



PhD thesis

# One Dimensional Dilute Quantum Gases and Their Ground State Energies

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# Contents

<b>Contents</b>	<b>ii</b>
<b>1 Introduction</b>	<b>1</b>
<b>2 Many-Body Quantum Mechanics</b>	<b>3</b>
2.1 Many-body Wave Functions . . . . .	3
Identical Particles: Bosons and Fermions . . . . .	4
2.2 Observables, Dynamics, and Energy . . . . .	5
Many-Body Hamiltonians . . . . .	7
2.3 The Scattering Length . . . . .	11
2.4 The Ground state Energy of Dilute Bose Gases . . . . .	12
2.5 The Lieb-Liniger Model: A Solvable Model in One Dimension . . . . .	12
The ground state . . . . .	15
Lower bound in the large $c$ limit . . . . .	17
2.6 The Yang-Gaudin Model . . . . .	18
<b>3 The ground state energy of the one dimensional dilute Bose gas (paper)</b>	<b>19</b>
<b>4 The ground state energy of the one dimensional dilute spin-<math>\frac{1}{2}</math> Fermi gas</b>	<b>65</b>
4.1 The model . . . . .	65
4.2 Upper bound . . . . .	66
Constructing a trial state . . . . .	66
Proof of Theorem 27 . . . . .	68
4.3 Extensions to other symmetries and spin dependent potentials . . . . .	80
Spin-1/2 bosons . . . . .	80
Spin dependent potentials . . . . .	81

<i>CONTENTS</i>	iii
4.4 Lower bound . . . . .	84
<b>A Periodic boundary conditions</b>	<b>85</b>
<b>Bibliography</b>	<b>87</b>



# Chapter 1

## Introduction

Introduction



## Chapter 2

# Many-Body Quantum Mechanics

In this chapter we give a brief introduction to many-body quantum mechanics. The chapter will serve to define relevant quantities, 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  $\Psi$  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

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

where  $S_i$  is the *spin* of the  $i$ th 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  $C_N := \{(x_1, \dots, x_N) \in \Omega^N \mid x_i \neq x_j \text{ if } i \neq j\}$  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.

**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  $d = 1$ ,  $C_{p,N} = \{x_1 < x_2 < \dots < x_N\}$ . 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  $C_N := \{(z_1, \dots, z_N) \in (\Omega \times \{-S, \dots, S\})^N \mid (z_i)_1 \neq (z_j)_1 \text{ if } i \neq j\}$ , and  $C_{p,N} := C_N/S_N$ . In this case  $C_{p,N}$  is not path connected, however, for each configuration of spins  $\sigma = (\sigma_1, \dots, \sigma_N) \in \{-S, \dots, S\}^N$  the configurations spaces  $C_{p,N,\sigma} = \{((x_1, \sigma_1), \dots, (x_N, \sigma_N)) \in (\Omega \times \{-S, \dots, S\})^N \mid x_i \neq x_j \text{ if } i \neq j\}$  are path connected and their fundamental groups are isomorphic to the fundamental group in the spinless case independent of  $\sigma$ .

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  $L_s^2\left((\Omega \times \{-S, \dots, S\})^N\right) \cong \vee_{i=1}^N L^2(\Omega; \mathbb{C}^{2S+1})$  and for fermions we restrict to wave-functions in the anti-symmetric (or fermionic) subspace  $L_a^2\left((\Omega \times \{-S, \dots, S\})^N\right) \cong \wedge_{i=1}^N L^2(\Omega; \mathbb{C}^{2S+1})$ .

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

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

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

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

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

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

## 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  $\mathcal{O} = \int_{\sigma(\mathcal{O})} \lambda dP_\lambda$ , 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  $P((\mathcal{O}, \Psi) \rightarrow \lambda \in M) = \int_{\lambda \in M} \langle \Psi, P_\lambda \Psi \rangle$ . Furthermore 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.

In 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

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

where we have set  $\hbar = 1$ .

**Remark 7.** *By Stone's theorem (ref Reed and Simon), the existence of a self-adjoint Hamiltonian,  $H$ , is guaranteed for any time evolution described by  $\Psi(t) = U(t - t_0)\Psi(t_0)$ , when  $U(t)$  is a strongly continuous one-parameter unitary group.*

Since the Hamiltonian,  $H$ , is self-adjoint, it represents an observable which we call *energy*. 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*

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

**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**,  $\mathcal{E}_H : \mathcal{D}(\mathcal{E}_H) \rightarrow \mathbb{R}$ , 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

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

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 very definition of the ground state energy. Furthermore, one can also define the dynamics of a quantum system by specifying an energy quadratic form in the following sense

**Remark 14** (Ref!!). Given a densely defined, lower bounded, closable, quadratic form  $\mathcal{E} : \mathcal{D}(\mathcal{E}) \rightarrow \mathbb{R}$  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  $\bar{\mathcal{E}}$ , 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

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

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<sup>1</sup>

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

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

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

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**

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

with domain  $\mathcal{D}(\mathcal{E}_{(v,\sigma)}) = \{\Psi \in (C_0^\infty(\Omega^N))_{b/f} | \mathcal{E}_{(v,\sigma)}(\Psi) < \infty\}$ . 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.

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<sup>1</sup>This is usually justified by going through a canonical quantization procedure for the classical Hamiltonian function of the system we are interested in modeling

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  $\mathcal{H}_{(v,\sigma)} := \overline{\mathcal{D}(\mathcal{E}_{(v,\sigma)})}^{\|\cdot\|_2}$  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  $\mathcal{H}_{(v,\sigma)} := \overline{\mathcal{D}(\mathcal{E}_{(v,\sigma)})}^{\|\cdot\|_2} \subset L^2_{s/a}(\Omega^N)$  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  $\geq 2$  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  $n \rightarrow \infty$*

and  $(\psi_n)_{n \in \mathbb{N}} \subset L^2 \left( \Omega^N, \underbrace{\sum_{i < j} v(x_i - x_j) d\lambda^N}_{:= d\mu_v} \right)$  Cauchy, implies  $\psi_n \xrightarrow{\|\cdot\|_{L^2(\Omega^N, d\mu_v)}} 0$ .

*0. This is evident from the fact that  $\psi_n \xrightarrow{\|\cdot\|_{L^2(\Omega^N, d\mu_v)}} f$  for some  $f \in L^2(\Omega^N, d\mu_v)$  by completeness. Now  $\psi_n$  has a subsequence that converges  $\lambda^N$ -almost everywhere to 0, and this subsequence further has a subsequence that converges  $\mu_v$ -almost everywhere to  $f$ . Hence  $f = 0$   $\mu_v$ -almost everywhere, as  $\mu_v \ll v$ . 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  $\sigma$ -finite measure  $v d\lambda^N$  is allowed as potential. Notice that we slightly abuse notation and write  $v(x_i - x_j) d\lambda^N$  even when

$v$  is a singular continuous measure and thus has no density. However, we do think of  $v$  as being a one-dimensional measure in the sense that

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

where we defined  $d\mu_{v_{ij}} := v(x_i - x_j) d(x_i - x_j)$  and  $\lambda_{(x_i - x_j) = \text{fixed}}^{N-1}$  to be the measure such that  $d\lambda^N = d(x_i - x_j) \times d\lambda_{(x_i - x_j) = \text{fixed}}^{N-1}$ . Uniqueness of the product measure is guaranteed by  $\sigma$ -finiteness of  $v$ . We will need the following essential lemma, where we use the notation  $\lambda_k^{N-1} := \prod_{i \neq k} dx_i$

**Lemma 19.** *Let  $(f_n)_{n \in \mathbb{N}} \subset H^1(\Omega^N)$  be a sequence such that  $\|f_n\|_{H^1} \rightarrow 0$  as  $n \rightarrow \infty$ . Then defining  $f_n^k(t, \bar{x}^k) := f_n(x_1, \dots, x_{k-1}, t, x_{k+1}, \dots, x_N)$  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,  $\lambda_k^{N-1}$ -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  $\lambda^N$ -a.e. to 0. Since  $f_n \in H^1(\Omega^N)$ , we know for any  $k = 1, \dots, N$  that  $f_n^k(t, \bar{x}^k)$  are in  $H^1(\Omega)$  (as functions of  $t$ )  $\lambda_k^{N-1}$ -a.e. [[EG91] Theorem 2 p. 164]. Now consider the  $H^1(\Omega)$  norms of  $g_n^k(\bar{x}^k) := \|f_n^k(\cdot, \bar{x}^k)\|_{H^1(\Omega)}$ . Clearly  $g_n^k$  constitute  $L^2$  functions, with norms converging to 0. Hence there exist a subsequence that converges pointwise  $\lambda_k^{N-1}$ -almost everywhere to 0. There there is a subsequence  $f_{n_i}^k$  such that for  $\lambda_k^{N-1}$ -a.e.  $\bar{x}^k$ ,  $f_{n_i}^k(\cdot, \bar{x}^k)$  converges to 0 in  $H^1(\Omega)$ . But then  $f_{n_i}^k(\cdot, \bar{x}^k)$  converges, by Morrey's inequality, pointwise to 0.  $\square$

