_i^2 \Psi_F)}{|x_2-x_1|} \right) \\ & \left. + E_F \int_{A_{12}^{23}} \left| \left(\xi_{12}^{23}\right)_a \frac{\Psi_F}{|x_2-x_1|} \right| \right].\end{aligned} \tag{4.2.50}$$

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

$$\begin{aligned}E_{12}^{23} \leq & 4 \sum_{a\in\{s,t\}} \int_{A_{12}^{23}} \left(\sum_{i=1}^{3} \partial_{y_i} \partial_{x_i} \frac{\overline{\left(\xi_{12}^{23}\right)_a (y)}}{|y_2-y_1|} \frac{\left(\xi_{12}^{23}\right)_a (x)}{|x_2-x_1|} \gamma^{(3)}(y_1,y_2,y_3;x_1,x_2,x_3) \right|_{y=x} \\ & + \left| \frac{\left(\xi_{12}^{23}\right)_a (x)}{|x_2-x_1|} \right|^2 \left| \left. \sum_{i=1}^{3} \partial_{y_i}^2 \gamma^{(3)}(y_1,y_2,y_3;x_1,x_2,x_3) \right|_{y=x} \right| \\ & \left. + E_F \left| \frac{\left(\xi_{12}^{23}\right)_a (x)}{|x_2-x_1|} \right|^2 \rho^{(3)}(x_1,x_2,x_3) \right) \\ \leq & \text{ const. } E_F \left((\rho b)^4 + N (\rho b)^6 \right)\end{aligned} \tag{4.2.51}$$

where we used the following bounds

$$
\begin{aligned}
\partial_{y_i}\partial_{x_i}\frac{\gamma^{(3)}(y_1,y_2,y_3;x_1,x_2,x_3)}{|x_2-x_1|\,|y_2-y_1|}\Bigg|_{y=x} &\le \text{const.}\rho^7,\\
\partial_{y_i}\frac{\gamma^{(3)}(y_1,y_2,y_3;x_1,x_2,x_3)}{|x_2-x_1|\,|y_2-y_1|}\Bigg|_{y=x} &\le \text{const.}\rho^7\,|x_3-x_4|\,,\\
\frac{\gamma^{(3)}(y_1,y_2,y_3;x_1,x_2,x_3)}{|x_2-x_1|\,|y_2-y_1|}\Bigg|_{y=x} &\le \text{const.}\rho^7\,|x_3-x_4|^2\,,\\
\left|\sum_{i=1}^{3}\partial^2_{y_i}\gamma^{(3)}(y_1,y_2,y_3;x_1,x_2,x_3)\Big|_{y=x}\right| &\le \text{const.}\rho^{11}\,|x_1-x_2|^2\,|x_2-x_3|^2\,|x_1-x_3|^2\,,
\end{aligned}
\tag{4.2.52}
$$

and

$$
\rho^{(3)}(x_1,x_2,x_3)\le \text{const.}\rho^9\,|x_1-x_2|^2\,|x_2-x_3|^2\,|x_1-x_3|^2\,, \tag{4.2.53}
$$

which all follows from Taylor expansion of the free Fermi reduced density (matrices). Furthermore, we used the bounds

$$
\sqrt{\left|\partial_i\left(\xi_{12}^{23}\right)_a\right|^2}\le b\max\left(\frac{\sqrt{2}}{b},\frac{1}{b-a_o}\right)\le 2,\qquad \sqrt{\left|\left(\xi_{12}^{23}\right)_a\right|^2}\le b \tag{4.2.54}
$$

which follows from properties of the scattering solution, monotonicity of its derivative, and Lemma 42. □

4.3 Extending the upper bound to other symmetries and spin dependent potentials

We present here corollaries that follows directly, *mutatis mutandis*, from the proof of Theorem 41. We also give an application of one the results, to a model where the new upper bound improves best up to now best known result.

