

One-dimensional Dilute Quantum Gases and Their Ground State Energies

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Motivation (Bosons)

- 2D and 3D dilute Bose gases are well-studied in the mathematical physics literature.
- 2D and 3D results are related to Bose-Einstein condensation (BEC).
- No BEC is expected in 1D.
- In 1D the hard core and Lieb-Liniger models are solvable.
- Our result is consistent with the absence of BEC in 1D.
- On the contrary it suggests that the 1D dilute bose gas shares features with the Fermi gas.

Motivation (Spin-1/2 fermions)

- 2D and 3D dilute Fermi gases are well-studied in the mathematical physics literature.
- In 1D the hard core and Yang-Gaudin models are solvable.
- In 1962 E. H. Lieb and D. C. Mattis showed that one-dimensional Fermi gases are antiferromagnetic (contradicting standard perturbative tight-binding methods).
- Hence the standard justification of the Heisenberg model of magnetism is too simple.
- Our result will break ground in rigorously justifying the Heisenberg antiferromagnet as an effective model in 1D.

Many-Body Quantum Mechanics

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**

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

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

Definition 1

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 $\sigma \in [0, \infty]$.

Proposition 1

Let $d = 1$, then any potential of the form $v = v_{\sigma\text{-finite}} + v_{\text{meas.}} + c\delta_0$, with $c \in \{0, \infty\}$, is allowed.

The Scattering Length

Theorem 2 (Lieb and Yngvason, 2001)

For $B_R = \{0 \leq |x| < R\} \subset \mathbb{R}^d$ with $R > R_0 := \text{range}(v)$, let $\phi \in H^1(B_R)$ satisfy

$$-\Delta\phi + \frac{1}{2}v\phi = 0, \quad \text{on } B_R, \quad (2)$$

with boundary condition $\phi(x) = 1$ for $|x| = R$. Then $\phi(x) = f(|x|)$ for some $f : (0, R] \rightarrow [0, \infty)$, and for $\text{range}(v) < r < R$, we have

$$f(r) = \begin{cases} (r - a)/(R - a) & \text{for } d = 1 \\ \ln(r/a)/\ln(R/a) & \text{for } d = 2 \\ (1 - ar^{2-d})/(1 - aR^{2-d}) & \text{for } d \geq 3, \end{cases} \quad (3)$$

with some constant a called the **(s-wave) scattering length**.

2D and 3D

For $\Lambda_L = [0, L]^d$, let $e(\rho) := \lim_{\substack{L \rightarrow \infty \\ N/L^d \rightarrow \rho}} E(N, L)/L^d$.

Theorem 3 ($d = 3$ result, Lee-Huang-Yang 1957¹)

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

Theorem 4 ($d = 2$ result²)

$$e(\rho) = 4\pi\rho^2 Y \left(1 - Y |\log Y| + \left(2\Gamma + \frac{1}{2} + \ln(\pi) \right) Y \right) + o(\rho^2 Y^2), \quad (5)$$

$$Y = |\ln(\rho a^2)|^{-1}.$$

^aUpper bound: Yau-Yin 2009, Basti-Cenatiempo-Schlein 2021. Lower bound: Fournais-Solovej 2021

^bFournais-Girardot-Junge-Morin-Olivieri 2022

Bosons Main Result

For the remainder of the presentation, $d = 1$.

Theorem 5 (A., R. Reuvers, J. P. Solovej, 2022)

Consider a Bose gas with repulsive interaction $v = v_{\text{reg}} + v_{\text{h.c.}}$. Define the density $\rho = N/L$. For $\rho|a|$ and ρR_0 sufficiently small, the ground state energy can be expanded as

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

where a is the scattering length of v .

Examples

The hard core gas

Energy behaves like free Fermi energy in volume $L - NR$, *i.e.*

$$\begin{aligned} E_{\text{hard core}}(N, L) &= N \frac{\pi^2}{3} \rho^2 (1 - NR/L)^{-2} \\ &= E_0 (1 + 2\rho R + \mathcal{O}((\rho R)^2)) . \end{aligned} \tag{7}$$

Scattering length is $a = R$.

Lieb-Liniger model

Energy behaves asymptotically like

$$E_{LL}(N, L, c) = N \frac{\pi^2}{3} \rho^2 (1 - 4\rho/c + \mathcal{O}((\rho/c)^2)) , \tag{8}$$

with scattering length $a = -\frac{2}{c}$.

Variational Principle

To obtain an upper bound, we use the variational principle, *i.e.*

$$E(N, L) \leq \frac{\mathcal{E}(\Psi)}{\|\Psi\|^2}, \quad \text{for any } \Psi \in \mathcal{D}(\mathcal{E}).$$

Trial State

Trial state has to capture free Fermi energy, as well as corrections due to scattering processes. Hence we consider

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

where ω is the suitably normalized solution to the two-body scattering equation, Ψ_F is the free Fermi ground state, and $\mathcal{R}(x) := \min_{i < j} (|x_i - x_j|)$ is uniquely defined a.e.