Using this lemma, we may prove the following Proposition

**Proposition 20.** *Let  $d = 1$ , then for any  $\sigma$ -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  $\mathcal{H}_{(v, \sigma)} := \overline{\mathcal{D}(\mathcal{E}_{(v, \sigma)})}^{\|\cdot\|_2}$  and  $d\mu_v = \sum_{1 \leq i < j \leq N} v(x_i - x_j) d\lambda^N$ . Clearly  $\mathcal{E}_{(v, \sigma)}$  is lower bounded and densely defined in  $\mathcal{H}_{(v, \sigma)}$ . Closability amounts to showing that  $\psi_n \xrightarrow{\|\cdot\|_{L^2(\Omega^N, d\lambda^N)}} 0$  and  $(\psi_n)_{n \in \mathbb{N}} \subset L^2(\Omega^N, d\mu_v)$  Cauchy w.r.t the norm  $\|\cdot\|_{\mathcal{E}_{(v, \sigma)}} = \sqrt{\mathcal{E}_{(v, \sigma)}(\cdot) + \|\cdot\|_2^2}$ , implies  $\psi_n \xrightarrow{\|\cdot\|_{L^2(\Omega^N, d\mu_v)}} 0$ . Now since  $(\psi_n)_{n \in \mathbb{N}}$  is a Cauchy sequence in  $L^2(\Omega^N, d\mu_v)$ , it has a subsequence that converges  $\mu_v$ -almost everywhere to some function  $f \in L^2(\Omega^N, d\mu_v)$ .

Furthermore, this subsequence has a further subsequence that converges  $\lambda^N$ -almost everywhere to 0. However, since  $(\psi_n)_{n \in \mathbb{N}}$  converges in  $H^1(\Omega^N, d\lambda^N)$ , Lemma 19 implies that for  $(x_i - x_j)$  fixed  $(\psi_n)_{n \in \mathbb{N}}$  converges  $\lambda^{N-1}$ -a.e. to 0. Hence  $(\psi_n)_{n \in \mathbb{N}}$  converges pointwise to 0 on  $\lambda^{N-1}$ -almost all lines. Now notice that  $d\mu_v = \sum_{1 \leq i < j \leq N} d\mu_{v_{ij}} \times d\lambda_{(x_i - x_j) = \text{fixed}}^{N-1}$ . Thus for  $\lambda_{(x_i - x_j) = \text{fixed}}^{N-1}$ -almost all lines in  $\Omega^N$  with  $x_i + x_j$  and  $x_k$  fixed for all  $k \neq i, j$ , by passing to a subsequence  $\psi_n$  converges pointwise to 0, by Lemma 19. But also on  $\lambda_{(x_i - x_j) = \text{fixed}}^{N-1}$ -almost all these lines  $\psi_n$  converges  $\mu_{v_{ij}}$ -almost everywhere to  $f$ , and hence  $f = 0$   $\mu_{v_{ij}}$ -almost everywhere. Thus we conclude that  $f = 0$   $\mu_v$ -almost everywhere. The lemma now follows from Remark 14.  $\square$

**Remark 21.** *Combining Lemma 20 and Remark 18 we conclude that potentials of the form  $v = v_{\sigma\text{-finite}} + v_{\text{abs.cont.}}$ , where  $v_{\sigma\text{-finite}}$  is a  $\sigma$ -finite measure and  $v_{\text{abs.cont.}}$  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  $\delta$ -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.

## 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.

## 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 [? ]. Their solution generalized the solution of the impenetrable bosons by Girardeau. The technique that was used is known as *Bethe ansatz* or *Bethe's hypothesis* after it was invented by Bethe to solve the one dimensional 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 [? ] and present a few more general results.

The Lieb-Liniger model is a model of bosons with dynamics given by the Hamiltonian

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

where the left-hand side is defined in the sense of quadratic forms. More precisely on a *sector*,  $\{\sigma\} = \{\sigma_1, \sigma_2, \dots, \sigma_N\} := \{0 < x_{\sigma_1} < x_{\sigma_2} < \dots < x_{\sigma_N} < L\}$ , where  $\sigma \in S_N$  is a permutation of  $\{1, \dots, N\}$ , 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

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

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

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

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  $P = (p_1, p_2, \dots, p_j = \alpha, p_{j+1} = \beta, \dots, p_N)$  and  $Q = (p_1, p_2, \dots, q_j = \beta, q_{j+1} = \alpha, \dots, p_N)$ , we have  $i(k_\beta - k_\alpha)(a(P) - a(Q)) = c(a(P) + a(Q))$  implying

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

where we have defined

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

We note that we will require  $k_i \neq k_j$  for  $i \neq j$  in order for  $\psi$  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  $\{1, 2, \dots, N\}$  take the form

$$\psi(0, x_2, x_3, \dots, x_N) = \psi(x_2, x_3, \dots, x_N, L), \\ (\partial_x \psi(x, x_2, x_3, \dots, x_N))|_{x=0} = (\partial_x \psi(x_2, x_3, \dots, x_N, x))|_{x=L}. \quad (2.5.5)$$

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

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

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  $(k_i)_{i \in \{1, \dots, N\}}$  solves the equations (2.5.6) then set  $(k'_i = k_i + 2\pi n_0/L)_{i \in \{1, \dots, N\}}$  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  $k_1 < k_2 < \dots < k_N$ , 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

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

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  $k_j - k_i = \frac{1}{L} \sum_{s=i}^{j-1} \delta_s$  for  $j > i$ , hence (2.5.7) is a set of equations determining  $(\delta_i)_{i \in \{1, \dots, N-1\}}$ . Given a set of  $(n_i)_{i \in \{1, \dots, N-1\}}$  and a solution of (2.5.7),  $(\delta_i)_{i \in \{1, \dots, N-1\}}$ , we merely choose  $k_1$  to satisfy (2.5.6) by having

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

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  $\delta$ s.

### 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 23.** *Let  $\Psi_V$  and  $\Psi_T$  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  $c \rightarrow \infty$ . Here it is easily verified that  $\Psi_V = |\Psi_F| = \Psi_T$ , where  $\Psi_F$  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  $\Psi_V$  is an eigenstate, we conclude that the variational ground state must remain the true ground state, as  $1/c$  varies.  $\square$

We note that while Lemma 23 holds for the ground state, its proof cannot be generalized to excited states, since there is no unique  $n$ th excited state in the Bose gas. In this case we refer to the more involved proof of completeness of the Bethe ansatz states by Dorlas [Dor93].

Interestingly, it is possible to study the thermodynamic limit ( $N, L \rightarrow \infty$  with  $N/L = \rho$ ) of system by the use of the Bethe ansatz solution. To do this, we define  $K(\gamma) := \lim_{\substack{N, L \rightarrow \infty \\ N/L = \rho}} k_N$  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)

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

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

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

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

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

Now let  $f$  be such that  $k_{i+1} - k_i = 1/(Lf(k_i))$ . Then by Poisson's summation formula we have

$$2\pi f(k) - 1 = 2c \int_{-K}^K \frac{f(p)}{c^2 + (p - k)^2} dp + \mathcal{O}(1/(cL)). \quad (2.5.12)$$

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

$$E = \sum_i k_i^2 = \int_{-K}^K k^2 f(k) dk, \quad (2.5.13)$$

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

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

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

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

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

$$1 = \frac{\gamma}{\lambda} \int_{-1}^1 g(x) dx. \quad (2.5.17)$$

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

**Proposition 24.** *Let  $E_c$  denote the ground state energy of  $H_{LL}$  with coupling  $c > 0$ . Then  $\lim_{c \rightarrow \infty} E_c = E_F$ , 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  $\Psi_c$  of  $H_{LL}$ , is uniformly (in  $c$ ) bounded in  $H^1$ . Hence  $\Psi_{c_n}$  is, by possibly passing to a subsequence, weakly convergent in  $H^1$ . By the Rellich-Kondrachov

theorem  $\Psi_{c_n}$  converges in  $L^2$  norm to the same limit. Now assuming  $c_n \rightarrow \infty$  as  $n \rightarrow \infty$  we have  $\Psi_{c_n}(x_i = x_j) \rightarrow 0$  in  $L^2(\Omega^{N-1})$  as  $n \rightarrow \infty$  for any  $i, j$  in order for the potential energy to stay finite. But then the limit  $\Psi$  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  $\Psi_{c_n}$ . 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.  $\square$