Spin-1/2 bosons

Going through the proof of Theorem 41 (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

$$\Psi_\chi = \begin{cases} \frac{\Psi_F}{\mathcal{R}} \left((\eta \omega_e^{\mathcal{R}} + (1-\eta)\omega_o^{\mathcal{R}}) \mathrm{P}_t^{\mathcal{R}} + \omega_o^{\mathcal{R}} \mathrm{P}_s^{\mathcal{R}} \right) \chi, & \mathcal{R}(x) < b \\ \Psi_F, & \mathcal{R}(x) \geq b \end{cases}. \tag{4.3.1}$$

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 50 (Bosonic version of Theorem 41)**.** *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 41 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 $v_{e/o} = v_{e/o,\text{h.c.}} + v_{e/o,\text{reg}}$ each satisfying the assumptions on v. In this case the $E_{1,e/o}$ becomes

$$\begin{aligned} E_{1,e} &:= \binom{N}{2} \left(\int_{A_{12}} \sum_{i=1}^N |\partial_i (\Psi_e)_{12}|^2 + \sum_{1 \leq i < j \leq N} (v_{e,\text{reg}})_{ij} \left| (\Psi_e)_{12} \right|^2 - \sum_{i=1}^N |\partial_i \Psi_F|^2 \right), \\ E_{1,o} &:= \binom{N}{2} \left(\int_{A_{12}} \sum_{i=1}^N |\partial_i (\Psi_o)_{12}|^2 + \sum_{1 \leq i < j \leq N} (v_{o,\text{reg}})_{ij} \left| (\Psi_o)_{12} \right|^2 - \sum_{i=1}^N |\partial_i \Psi_F|^2 \right), \end{aligned} \tag{4.3.4}$$

Consequently, Theorem 41 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 51 (Spin dependent version of Theorem 41)**.** *Let $v = v_e \,\mathrm{P}_s + v_o \,\mathrm{P}_t \geq 0$ 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 41 but change $\omega_{e/o}$ to even/odd wave scattering solutions of $v_{e/o}$. Notice that it is no longer clear that $a_o > a_e$ 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. □

An interesting application of a version of Corollary 51 given below in Corollary 52 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 $c > c'$

$$E_{LLH} \leq E_{LL}(\ln(2)c' + (1-\ln(2))c), \tag{4.3.7}$$

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

$$H_{LLH} = -\sum_i \partial_i^2 + 2\sum_{i<j}\left(c' \,\mathrm{P}_s^{i,j} + c\,\mathrm{P}_t^{i,j}\right)\delta(x_i - x_j), \tag{4.3.8}$$

However the domain is taken to be wave functions that are *symmetric in the spacial coordinates* meaning 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. This of course implies that Corollary 51 is not directly useful in this case. However, Going through the proof of Theorem 41, we see that we may as well get the following corollary

Corollary 52 (Spatially symmetric, spin dependent version of Theorem 41)**.** *Let* $v = v_s \,\mathrm{P}_s + v_t \,\mathrm{P}_t \geq 0$ *satisfy the assumption from above, then the ground state energy of the dilute spin–*$1/2$ *spacially symmetric gas satisfies*

$$E \leq N\frac{\pi^2}{3}\rho^2\left(1 + 2\rho\left(\ln(2)a_s + (1-\ln(2))a_t\right) + \mathcal{O}\left((\rho R)^{6/5} + N^{-1}\right)\right), \tag{4.3.9}$$

if $a_t \geq a_s$ *and*

$$E \leq N\frac{\pi^2}{3}\rho^2\left(1 + 2\rho a_t + \mathcal{O}\left((\rho R)^{6/5} + N^{-1}\right)\right), \tag{4.3.10}$$

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 41 (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 41 the same step may be justified by spacial symmetry. To see this, we note that (4.2.10) can be derived by use of only spatial symmetry. However, in (4.2.12) we find instead

$$\begin{aligned}\int_{B_{12}^{\geq}} |\partial_i \Psi_\chi|^2 \leq & \sum_{\{\sigma\}\in S_{12}} \left(\int_{A_{12}\cap\{\sigma\}} |\partial_i (\Psi_e)_{12}|^2\right) \left\langle \chi \left| \mathrm{P}_s^{\sigma^{-1}(1),\sigma^{-1}(2)} \right| \chi \right\rangle \\ &+ \sum_{\{\sigma\}\in S_{12}} \left(\int_{A_{12}\cap\{\sigma\}} |\partial_i (\Psi_o)_{12}|^2\right) \left\langle \chi \left| \mathrm{P}_t^{\sigma^{-1}(1),\sigma^{-1}(2)} \right| \chi \right\rangle,\end{aligned} \tag{4.3.11}$$