One-particle Reduced Density Matrix

For the free Fermi gas we have

$$\begin{aligned}\gamma^{(1)}(x, y) &= \frac{2}{L} \sum_{j=1}^N \sin\left(\frac{\pi}{L} jx\right) \sin\left(\frac{\pi}{L} jy\right) \\ &= \frac{\pi}{L} \left(D_N\left(\pi \frac{x-y}{L}\right) + D_N\left(\pi \frac{x+y}{L}\right) \right),\end{aligned}\tag{9}$$

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.

By Wick's theorem all derivatives of reduced density matrices are bounded by a constant times an appropriate power of ρ .

Some Useful Bounds

Lemma 1

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

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

Lemma 2

We have the following bounds

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

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

$$\left| \sum_{i=1}^2 \partial_{y_i}^2 \gamma^{(2)}(x_1, x_2; y_1, y_2) \Big|_{y=x} \right| \leq \text{const. } \rho^6 (x_1 - x_2)^2,$$
$$\vdots$$

Collecting Everything

Upper bound

$$E \leq N \frac{\pi^2}{3} \rho^2 \frac{\left(1 + 2\rho a \frac{b}{b-a} + \text{const.} \left[\frac{1}{N} + N(b\rho)^3 (1 + \rho b^2 \int v_{\text{reg}}) \right]\right)}{\|\Psi\|^2}, \quad (10)$$

where the finite measure v_{reg} is v with any hard core removed. By lemma 1 we know $\|\Psi\|^2 \geq 1 - \text{const. } N(\rho b)^3$.

Localization

Divide into M smaller boxes with $\tilde{N} = N/M$ particles in each, and make distance b between boxes (no interaction between boxes), and choose M such that $\tilde{N} = (\rho b)^{-3/2} \gg 1$.

Upper Bound

After localization

$$E(N, L) \leq N \frac{\pi^2}{3} \rho^2 \frac{\left(1 + 2\rho a \frac{b}{b-a} + \text{const.} \frac{M}{N} + \text{const.} \tilde{N}(b\rho)^3 (1 + \rho b^2 \int v_{\text{reg}})\right)}{1 - \tilde{N}(\tilde{\rho}b)^3} \quad (11)$$

Choosing $b = \max(\rho^{-1/5} |a|^{4/5}, R_0)$ we find

Proposition 2 (Upper bound Theorem 5)

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

$$E^D(N, L) \leq N \frac{\pi^2}{3} \rho^2 \left(1 + 2\rho a + C_U \left((\rho|a|)^{6/5} + (\rho R_0)^{3/2} + N^{-1}\right)\right). \quad (12)$$

Lower Bound

Proof of lower bound consists of the following steps:

- 1 Use Dyson's lemma to reduce to a nearest neighbor double delta-barrier potential.
- 2 Reduce to the Lieb Liniger model by discarding **a small part** of the wave function.
- 3 Use a known lower bound for the Lieb Liniger model.

The Lieb-Liniger (LL) model

$$H_{LL} = - \sum_{i=1}^n \partial_i^2 + 2c \sum_{i < j} \delta(x_i - x_j). \quad (13)$$

Behavior in thermodynamic limit: $\lim_{\substack{\ell \rightarrow \infty, \\ n/\ell \rightarrow \rho}} E_{LL}(n, \ell, c)/\ell = \rho^3 e(\gamma)$

with $\gamma = c/\rho$.

Lemma 3 (Lieb-Liniger lower bound)

Let $\gamma > 0$, then

$$e(\gamma) \geq \frac{\pi^2}{3} \left(\frac{\gamma}{\gamma + 2} \right)^2 \geq \frac{\pi^2}{3} \left(1 - \frac{4}{\gamma} \right). \quad (14)$$

Reducing to the LL Model

Lemma 4 (Dyson)

Let $R > R_0 = \text{range}(v)$ and $\varphi \in H^1(\mathbb{R})$, then for any interval $\mathcal{I} \ni 0$

$$\int_{\mathcal{I}} |\partial \varphi|^2 + \frac{1}{2} v |\varphi|^2 \geq \int_{\mathcal{I}} \frac{1}{R-a} (\delta_R + \delta_{-R}) |\varphi|^2, \quad (15)$$

where a is the s -wave scattering length.

Hence we have, denoting $\mathfrak{r}_i(x) = \min_j (|x_i - x_j|)$

$$\begin{aligned} \int \sum_i |\partial_i \Psi|^2 + \sum_{i \neq j} \frac{1}{2} v_{ij} |\Psi|^2 \geq \\ \int \sum_i |\partial_i \Psi|^2 \chi_{\mathfrak{r}_i(x) > R} + \sum_i \frac{1}{R-a} \delta(\mathfrak{r}_i(x) - R) |\Psi|^2. \end{aligned} \quad (16)$$

Reducing to the LL Model

Define $\psi \in L^2([0, \ell - (n-1)R]^n)$ by

$$\psi(x_1, x_2, \dots, x_n) = \Psi(x_1, R + x_2, \dots, (n-1)R + x_n),$$

for $x_1 \leq x_2 \leq \dots \leq x_n$ and symmetrically extended.