*Proof in the thermodynamic limit by Bethe ansatz.* It follows from (2.5.17) that  $\lambda \rightarrow \infty$  as  $c \rightarrow \infty$ . 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  $\square$

**Proposition 25.** *Let  $\Psi_c$  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  $\Psi_{c_{n_i}} \rightarrow \Psi$  in  $C^\infty(\overline{\{1, 2, \dots, N\}})$  as  $i \rightarrow \infty$ .*

*Proof.* Since  $\Psi_{c_n}$  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  $\overline{\{1, 2, \dots, N\}}$  is convex, we have by elliptic regularity ([Gri11], Theorem 3.2.3.1) that  $\|\Psi_{c_n}\|_{H^{2m}(\{1, 2, \dots, N\})} \leq C_m \lambda_n^m \|\Psi_{c_n}\|_{L^2(\{1, 2, \dots, N\})} \leq C_m E_F^m$ . By Rellich–Kondrachov, there exist for each  $m \in \mathbb{N}$  a subsequence  $\Psi_{c_{n_i}}^m$  such that  $\Psi_{c_{n_i}}^m$  converges in  $H^{2m-1}(\{1, 2, \dots, N\})$ . By a diagonal argument we find a subsequence,  $\Psi_{c_{n_i}}^i$ , which converges in  $H^k(\{1, 2, \dots, N\})$  for all  $k \in \mathbb{N}$ . Hence, by the Sobolev embedding theorem ([Ada75], Theorem 5.4),  $\Psi_{c_{n_i}}^i$  converges to  $\Psi$  in  $C^\infty(\overline{\{1, 2, \dots, N\}})$ .  $\square$

### 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 25 to give an asymptotic (in  $c$ ) bound in a finite box. The strategy is as follows: Consider the ground state,  $\Psi_c$  of the Lieb-Liniger model in a box of size  $L$ . We define  $\tilde{\Psi}_c : [0, L + (N - 1)R]^N \rightarrow \mathbb{C}$

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  $\{y_{k+1} - kR > y_k \text{ for all } k = 1, \dots, N\} := \Gamma$ . 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  $\Gamma$ . Indeed it is an eigenfunction on  $\Gamma$  with eigenvalue  $E_c$ . Then we have

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

where  $\nabla_n$  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

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

## 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.

## Chapter 3

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

## 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  $\rho$ , 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

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

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  $a$ ,

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

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

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

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  $2c > 0$ ,

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

The ground state can be found explicitly [32], and in the thermodynamic

limit  $L \rightarrow \infty$  with density  $\rho = N/L$  fixed, its energy is

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

where  $e(c/\rho)$  is described by integral equations. Since  $c/\rho$  is the only relevant parameter, diluteness, or low density  $\rho$ , should imply  $c/\rho \gg 1$ . In this case, the ground state energy can be expanded as ([32]; see, for example, [20, 24]),

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

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

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

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]

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

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,  $\text{supp}(v) \subset [-R_0, R_0]$ . Furthermore, we assume  $v = v_{\text{reg}} + v_{\text{h.c.}}$ , where  $v_{\text{reg}}$  is a finite measure, and  $v_{\text{h.c.}}$  is a positive linear combination of ‘hard-core’ potentials of the form

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

for  $0 \leq x_1 \leq x_2 \leq R_0$ .<sup>1</sup> We will consider the  $N$ -body Hamiltonian

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

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

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

with energy functional

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

**Theorem 1** (bosons). *Consider a Bose gas with repulsive interaction  $v = v_{\text{reg}} + v_{\text{h.c.}}$  as defined above. Write  $\rho = N/L$ . For  $\rho|a|$  and  $\rho R_0$  sufficiently small, the ground state energy can be expanded as*

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

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

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<sup>1</sup>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  $h \rightarrow \infty$  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).<sup>2</sup> 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  $\text{supp}(v) \subset [-R_0, R_0]$ ). Let  $R > R_0$ . For*

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<sup>2</sup>Note that Girardeau studied the  $c/\rho \rightarrow \infty$  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  $f(R) = f(-R) = 1$ ,

$$\int_{-R}^R 2|\partial_x f|^2 + v(x)|f(x)|^2 dx \geq \frac{4}{R-a}. \quad (1.14)$$

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  $\rho|a| \rightarrow 0$ . Here, we can rely on Girardeau's solution [16] of the  $c/\rho \rightarrow \infty$  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  $0 \leq x_1 \leq \dots \leq x_N \leq L$  (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<sup>3</sup>

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

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

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

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<sup>3</sup>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.<sup>4</sup>

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

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

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

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

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  $\Psi$ , 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  $\Psi$  from the thrown-out regions).

All this may seem rather radical, but the heuristics work out: starting

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<sup>4</sup>The wave functions  $\Psi_F^{\text{per}}$  and  $|\Psi_F^{\text{per}}|$  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  $v = v_{\text{reg}} + v_{h.c.}$  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  $\rho a_o$  and  $\rho R_0$  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  $c/\rho$  [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]*

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

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

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

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  $0 \leq x_1 < \dots < x_N \leq L$ , we want to add anyonic phases  $e^{i\kappa}$  with  $0 \leq \kappa \leq \pi$  whenever two particles are interchanged? It turns out this can be made to work, going back to, amongst others, [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  $c/\rho \rightarrow \infty$  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  $\kappa$  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  $2c\delta_0/\cos(\kappa/2)$ .<sup>5</sup> 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  $v_{\text{reg}}$  is a finite measure with  $v_{\text{reg}}(\{0\}) = 0$ . Define  $a_\kappa$  to be the scattering length associated with potential  $v_\kappa = v_{\text{h.c.}} + v_{\text{reg}} + \frac{2c}{\cos(\kappa/2)}\delta_0$ . Write  $\rho = N/L$ . For  $\rho|a_\kappa|$  and  $\rho R_0$  sufficiently small, the ground state energy  $E_{(\kappa,c)}(N, L)$  of the anyon gas can be expanded as*

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

## 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

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<sup>5</sup>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  $\lambda_0$  in the limit  $c/\rho \gg 1$  is predicted to be

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

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]

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

3. **Positive temperature.** For  $T > 0$ , one can again ask if quantities like the chemical potential and free energy only depend on  $\rho a$  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  $v = v_{\text{reg}} + v_{\text{h.c.}}$  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

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

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  $|\Psi_F^{\text{per}}|$  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

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

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  $\Psi_\omega$  defined in (2.2). This is done in Section 2.4 by dividing  $[0, L]$  into small intervals, and patching copies of  $\Psi_\omega$ .

First, we focus on the small- $N$  trial state  $\Psi_\omega$ . 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  $\Psi_\omega$  defined in (2.2) can be estimated as*

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

To prove this lemma, it is useful divide the configuration space into

various sets. For  $i < j$ , define

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

Note that  $\Psi_\omega$  equals  $|\Psi_F|$  on the complement of  $B$ , and that  $B_{ij}$  equals  $B$  intersected with the set  $\{\text{“particles } i \text{ and } j \text{ are closer than any other pair”}\}$ . 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

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

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.**

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

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  $\Psi_F$  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  $N$  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  $B = \{x \in \mathbb{R}^N \mid \mathcal{R}(x) < b\}$ , we may rewrite this, using the diamagnetic inequality, as

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

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

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

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

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

We may, by an inclusion-exclusion argument, estimate

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

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

## 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

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

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

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

Notice that  $(z + z^{-1})^n = \sum_{k=0}^n \binom{n}{k} z^{2k-n}$ . For  $1 \leq i \leq N-1$ , 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

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

For  $1 \leq i \leq N-2$ , 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  $3 \leq j \leq N$  and  $1 \leq i \leq N-j$ , 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

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

This is a Vandermonde determinant and we conclude

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

### 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  $\tilde{\gamma}^{(1)}(x, y)$

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

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



### 2.1.3 Useful bounds on various reduced density matrices of $\Psi_F$

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

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

with  $\int |f(x_2)| dx_2 \leq \text{const. } \rho^3 \ln(N)$ .

*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,

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

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

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

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

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

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

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  $\rho^{(1)'} : [0, L] \rightarrow \mathbb{R}$ , and  $\int_{[0, L]} |\rho^{(1)''}| \leq \text{const. } \rho^2 \ln(N)$ , and finally that  $\int_{[0, L]} |\rho^{(1)'}| \leq \text{const. } \rho \ln(N)$ , which follows

from the bound on Dirichlet's kernel  $\|D_N^{(k)}\|_{L^1([0,2\pi])} \leq \text{const. } N^k \ln(N)$ , to conclude that

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

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

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

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

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

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.*

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

*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  $\rho^k$  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  $\rho$  can be found by simple dimensional analysis.  $\square$

**Lemma 13.** *We have the following bounds.*

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

*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

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

We prove the following bound.