where $\sigma^{-1}(i)$ is defined such that $\sigma_{\sigma^{-1}(i)} = i$. This is a consequence of the fact that the spins are not permuted when defining the trial state using the spatial symmetry. A similar modification is made in the proofs of Lemmas 43 and 44. 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 52 (up to a small error in the dilute limit) is

$$E_{LLH} \leq E_{LL}\left(\left(\frac{\ln(2)}{c'} + \frac{1-\ln(2)}{c}\right)^{-1}\right), \tag{4.3.12}$$

when $c > c'$. By the weighted harmonic-arithmetic mean inequality it is clear that our bound improves (4.3.7). The two bounds agree in the limit $\frac{c-c'}{c'} \to 0$. However, (4.3.7) 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.

4.4 Lower bound

In this section, we will further motivate the Conjecture 40, however a complete proof of a lower bound matching the upper bound in Theorem 41 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 40.

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 30. In this case we have

$$E = E_F\left(L \to \frac{1}{1-\rho a}L\right) = N\frac{\pi^2}{3}\rho^2\left(1-\rho a\right)^{-2} + \rho^2\mathcal{O}(1), \tag{4.4.1}$$

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

$$E = N\frac{\pi^2}{3}\rho^2\left(1-\ln(2)\rho a_e - (1-\ln(2))\rho a_o\right)^{-2} + \rho^2\mathcal{O}(1), \tag{4.4.2}$$

which match Conjecture 40.

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 29 Of course the upper bound from Theorem 41 applies. Furthermore, we found in Proposition 39 the bound

$$e = \lim_{\substack{N,L\to\infty \\ N/L=\rho}} E/L \geq \frac{\pi^2}{3}\rho^3 \left[(1 - \ln(2)\rho a_e)^{-2}\right]. \tag{4.4.3}$$

Hence we conclude $e = \frac{\pi^2}{3}\rho^3\left(1 + 2\ln(2)\rho a_e + \mathcal{O}(\rho R)^{6/5}\right)$, which is in agreement with Conjecture 40.

The general case

In the case of a general potential, v, where the resulting model is not solvable, we migth 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 20 and 21 of Chapter 3 does not depend on any symmetry of the wave function. Dyson's lemma (Lemma 22 of Chapter 3) is modifed slightly in the following way: Let $H^1_{\text{even/odd}}$ denote even/odd H^1 functions, then we have the following lemma.

Lemma 53 (Dyson's lemma spin–1/2 fermions)**.** *Let* $R > R_0 = \text{range}(v)$ *and* $\varphi \in \left(H^1_{\text{even}}(\mathbb{R}) \otimes \mathrm{P}_s\left(\mathbb{C}^2\right)^2\right) \oplus \left(H^1_{\text{odd}}(\mathbb{R}) \otimes \mathrm{P}_t\left(\mathbb{C}^2\right)^2\right)$, *then for any interval* $\mathcal{I} \ni 0$

$$\int_{\mathcal{I}} |\partial\varphi|^2 + \frac{1}{2}v|\varphi|^2 \geq \int_{\mathcal{I}} \overline{\varphi}\left(\frac{1}{R-a_e}\,\mathrm{P}_s + \frac{1}{R-a_o}\,\mathrm{P}_t\right)(\delta_R + \delta_{-R})\,\varphi, \tag{4.4.4}$$

where a *is the s-wave scattering length.*

Proof. The lemma follows straigthforwardly from the Definitions 24 and 25. □

Thus we may prove the equivalent of Lemma 23 of Chapter 3: In the following Ψ denotes the spin–1/2 fermionic (Neumann) ground state of

$$H = -\sum_{i=1}^{N}\partial_i^2 + \sum_{1\leq i<j\leq N} v(x_i - x_j). \tag{4.4.5}$$

We shall also define the contionuous 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 $0 \leq x_1 \leq \cdots \leq x_n \leq L-(n-1)R$

$$\psi(x_1, x_2, \dots, x_n) := \Psi(x_1, R + x_2, \dots, (n-1)R + x_n), \tag{4.4.6}$$

and extended by spacial symmtry.