**Lemma 14.**

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

*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

$$\begin{aligned} E_1^{(1)} &= 2 \binom{N}{2} \int_{A_{12}} |\partial_1 \Psi_{12}|^2 \\ &= 2 \binom{N}{2} \int_{A_{12}} \overline{\Psi}_{12} (-\partial_1^2 \Psi_{12}) + 2 \binom{N}{2} \int [\overline{\Psi}_{12} \partial_1 \Psi_{12}]_{x_1=x_2-b}^{x_1=x_2+b} dx_2 \dots dx_N, \end{aligned} \quad (2.30)$$

The boundary term can be calculated explicitly, and we find

$$\begin{aligned} 2 \binom{N}{2} \int [\overline{\Psi}_{12} \partial_1 \Psi_{12}]_{x_1=x_2-b}^{x_1=x_2+b} dx_2 \dots dx_N &= \int \left[ \frac{\omega(x_1 - x_2)}{|x_1 - x_2|} \partial_{x_1} \left( \frac{\omega(x_1 - x_2)}{|x_1 - x_2|} \right) \rho^{(2)}(x_1, x_2) \right]_{x_2-b}^{x_2+b} dx_2 \\ &\quad + \int \left[ \left( \frac{\omega(x_1 - x_2)}{|x_1 - x_2|} \right)^2 \partial_{x_1} \left( \gamma^{(2)}(x_1, x_2; y, x_2) \right) \right]_{y=x_1}^{x_2+b} dx_2 \end{aligned} \quad (2.31)$$

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

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

Using Lemma 11, we find

$$\int \left[ \frac{\omega(x_1 - x_2)}{|x_1 - x_2|} \partial_{x_1} \left( \frac{\omega(x_1 - x_2)}{|x_1 - x_2|} \right) \rho^{(2)}(x_1, x_2) \right]_{x_2-b}^{x_2+b} dx_2 \leq 2a \frac{b}{b-a} N \frac{\pi^2}{3} \rho^3 \left( 1 + \text{const.} \frac{\ln(N)}{N} \right). \quad (2.33)$$

Furthermore, we denote

$$\begin{aligned} &\int \left[ \left( \frac{\omega(x_1 - x_2)}{|x_1 - x_2|} \right)^2 \partial_{x_1} \left( \gamma^{(2)}(x_1, x_2; y, x_2) \right) \right]_{y=x_1}^{x_2+b} dx_2 \\ &= \int \left[ \partial_{x_1} \left( \gamma^{(2)}(x_1, x_2; y, x_2) \right) \right]_{y=x_1}^{x_2+b} dx_2 =: \kappa_1. \end{aligned} \quad (2.34)$$

Thus, we have

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

Another contribution to  $E_1$  is

$$\begin{aligned}
E_1^{(2)} &= -\binom{N}{2} \int_{A_{12}} \left( 2|\partial_1 \Psi_F|^2 + \sum_{i=3}^N |\partial_i \Psi_F|^2 \right) \\
&= -\binom{N}{2} \int_{A_{12}} \sum_{i=1}^N \overline{\Psi_F} (-\partial_i^2 \Psi_F) - 2\binom{N}{2} \int [\overline{\Psi_F} \partial_1 \Psi_F]_{x_1=x_2-b}^{x_1=x_2+b} \\
&= -E_0 \binom{N}{2} \int_{A_{12}} |\Psi_F|^2 - \underbrace{\int \left[ \partial_y \gamma^{(2)}(x_1, x_2; y, x_2) \Big|_{y=x_1} \right]_{x_2-b}^{x_2+b} dx_2}_{\kappa_1},
\end{aligned} \tag{2.36}$$

and using Lemma 11, we find

$$E_1^{(2)} = -\text{const. } E_0 N \rho^3 b^3 - \kappa_1. \tag{2.37}$$

The last contributions are

$$E_1^{(3)} = \binom{N}{2} \int_{A_{12}} \sum_{1 \leq i < j \leq N} (v_{\text{reg}})_{ij} |\Psi_{12}|^2 = \binom{N}{2} \int_{A_{12}} v_{12} |\Psi_{12}|^2 + 2\binom{N}{2} \int_{A_{12}} \sum_{2 \leq i < j}^N (v_{\text{reg}})_{ij} |\Psi_{12}|^2$$

and

$$E_1^{(4)} = \int_{A_{12}} \sum_{i=3}^N |\partial_i \Psi_{12}|^2. \text{ First, notice that}$$

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

By Lemma 12,

$$\begin{aligned}
&\binom{N}{2} \int_{A_{12}} \sum_{2 \leq i < j}^N (v_{\text{reg}})_{ij} |\Psi_{12}|^2 \\
&\leq \text{const. } \left( N^2 (\rho b)^3 \rho^3 \int x^2 v_{\text{reg}}(x) dx + N (\rho b)^3 \rho^5 \int x^4 v_{\text{reg}}(x) dx + N (\rho b)^4 \rho^4 \int x^3 v_{\text{reg}}(x) dx \right. \\
&\quad \left. + N (\rho b)^5 \rho^3 \int x^2 v_{\text{reg}}(x) dx \right) \\
&\leq \text{const. } N^2 (\rho b)^5 \rho \int v_{\text{reg}} = \text{const. } E_0 N (\rho b)^3 \left( \rho b^2 \int v_{\text{reg}} \right),
\end{aligned} \tag{2.39}$$

and so

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

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

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

Furthermore, we have

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

By Lemma 11, it follows that

$$\binom{N}{2} \int_{A_{12}} \left| \frac{\omega}{(x_1 - x_2)} \Psi_F \right|^2 \leq b^2 \int_{\{|x_1 - x_2| < b\}} \frac{\rho^{(2)}(x_1, x_2)}{|x_1 - x_2|^2} dx_1 dx_2 \leq \text{const.} \quad b^2 \rho^4 L b = \text{const.} \quad N \rho^3 b^3 \tag{2.43}$$

and by Lemma 12, it follows that

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

so that we find

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

Finally, again by Lemma 12, we have

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

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

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

Combining everything, we get the desired result.  $\square$

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

Recall that

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

We now prove the following bound.

**Lemma 15.**

$$E_2^{(1)} + E_2^{(2)} \leq E_0 (N(\rho b)^4 + N^2(\rho b)^6). \quad (2.49)$$

*Proof.* We start by splitting  $E_2^{(1)}$  and  $E_2^{(2)}$  in two terms each and using

partial integration. Consider first  $E_2^{(1)}$ ,

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

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

$$\begin{aligned} \binom{N}{2} 2N \int_{A_{12} \cap A_{23}} \sum_{i=4}^N |\partial_i \Psi_F|^2 &= \binom{N}{2} 2N \int_{A_{12} \cap A_{23}} \sum_{i=4}^N \overline{\Psi_F} (-\partial_i^2 \Psi_F) \\ &\leq E_0 N^3 \int_{A_{12} \cap A_{23}} |\Psi_F|^2 - N^3 \int_{A_{12} \cap A_{23}} \sum_{i=1}^3 \overline{\Psi_F} (-\partial_i^2 \Psi_F) \\ &\leq 2E_0 \int_{[0,L]} \int_{[x_2-b, x_2+b]} \int_{[x_2-b, x_2+b]} \rho^{(3)}(x_1, x_2, x_3) dx_3 dx_1 dx_2 - N^3 \int_{A_{12} \cap A_{23}} \sum_{i=1}^3 \overline{\Psi_F} (-\partial_i^2 \Psi_F) \end{aligned} \quad (2.51)$$

Using Lemma 12, we find

$$2E_0 \int_{[0,L]} \int_{[x_2-b, x_2+b]} \int_{[x_2-b, x_2+b]} \rho^{(3)}(x_1, x_2, x_3) dx_3 dx_1 dx_2 \leq NE_0(\rho b)^6. \quad (2.52)$$

Furthermore, we find by Lemma 13 that

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

Collecting everything, we find

$$E_2^{(1)} \leq \text{const. } NE_0(\rho b)^6. \quad (2.54)$$



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

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

By Lemma 13, we get

$$4 \int_{x_2 \in [0, L]} \int_{|x_3-x_4|<b} \left[ \partial_{y_1} \gamma^{(4)}(x_1, x_2, x_3, x_4; y_1, x_2, x_3, x_4) \right]_{y_1=x_1}^{x_1=x_2+b}_{x_1=x_2-b} = \text{const. } E_0 N (\rho b)^4. \tag{2.56}$$

Furthermore, by Lemma 13 again, it follows that

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

□

## 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  $\Psi_\omega$  (2.2). To construct a trial state for arbitrary  $N$ , we glue together copies of  $\Psi_\omega$  on small intervals. This is straightforward with Dirichlet boundary conditions since the wave functions vanish at the boundaries. We therefore consider the state  $\Psi_{\text{full}} = \prod_{i=1}^M \Psi_{\omega, \ell}(x_1^i, \dots, x_{\tilde{N}}^i)$ , where  $(x_1^i, \dots, x_{\tilde{N}}^i)$  are the particles in box  $i$  and  $\ell$  is the length of each box. Of course,  $\cup_{i=1}^M \{x_1^i, \dots, x_{\tilde{N}}^i\} = \{x_1, \dots, x_N\}$  and  $\{x_1^i, \dots, x_{\tilde{N}}^i\} \cap \{x_1^j, \dots, x_{\tilde{N}}^j\} = \emptyset$  for  $i \neq j$ , such that  $M\tilde{N} = N$ . 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

$$E \leq M e_0 \left( 1 + 2\tilde{\rho} a \frac{b}{b-a} + \text{const. } \tilde{N}(b\tilde{\rho})^3 \left( 1 + \rho b^2 \int v_{\text{reg}} \right) \right) / \|\Psi_\omega\|^2, \quad (2.58)$$

with  $e_0 = \frac{\pi^2}{3} \tilde{N} \tilde{\rho}^2 (1 + \text{const. } \frac{1}{N})$  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  $\|\Psi_\omega\|^2 \geq 1 - \int_B |\Psi_F|^2 \geq 1 - \int_{|x_1-x_2|<b} \rho^{(2)}(x_1, x_2) \geq 1 - \text{const. } \tilde{N}(\rho b)^3$ , where the last inequality follows from Lemma 11. Thus, choosing  $M$  such that  $bM/L \ll 1$ , we have

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

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

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

Here, we used the fact that  $\tilde{N}(\rho b)^3 \leq 1/2$ , so that we have

$$1/(1 - \tilde{N}(\rho b)^3) \leq 1 + 2\tilde{N}(\rho b)^3. \text{ Optimizing in } x, \text{ we find } x = M/N = \frac{(b\rho)^{3/2} (1 + \rho b^2 \int v_{\text{reg}})^{1/2}}{1 + 2\rho^2 ab} \simeq (b\rho)^{3/2} (1 + \rho b^2 \int v_{\text{reg}})^{1/2}, \text{ which gives the error}$$

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

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

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

Notice that

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

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

### 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*

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

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]

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

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

$$\lambda = \gamma \int_{-1}^1 g(x) dx. \quad (3.4)$$

This allows for a rigorous lower bound.

**Lemma 17** (Lieb-Liniger lower bound). *For  $\gamma > 0$ ,*

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

*Proof.* Neglecting  $(x - y)^2$  in the denominator of (3.3), we see that  $g \leq \frac{1}{2\pi} + 2\frac{1}{\lambda} \int_{-1}^1 g(x) dx$ . On the other hand, (3.4) shows that  $e(\gamma) = \frac{\int_{-1}^1 g(x) x^2 dx}{\left( \int_{-1}^1 g(x) dx \right)^3}$ . We denote  $\int_{-1}^1 g(x) dx = M$ , 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  $\int_{-1}^1 g(x)x^2 dx = \frac{1}{3} \frac{M^3}{4K^2}$ . 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*

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

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  $b > 0$ ,*

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

*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  $\Lambda_{3L}$ ,
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.  $\left|\frac{dh}{dx}\right|^2 \leq \frac{1}{b^2}$ , and  $h^2 \leq 1$ .

Let  $f \in \mathcal{D}(\mathcal{E}_{\Lambda_L}^N)$ . Define  $\tilde{f}$  by extending  $f$  to  $\Lambda_{3L}$  by reflecting  $f$  across each face of its domain in  $\Lambda_{3L}$ . Define then  $V : L^2(\Lambda_L) \rightarrow L^2(\Lambda_{L+2b})$  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  $Vf \in \mathcal{D}(\mathcal{E}_{\Lambda_{L+2b}}^D)$ . Let  $\psi$  be the ground state of  $\mathcal{E}_{\Lambda_L}^N$ , 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  $\psi$  extended by reflection as above and notice that for  $|x_2| < L/2 - b$ , we have

$$\begin{aligned} & \int_{-L/2-b}^{L/2+b} v(|x_1 - x_2|) \left| \tilde{\psi}(x) \right|^2 h(x_1)^2 h(x_2)^2 dx_1 \leq \\ & \int_{-L/2+b}^{L/2-b} v(|x_1 - x_2|) \left| \tilde{\psi} \right|^2 dx_1 + \sum_{s \in \{-1, 1\}} s \int_{s(L/2-b)}^{s(L/2)} v(|x_1 - x_2|) \left| \tilde{\psi} \right|^2 (h(x)^2 + h(L-x)^2) dx_1 \\ & = \int_{-L/2}^{L/2} v(|x_1 - x_2|) \left| \tilde{\psi} \right|^2 dx_1, \end{aligned} \tag{3.8}$$

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  $h$ .

$$\begin{aligned} & \sum_{(s_1, s_2) \in \{-1, 1\}^2} s_1 s_2 \int_{L/2-s_1b}^{L/2} \int_{L/2-s_2b}^{L/2} v(|x_1 - x_2|) \left| \tilde{\psi}(x) \right|^2 h(x_1)^2 h(x_2)^2 dx_2 dx_1 \\ & = \sum_{(s_1, s_2) \in \{-1, 1\}^2} \int_0^b \int_0^b v(|s_1 y_1 - s_2 y_2|) \left| \tilde{\psi}(L/2 - s_1 y_1, L/2 - s_2 y_2, \bar{x}^{1,2}) \right|^2 \\ & \quad \times h(L/2 - s_1 y_1)^2 h(L/2 - s_2 y_2)^2 dy_2 dy_1 \\ & \leq \int_0^b \int_0^b v(|y_1 - y_2|) \left| \tilde{\psi}(L/2 - y_1, L/2 - y_2, \bar{x}^{1,2}) \right|^2 \\ & \quad \times \sum_{(s_1, s_2) \in \{-1, 1\}^2} h(L/2 - s_1 y_1)^2 h(L/2 - s_2 y_2)^2 dy_2 dy_1 \\ & = \int_0^b \int_0^b v(|y_1 - y_2|) \left| \tilde{\psi}(L/2 - y_1, L/2 - y_2, \bar{x}^{1,2}) \right|^2 dy_2 dy_1, \end{aligned} \tag{3.9}$$

where we write  $\bar{x}^{1,2}$  as shorthand for  $(x_3, \dots, x_N)$ . 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

$$\begin{aligned} & \int_{-L/2-b}^{L/2+b} \int_{-L/2-b}^{L/2+b} v(|x_1 - x_2|) \left| \tilde{\psi}(x) \right|^2 h(x_1)^2 h(x_2)^2 dx_1 dx_2 \\ & \leq \int_{-L/2}^{L/2} \int_{-L/2}^{L/2} v(|x_1 - x_2|) \left| \tilde{\psi}(x) \right|^2 dx_1 dx_2. \end{aligned} \quad (3.10)$$

The result now follows from the fact that  $V$  is an isometry.  $\square$

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

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

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  $E_{LL}^D(2^m n, 2^m \ell) \leq 2 E_{LL}^D(2^{m-1} n, 2^{m-1} \ell)$ . Since we also have  $e_{LL}^D(2^m n, 2^m \ell, c) \geq e_{LL}(2^m n, 2^m \ell, c) \rightarrow e_{LL}(n/\ell, c)$  as  $m \rightarrow \infty$  [32], we see that

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

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

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

$\square$

### 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  $\Psi$  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

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

extended symmetrically to other orderings of the particles. Our first goal is to prove that almost no weight is lost in going from  $\Psi$  to  $\psi$ , 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  $\phi(0) = 0$ ,*

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

*Proof.* Write  $\phi(x) = \int_0^x \phi'(t) dt$ , and find that

$$|\phi(x)| \leq \int_0^x |\phi'(t)| dt. \quad (3.16)$$

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

We can estimate the norm loss in the following way

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

where  $B := \{x \in \mathbb{R}^n | \min_{i,j} |x_i - x_j| < R\}$  and  $D_{ij} := \{x \in \mathbb{R}^n | \mathbf{r}_i(x) = |x_i - x_j| < R\}$  with  $\mathbf{r}_i(x) := \min_{j \neq i} (|x_i - x_j|)$ . 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  $\psi$  be defined in (3.14),*

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

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

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

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

$$|\phi(x)|^2 - |\phi(x')|^2 = (|\phi(x)| - |\phi(x')|)^2 + 2(|\phi(x)| - |\phi(x')|)|\phi(x')| \leq 2(|\phi(x)| - |\phi(x')|)^2 + |\phi(x')|^2 \quad (3.20)$$