Lemma 54. *Let $R > \max(R_0, 2|a|)$ and $\epsilon \in [0,1]$. For ψ defined in (4.4.6),*

$$\begin{aligned}\int \sum_i |\partial_i \Psi|^2 + \sum_{i \neq j} \frac{1}{2} v_{ij} |\Psi|^2 \geq E^N_{LLH}\left(N, \tilde{L}, \frac{2\epsilon}{R - a_e}, \frac{2\epsilon}{R - a_o}\right) \langle \psi | \psi \rangle \\ + \frac{(1-\epsilon)}{R^2} \text{const. } (1 - \langle \psi | \psi \rangle).\end{aligned} \tag{4.4.7}$$

where $\tilde{L} := L - (n-1)R$, the superscirpt "N" denotes Neumann boundary condition, and $E_{LLH}(N, L, c', c)$ is the ground state energy of the Lieb-Liniger-Heisenberg model in (4.3.8).

Proof. We mimic the proof of Chapter 3: Splitting the energy functional in two parts, and using Lemma 21 from Chapter 3 on one term and Lemma 53 on the other, we find

$$\begin{aligned}&\int \sum_i |\partial_i \Psi|^2 + \sum_{i \neq j} \frac{1}{2} v_{ij} |\Psi|^2 \geq \\ &\int \sum_i |\partial_i \Psi|^2 \mathbb{1}_{\mathfrak{r}_i(x) > R} + \overline{\Psi} \epsilon \sum_i \delta(\mathfrak{r}_i(x) - R) \left(\frac{1}{R - a_e} \mathrm{P}_s^{i,j_i} + \frac{1}{R - a_o} \mathrm{P}_t^{i,j_i} \right) \Psi \\ &\qquad + (1-\epsilon) \left(\sum_{i<j} \int_{D_{ij}} |\partial_i \Psi|^2 + \int \sum_{i<j} v_{ij} |\Psi|^2 \right),\end{aligned} \tag{4.4.8}$$

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 53 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 use of Lemma 21 of Chapter 3 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-Heisenberg model (since the two delta functions collapse to a single delta of twice the strength when volume R is removed between particles), we obtain

$$\int \sum_i |\partial_i \Psi|^2 + \sum_{i\neq j} \frac{1}{2} v_{ij} |\Psi|^2 \geq E^N_{LLH}\left(N, \tilde{L}, \frac{2\epsilon}{R-a_e}, \frac{2\epsilon}{R-a_o}\right)\langle\psi|\psi\rangle + \frac{(1-\epsilon)}{R^2}\text{const. } (1-\langle\psi|\psi\rangle),$$

which is the desired result. □

We may also prove the equivalent of Lemma 24 of Chapter 3, by using that $E_{LLH}(N, \tilde{L}, c', c) \geq E_{LL}(N.\tilde{L}, c')$ when $c > c'$.

Lemma 55. *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 24 in Chapter 3: From the known upper bound, *i.e.* Theorem 41, and by Lemma 54 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 18 of Chapter 3 on the left-hand side, we find

$$\begin{aligned} &n\frac{\pi^2}{3}\Bigg(\rho^2\left(1 + 2\rho\left(\ln(2)a_e + (1-\ln(2)a_o)\right) + \text{const. } (\rho R)^{6/5}\right) \\ &\qquad - \tilde{\rho}^2\left(1 - 4\tilde{\rho}(R-a_e) - \text{const. } n^{-2/3}\right)\Bigg) \\ &\geq \left(\frac{1}{16R^2} - E^N_{LLH}\left(N, \tilde{L}, \frac{1}{R-a_e}, \frac{1}{R-a_o}\right)\right)(1-\langle\psi|\psi\rangle), \end{aligned} \tag{4.4.11}$$

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

$$\text{const. } n\rho^2 R^2 \left(\rho R + (\rho R)^{6/5} + n^{-2/3}\right) \geq \left(\frac{1}{16} - R^2 n \frac{4\pi^2}{3}\rho^2\right)(1 - \langle\psi|\psi\rangle)\,. \tag{4.4.12}$$

It follows that we have

$$\langle\psi|\psi\rangle \geq 1 - \text{const. } \left(n(\rho R)^3 + n^{1/3}(\rho R)^2\right). \tag{4.4.13}$$

□

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Appendix A

Periodic boundary conditions

If we consider the case with periodic boundary conditions in the box, one may actually 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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