It follows that

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

Viewing  $\Psi$  as a function of  $x_i$ , we have

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

Hence,

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

where  $D'_{ij} := \{x_i \in \mathbb{R} | \mathbf{r}_i(x) = |x_i - x_j| < R\}$  and  $d\bar{x}^i$  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  $R > R_0 = \text{range}(v)$  and  $\varphi \in H^1(\mathbb{R})$ , then*



for any interval  $\mathcal{I} \ni 0$

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

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

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

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

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

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

where  $\mathbf{r}_i(x) = \min_{j \neq i} (|x_i - x_j|)$  and the nearest neighbor delta interaction can be written  $\delta(\mathbf{r}_i(x) - R) = \left( \sum_{j \neq i} [\delta(x_i - x_j - R) + \delta(x_i - x_j + R)] \right) \mathbb{1}_{\mathbf{r}_i(x) \geq R}$ . 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  $\psi$  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

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

□

The next lemma will continue the process of bounding the norm loss in

going from  $\Psi$  of norm 1 to  $\psi$  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

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

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

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

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

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

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

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

It follows that we have

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

□

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

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

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

**Proposition 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

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

*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,

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

□

**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  $\rho R \leq \frac{1}{2}$ ,

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

### 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  $\mu$ .

**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  $\mu = \pi^2 \rho^2 (1 + \frac{8}{3}\rho a)$ . Then,

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

*Proof.* By Corollary 26, we have

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

Superadditivity caused by the positive potential implies

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

The result therefore follows from the fact that

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

□

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

$$E^N(N, L) \geq F^N(\mu, L) + \mu N, \quad (3.41)$$

where  $F^N(\mu, L) = \inf_{N'} (E^N(N', L) - \mu N')$ . Clearly,

$$F^N(\mu, L) \geq M F^N(\mu, \ell), \quad (3.42)$$

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  $\mu = \pi^2 \rho^2 (1 + \frac{8}{3} \rho a)$  (notice that  $\mu = \frac{d}{d\rho} (\frac{\pi^2}{3} \rho^3 (1 + 2\rho a))$ ). By Lemma 27,

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

It is known from Proposition 25 that for  $n < \Xi n^*$ ,

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

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

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

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,

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

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

## 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  $\Sigma_\sigma := \{x_{\sigma_1} < x_{\sigma_2} < \dots < x_{\sigma_N}\} \subset \mathbb{R}^N$  indexed by permutations  $\sigma = (\sigma_1, \dots, \sigma_N)$ , and the diagonal  $\Delta_N := \bigcup_{1 \leq i < j \leq N} \{x_i = x_j\}$ . Consider the kinetic energy operator on  $\mathbb{R}^N \setminus \Delta_N$ ,

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

with domain

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

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

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

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*

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

*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  $\varphi = e^{-i\frac{\kappa}{2}\Lambda} f$  and  $\vartheta = e^{-i\frac{\kappa}{2}\Lambda} g$ . 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

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

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

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

so that

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

Hence, it follows that

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

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

**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  $\kappa$  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  $U_\kappa : f \mapsto e^{-i\frac{\kappa}{2}\Lambda}f$  provides a unitary equivalence of the bosonic and anyonic set-ups. That is,  $U_\kappa \mathcal{D}(\mathcal{E}_{c/\cos(\kappa/2)}) = \mathcal{D}(\mathcal{E}_{\kappa,c})$  with  $\mathcal{E}_{\kappa,c}(U_\kappa f) = \mathcal{E}_{c/\cos(\kappa/2)}(f)$ . Hence, the result follows from Theorem 1.  $\square$

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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- $\frac{1}{2}$  Fermi gas. Due to an important theorem of Lieb and Mattis, [LM62b], it is known that the ground state of a repulsively interacting spin- $\frac{1}{2}$  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- $\frac{1}{2}$  Fermi gas.

### 4.1 The model

We consider a gas of fermions, each with spin- $\frac{1}{2}$ , 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  $v_{\text{reg}}$  is a finite measure and  $v_{\text{h.c.}}$  is a positive linear combination of hard cores. Formally, we write the Hamiltonian

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

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

**Conjecture 26.** *Let  $v \geq 0$  satisfy the assumption from above, then the ground state energy of the dilute spin-1/2 Fermi gas satisfies*

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

## 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 26. 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 27.** *Let  $v \geq 0$  satisfy the assumption from above, then the ground state energy of the dilute spin-1/2 Fermi gas satisfies*

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

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  $\{\sigma\} = \{\sigma_1, \sigma_2, \dots, \sigma_N\} = \{0 < x_{\sigma_1} < x_{\sigma_2} < \dots < x_{\sigma_N} < L\}$ , 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  $P_t^{i,i+1} \Psi|_{\{x_{\sigma_i}=x_{\sigma_{i+1}}\}} = 0$ . Here  $P_t^{i,j}$  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  $P_s^{i,j}$ . 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

$$\Psi_\chi = \begin{cases} \frac{\Psi_F}{\mathcal{R}} ((\eta\omega_e^{\mathcal{R}} + (1-\eta)\omega_o^{\mathcal{R}}) P_s^{\mathcal{R}} + \omega_o^{\mathcal{R}} P_t^{\mathcal{R}}) \chi, & \mathcal{R}(x) < b \\ \Psi_F, & \mathcal{R}(x) \geq b \end{cases}, \quad (4.2.2)$$

where  $\chi$  is some spin state,  $b > R_0$ ,  $\omega_{s/o}^{\mathcal{R}}(x) := \omega_{s/o}(\mathcal{R}(x))$ , and  $P_{s/t}^{\mathcal{R}(x)} := P_{s/t}^{i,j}$  when  $\mathcal{R}(x) = |x_i - x_j|$ , and  $\eta$  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

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

In this case, we see that  $P_t^{i,j} \Psi|_{x_i=x_j} = 0$  due to the boundary condition satisfied by  $\omega_o$ . We notice that a potential discontinuity could arise from  $P_{s/t}^{\mathcal{R}(x)}$ , since these projection are discontinuous at points where  $\mathcal{R}_2(x) = \mathcal{R}(x)$ . However, since  $P_s^{\mathcal{R}(x)} + P_t^{\mathcal{R}(x)} = 1$ , we see that  $\Psi$  is continuous due to the inclusion of  $\eta$ . The extension of  $\Psi$  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 27. 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

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

where  $\tilde{N} = N/M$  and  $x_i^m := x_{m\tilde{N}+i}$  and the superscript  $I_m$  in  $\Psi_{\chi}^{I_m}$  means that we take the state  $\Psi_{\chi}$  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  $P_s^{i,j} = 1/4 - S_i \cdot S_j$  and  $P_t^{i,j} = 3/4 + S_i \cdot S_j$ , we expect (ignoring the effect of  $\eta$ ) that the correction we obtain from the variational state  $\Psi_{\chi}$  is of the order

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

The minimizer (in  $\chi$ ),  $\chi_0$ , 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  $\chi_0 = |\text{GS}_{\text{HAF}}\rangle$ . 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]

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

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

### Proof of Theorem 27

In this section, we give the formal proof of Theorem 27. 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 28.** *Let  $\eta$  be defined as above, then we have*

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

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



state

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

We will henceforth assume  $\chi$  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

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

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  $\eta$  in the trial state, we need to further divide the integration domain. We list here different domains of integration that will be relevant in this section

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

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  $v_{\text{reg}}$ , 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)

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

Defining

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

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

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

where  $P_{s/t}^{N,N+1} := P_{s/t}^{N,1}$  and  $\chi_\sigma$  is the spin state  $\chi$  with spins relabeled by  $(1, \dots, N) \mapsto (\sigma_1, \dots, \sigma_N)$  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 that  $\langle \chi_\sigma | P_t^{1,2} | \chi_\sigma \rangle$  is independent of  $\sigma \in S_{12}$  and the translation invariance of  $\chi$ , we see that

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

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

$$\frac{1}{N} \left( \sum_{k=1}^N \langle \chi | P_s^{k,k+1} | \chi \rangle + \sum_{k=1}^N \langle \chi | P_t^{k,k+1} | \chi \rangle \right) = 1,$$

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

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

We see that this reduces proving an upper bound to a case we have already analyzed in Chapter 3, except 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 29.** *Let  $E_{12}^{34}$  and  $\Psi_\chi$  be defined as above, then we have the following*

bound:

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

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

**Lemma 30.** Let  $E_{12}^{23}$  and  $\Psi_\chi$  be defined as above, then we have the following bound:

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

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

Using Lemmas 29 and 30, we deduce, from (4.2.14) the following bound upper bound on the trial state energy

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

Defining the quantities

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

and the quantities from Chapter 3:

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

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

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

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

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

We also recall the lemma

**Lemma 32** (Lemma 15 of Chapter 3).

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

Using Lemmas 31 and 32 we find the result

**Lemma 33.** *For  $N(\rho b)^3 \leq 1$  and  $b > 2a_o$  we have*

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

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 31 and 32.  $\square$

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  $\chi$  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  $\chi$  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 34** ([Mat12], Eq. (5.171)). *Let  $|\text{GS}_{\text{HAF}}\rangle$  denote the ground state of the periodic antiferromagnetic Heisenberg chain. Then*

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

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

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

*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

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

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

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

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

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

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

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

where  $e_P = \lim_{N \rightarrow \infty} \frac{1}{N}E_P^N$ . The desired result follows from Lemma 34.  $\square$

We are now ready to give the proof of Theorem 27:

*Proof of Theorem 27.* 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

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

Combining lemmas 33 and 35, we find

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

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

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

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

Furthermore choosing  $b = \max(\rho^{-1/5} |a_e|^{4/5}, \rho^{-1/5} a_o^{4/5}, R_0)$  we see that  $a_{e/o} \leq \tilde{a}_{e/o} = a_{e/o} \frac{b}{b - a_{e/o}} \leq a_{e/o} (1 + 2(\rho R)^{1/5})$  for  $(\rho R)^{1/5} \leq 1/2$  and the desired result follows from the simple estimate on the norm

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

□

### Estimating $E_{12}^{34}$ (proof of lemma 29)

*Proof of Lemma 29.* Estimating  $E_{12}^{34}$  is a straightforward computation that goes as follows:

Defining  $\xi_{12}^{34} := \left( (\eta\omega_e^{12} + (1 - \eta)\omega_o^{12}) P_s^{1,2} + \omega_o^{12} P_t^{1,2} \right) \chi$  on  $B_{12}^{34} \cap \{1, 2, \dots\}$  and (space-spin)-symmetrically extended to  $B_{12}^{34}$ , we see that  $\Psi_{\chi} = \xi_{12}^{34} \frac{\Psi_F}{|x_2 - x_1|}$  on



$B_{12}^{34}$ : Hence we find

$$\begin{aligned}
E_{12}^{34} &= \binom{N}{2} \binom{N-2}{2} \int_{B_{12}^{34}} \sum_{i=1}^N \left| \partial_i \left( \xi_{12}^{34} \frac{\Psi_F}{|x_2 - x_1|} \right) \right|^2 \\
&\leq \binom{N}{2} \binom{N-2}{2} \left[ \int_{A_{12}^{34}} \sum_{i=1}^4 \left| \partial_i \left( \xi_{12}^{34} \frac{\Psi_F}{|x_2 - x_1|} \right) \right|^2 \right. \\
&\quad \left. + \int_{A_{12}^{34}} \sum_{i=5}^N \overline{\xi_{12}^{34} \frac{\Psi_F}{|x_2 - x_1|}} \left( \xi_{12}^{34} \frac{(-\partial_i^2 \Psi_F)}{|x_2 - x_1|} \right) \right] \\
&= \binom{N}{2} \binom{N-2}{2} \left[ \int_{A_{12}^{34}} \sum_{i=1}^4 \left| \partial_i \left( \xi_{12}^{34} \frac{\Psi_F}{|x_2 - x_1|} \right) \right|^2 \right. \\
&\quad \left. - \int_{A_{12}^{34}} \sum_{i=1}^4 \overline{\xi_{12}^{34} \frac{\Psi_F}{|x_2 - x_1|}} \left( \xi_{12}^{34} \frac{(-\partial_i^2 \Psi_F)}{|x_2 - x_1|} \right) \right. \\
&\quad \left. + E_F \int_{A_{12}^{34}} \left| \xi_{12}^{34} \frac{\Psi_F}{|x_2 - x_1|} \right|^2 \right], \tag{4.2.35}
\end{aligned}$$

where we used  $B_{12}^{34} \subset A_{12}^{34}$ , integration by parts, and the fact that  $\Psi_F$  is an eigenfunction of  $(-\Delta)$ , with eigenvalue  $E_F$ .

Thus, using  $|\xi_{12}^{34}|^2 \leq b^2$  and restricting to  $b \geq 2a_0 \geq 2a_e$ , we find

$$\begin{aligned}
E_{12}^{34} &\leq 4 \int_{A_{12}^{34}} \left( \sum_{i=1}^4 \partial_{y_i} \partial_{x_i} \frac{\overline{\xi_{12}^{34}(y)}}{|y_2 - y_1|} \frac{\xi_{12}^{34}(x)}{|x_2 - x_1|} \gamma^{(4)}(y_1, y_2, y_3, y_4; x_1, x_2, x_3, x_4) \right) \Big|_{y=x} \\
&\quad + \left| \frac{\xi_{12}^{34}(x)}{|x_2 - x_1|} \right|^2 \left| \sum_{i=1}^4 \partial_{y_i}^2 \gamma^{(4)}(y_1, y_2, y_3, y_4; x_1, x_2, x_3, x_4) \right| \Big|_{y=x} \\
&\quad + E_F \left| \frac{\xi_{12}^{34}(x)}{|x_2 - x_1|} \right|^2 \rho^{(4)}(x_1, x_2, x_3, x_4) \\
&\leq \text{const. } E_F \left( N (\rho b)^4 + N^2 (\rho b)^6 \right) \tag{4.2.36}
\end{aligned}$$

where we used the following bounds

$$\begin{aligned}
 \left. \partial_{y_i} \partial_{x_i} \frac{\gamma^{(4)}(y_1, y_2, y_3, y_4; x_1, x_2, x_3, x_4)}{|x_2 - x_1| |y_2 - y_1|} \right|_{y=x} &\leq \text{const.} \rho^8, \\
 \left. \partial_{y_i} \frac{\gamma^{(4)}(y_1, y_2, y_3, y_4; x_1, x_2, x_3, x_4)}{|x_2 - x_1| |y_2 - y_1|} \right|_{y=x} &\leq \text{const.} \rho^8 |x_3 - x_4|, \\
 \left. \frac{\gamma^{(4)}(y_1, y_2, y_3, y_4; x_1, x_2, x_3, x_4)}{|x_2 - x_1| |y_2 - y_1|} \right|_{y=x} &\leq \text{const.} \rho^8 |x_3 - x_4|^2, \\
 \left| \sum_{i=1}^4 \partial_{y_i}^2 \gamma^{(4)}(y_1, y_2, y_3, y_4; x_1, x_2, x_3, x_4) \right|_{y=x} &\leq \text{const.} \rho^{10} |x_1 - x_2|^2 |x_3 - x_4|^2,
 \end{aligned} \tag{4.2.37}$$

and

$$\rho^{(4)}(x_1, x_2, x_3, x_4) \leq \text{const.} \rho^8 |x_1 - x_2|^2 |x_3 - x_4|^2, \tag{4.2.38}$$

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

$$\sqrt{|\partial_i \xi_{12}^{34}|^2} \leq b \max \left( \frac{\sqrt{2}}{b}, \frac{1}{b - a_o} \right) \leq 2, \quad \sqrt{|\xi_{12}^{34}|^2} \leq b \tag{4.2.39}$$

which follows from properties of the scattering solution, monotonicity of its derivative, and Lemma 28.  $\square$

### Estimating $E_{12}^{23}$ (proof of Lemma 30)

*Proof of Lemma 30.* 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  $\xi_{12}^{23} := \left( (\eta \omega_e^{12} + (1 - \eta) \omega_o^{12}) P_s^{1,2} + \omega_o^{12} P_t^{1,2} \right) \chi$  on  $B_{12}^{23} \cap \{1, 2, \dots\}$  and (space-spin)-symmetrically extended to  $B_{12}^{23}$ , we see that  $\Psi_\chi = \xi_{12}^{23} \frac{\Psi_F}{|x_2 - x_1|}$  on

$B_{12}^{23}$ : Hence we find

$$\begin{aligned}
E_{12}^{23} &= \binom{N}{2} 2(N-2) \int_{B_{12}^{23}} \sum_{i=1}^N \left| \partial_i \left( \xi_{12}^{23} \frac{\Psi_F}{|x_2 - x_1|} \right) \right|^2 \\
&\leq \binom{N}{2} 2(N-1) \left[ \int_{A_{12}^{23}} \sum_{i=1}^3 \left| \partial_i \left( \xi_{12}^{23} \frac{\Psi_F}{|x_2 - x_1|} \right) \right|^2 \right. \\
&\quad \left. + \int_{A_{12}^{23}} \sum_{i=4}^N \overline{\xi_{12}^{23} \frac{\Psi_F}{|x_2 - x_1|}} \left( \xi_{12}^{23} \frac{(-\partial_i^2 \Psi_F)}{|x_2 - x_1|} \right) \right] \\
&= \binom{N}{2} 2(N-2) \left[ \int_{A_{12}^{23}} \sum_{i=1}^3 \left| \partial_i \left( \xi_{12}^{23} \frac{\Psi_F}{|x_2 - x_1|} \right) \right|^2 \right. \\
&\quad \left. - \int_{A_{12}^{23}} \sum_{i=1}^3 \overline{\xi_{12}^{23} \frac{\Psi_F}{|x_2 - x_1|}} \left( \xi_{12}^{23} \frac{(-\partial_i^2 \Psi_F)}{|x_2 - x_1|} \right) \right. \\
&\quad \left. + E_F \int_{A_{12}^{23}} \left| \xi_{12}^{23} \frac{\Psi_F}{|x_2 - x_1|} \right|^2 \right], \tag{4.2.40}
\end{aligned}$$

where we used  $B_{12}^{23} \subset A_{12}^{23}$ , integration by parts, and the fact that  $\Psi_F$  is an eigenfunction of  $(-\Delta)$ , with eigenvalue  $E_F$ .

Thus, using  $|\xi_{12}^{23}|^2 \leq b^2$  and restricting to  $b \geq 2a_o \geq 2a_e$ , we find

$$\begin{aligned}
E_{12}^{23} &\leq 4 \int_{A_{12}^{23}} \left( \sum_{i=1}^3 \partial_{y_i} \partial_{x_i} \overline{\frac{\xi_{12}^{23}(y)}{|y_2 - y_1|}} \frac{\xi_{12}^{23}(x)}{|x_2 - x_1|} \gamma^{(3)}(y_1, y_2, y_3; x_1, x_2, x_3) \right) \Big|_{y=x} \\
&\quad + \left| \frac{\xi_{12}^{23}(x)}{|x_2 - x_1|} \right|^2 \left| \sum_{i=1}^3 \partial_{y_i}^2 \gamma^{(4)}(y_1, y_2, y_3; x_1, x_2, x_3) \right| \Big|_{y=x} \\
&\quad + E_F \left| \frac{\xi_{12}^{23}(x)}{|x_2 - x_1|} \right|^2 \rho^{(3)}(x_1, x_2, x_3) \\
&\leq \text{const. } E_F \left( (\rho b)^4 + N (\rho b)^6 \right) \tag{4.2.41}
\end{aligned}$$

where we used the following bounds

$$\begin{aligned}
 \left| \partial_{y_i} \partial_{x_i} \frac{\gamma^{(3)}(y_1, y_2, y_3; x_1, x_2, x_3)}{|x_2 - x_1| |y_2 - y_1|} \right|_{y=x} &\leq \text{const.} \rho^7, \\
 \left| \partial_{y_i} \frac{\gamma^{(3)}(y_1, y_2, y_3; x_1, x_2, x_3)}{|x_2 - x_1| |y_2 - y_1|} \right|_{y=x} &\leq \text{const.} \rho^7 |x_3 - x_4|, \\
 \left| \frac{\gamma^{(3)}(y_1, y_2, y_3; x_1, x_2, x_3)}{|x_2 - x_1| |y_2 - y_1|} \right|_{y=x} &\leq \text{const.} \rho^7 |x_3 - x_4|^2, \\
 \left| \sum_{i=1}^3 \partial_{y_i}^2 \gamma^{(3)}(y_1, y_2, y_3; x_1, x_2, x_3) \right|_{y=x} &\leq \text{const.} \rho^{11} |x_1 - x_2|^2 |x_2 - x_3|^2 |x_1 - x_3|^2,
 \end{aligned} \tag{4.2.42}$$

and

$$\rho^{(3)}(x_1, x_2, x_3) \leq \text{const.} \rho^9 |x_1 - x_2|^2 |x_2 - x_3|^2 |x_1 - x_3|^2, \tag{4.2.43}$$

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

$$\sqrt{|\partial_i \xi_{12}^{23}|^2} \leq b \max \left( \frac{\sqrt{2}}{b}, \frac{1}{b - a_o} \right) \leq 2, \quad \sqrt{|\xi_{12}^{23}|^2} \leq b \tag{4.2.44}$$

which follows from properties of the scattering solution, monotonicity of its derivative, and Lemma 28.  $\square$

### 4.3 Extensions to other symmetries and spin dependent potentials

We present here corollaries that follows directly, *mutatis mutandis*, from the proof of Theorem 27. 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 27 (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

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

The proof is unchanged except for the choice of  $\chi$ . In this case, since  $a_o \geq a_e$  and the roles of  $a_o$  and  $a_e$  are exchanged, the optimal choice for  $\chi$  is a spin polarized state. Hence we get the following corollary:

**Corollary 36** (Bosonic version of Theorem 27). *Let  $v$  satisfy the assumption from above, then the ground state energy of the dilute spin-1/2 Bose gas satisfies*

$$E \leq N \frac{\pi^2}{3} \rho^2 \left( 1 + 2\rho a_e + \mathcal{O} \left( (\rho R)^{6/5} + N^{-1} \right) \right) \quad (4.3.2)$$

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

### Spin dependent potentials

Interestingly, the proof of Theorem 27 we gave in the last section, allows for a slight generalization to potentials that are of the form

$$v(x_i - x_j) = v_e(x_i - x_j) P_s^{i,j} + v_o(x_i - x_j) P_t^{i,j} \quad (4.3.3)$$

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

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

Consequently, Theorem 27 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 37** (Spin dependent version of Theorem 27). *Let  $v = v_e P_s + v_o P_t \geq 0$  satisfy the assumption from above, then the ground state energy of the dilute spin-1/2 Fermi gas satisfies*

$$E \leq N \frac{\pi^2}{3} \rho^2 \left( 1 + 2\rho (\ln(2)a_e + (1 - \ln(2))a_o) + \mathcal{O}\left((\rho R)^{6/5} + N^{-1}\right) \right), \quad (4.3.5)$$

if  $a_o \geq a_e$  and

$$E \leq N \frac{\pi^2}{3} \rho^2 \left( 1 + 2\rho a_o + \mathcal{O}\left((\rho R)^{6/5} + N^{-1}\right) \right), \quad (4.3.6)$$

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 27 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  $\chi$  is the periodic antiferromagnetic Heisenberg chain when  $a_o \geq a_e$  and a spin polarized state when  $a_e > a_o$ .  $\square$

An interesting application of a version of Corollary 37 given below in Corollary 38 is the Lieb-Liniger-Heisenberg model introduced by Girardeau in [Gir06]. In this paper, an upper bound is given by a trial state argument in the case  $c > c'$

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

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

$$H_{LLH} = - \sum_i \partial_i^2 + 2 \sum_{i < j} (c' P_s + c P_t) \delta(x_i - x_j), \quad (4.3.8)$$

However the domain is taken to be spin 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 37 is not directly useful in this case. However, Going through the proof of Theorem 27, we see that we may as well get the following corollary

**Corollary 38** (Spatially symmetric, spin dependent version of Theorem 27).

Let  $v = v_s P_s + v_t P_t \geq 0$  satisfy the assumption from above, then the ground state energy of the dilute spin-1/2 spacially symmetric gas satisfies

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

if  $a_t \geq a_s$  and

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

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 27 (including lemmas used) but change  $\omega_{e/o}$  to the even wave scattering solution of  $v_{s/t}$ . The choice of  $\chi$  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 27 the same step may be justified by spacial symmetry, however, this is not completely obvious. It is easily seen that (4.2.10) can be derived by use of only spatial symmetry. However, in (4.2.12) we get instead

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

since the spins are not permuted when using spatial symmetry (CHECK THIS)

□

We see that the upper bound given by Corollary 38 (up to a small error in the dilute limit) is

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

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  $\frac{c-c'}{c'} \rightarrow 0$ .

However, (4.3.7) gives just the free Fermi energy on the right-hand side when  $c \rightarrow \infty$ , whereas our bound reduces to the correct Yang-Gaudin energy to leading order in this limit.

## 4.4 Lower bound



## 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 (??), where no properties of  $\chi$  have been used, we find

$$\int_{B_{12}^{\geq}} |\partial_i \Psi_\chi|^2 \leq \int_{A_{12}} |\partial_i (\Psi_e)_{12}|^2 \frac{1}{N} \sum_k \langle \chi | P_s^{k,k+1} | \chi \rangle + |\partial_i (\Psi_o)_{12}|^2 \frac{1}{N} \sum_k \langle \chi | P_t^{k,k+1} | \chi \rangle \quad (\text{A.0.1})$$

where we defined

$$(\Psi_e)_{12} := \frac{\Psi_F}{|x_2 - x_1|} \omega_e \text{ and } (\Psi_o)_{12} := \frac{\Psi_F}{|x_2 - x_1|} \omega_o, \quad (\text{A.0.2})$$

and we used that

$$\int_{A_{12} \cap \{\dots, 1, 2, \dots\}} |\partial_i (\Psi_{e/o})_{12}|^2 = \frac{1}{N} \int_{A_{12}} |\partial_i (\Psi_{e/o})_{12}|^2. \quad (\text{A.0.3})$$

But from (A.0.1) it is clear that the antiferromagnetic Heisenberg ground state is optimal.



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