Then

$$\begin{aligned} \mathcal{E}(\Psi) &\geq E_{LL}^N(n, \ell - (n-1)R, 2/(R-a)) \langle \psi | \psi \rangle \\ &\geq n \frac{\pi^2}{3} \rho^2 \left(1 + 2\rho(a - R) + 2\rho R - \text{const.} \frac{1}{n^{2/3}} \right) \langle \psi | \psi \rangle. \end{aligned} \tag{17}$$

Lower Bound for Mass of ψ

Lemma 5

Let ψ be defined as above, then

$$1 - \langle \psi | \psi \rangle \leq 8 \left(R^2 \sum_{i < j} \int_{B_{ij}} |\partial_i \Psi|^2 + R(R - a) \sum_{i < j} \int v_{ij} |\Psi|^2 \right), \quad (18)$$

Combining lemmas 4 and 5 we have the following lemma:

Lemma 6

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

$$\langle \psi | \psi \rangle \geq 1 - \text{const.} \left(n(\rho R)^3 + n^{1/3}(\rho R)^2 \right). \quad (19)$$

Lower Bound

By the reduction to the LL model we find

Proposition 3

For assumptions as in lemma 6 we have

$$E^N(n, \ell) \geq n \frac{\pi^2}{3} \rho^2 \left(1 + 2\rho a + \text{const.} \left(\frac{1}{n^{2/3}} + n(\rho R)^3 + n^{1/3}(\rho R)^2 \right) \right). \quad (20)$$

Corollary 1

For $n = \text{const.}$ $(\rho R)^{-9/5}$ we have

$$E^N(n, \ell) \geq n \frac{\pi^2}{3} \rho^2 \left(1 + 2\rho a - \text{const.} \left((\rho R)^{6/5} + (\rho R)^{7/5} \right) \right). \quad (21)$$

Lower Bound Localization

To prove the lower bound, we localize, as in the upper bound, to smaller boxes. In the following C denotes the constant in Corollary 1.

Lemma 7

Let $\Xi \geq 4$ be fixed and let $n = m\Xi\rho\ell + n_0$ with $n_0 \in [0, \Xi\rho\ell)$ for some $m \in \mathbb{N}$ with $n^ := \rho\ell = \mathcal{O}(\rho R)^{-9/5}$. Furthermore, assume that $\rho R < 1$ and $C(\rho R)^{6/5} \leq 1/4$ and let $\mu = \pi^2\rho^2(1 + \frac{8}{3}\rho a)$, then*

$$E^N(n, \ell) - \mu n \geq E^N(n_0, \ell) - \mu n_0. \quad (22)$$

Proposition 4 (Lower bound Theorem 5)

There exists a constant $C_L > 0$ such that the ground state energy $E^N(N, L)$ satisfies

$$E^N(N, L) \geq N \frac{\pi^2}{3} \rho^2 \left(1 + 2\rho a - C_L \left((\rho|a|)^{6/5} + (\rho R_0)^{6/5} + N^{-2/3} \right) \right). \quad (23)$$

Spinless/Spin-Polarized Fermions

Spinless fermions are unitarily equivalent to bosons with a zero b.c. at all planes of intersection, *i.e.* with an infinite delta potential. As a consequence we have the following corollary.

Theorem 6 (Spin-polarized fermions)

Consider a spin-polarized Fermi gas with repulsive interaction $v = v_{\text{reg}} + v_{\text{h.c.}}$ as defined before. Let $E_F(N, L)$ be its associated ground state energy. Write $\rho = N/L$. For ρa_o and ρR_0 sufficiently small, the ground state energy can be expanded as

$$E_F(N, L) = N \frac{\pi^2}{3} \rho^2 \left(1 + 2\rho a_o + \mathcal{O} \left((\rho R_0)^{6/5} + N^{-2/3} \right) \right), \quad (24)$$

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

This is consistent with lower bound $E_F(N, L) \geq E_0$, since $a_o \geq 0$.

Two solvable model for spin-1/2 fermions

The hard core gas

Ground state energy is independent of spin so

$$E_{\text{hard core}}(N, L) = N \frac{\pi^2}{3} \rho^2 (1 - NR/L)^{-2} \approx E_0(1 + 2\rho R). \quad (25)$$

Scattering length is $a_e = a_o = R$.

Yang-Gaudin model

Is the spin-1/2 version of the LL model, *i.e.* $H_{YG} = H_{LL}$. Behaves asymptotically like

$$E_{YG}(N, L, c) = N \frac{\pi^2}{3} \rho^2 \left(1 - 4\rho \ln(2)/c + \mathcal{O}((\rho/c)^2) \right), \quad (26)$$

with scattering length $a_e = -\frac{2}{c}$, $a_o = 0$.

A Conjecture for Spin-1/2 Fermions

Based on the two solvable cases, we expect

Conjecture 1

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

$$E = N \frac{\pi^2}{3} \rho^2 \left(1 + 2\rho (\ln(2)a_e + (1 - \ln(2))a_o) + \mathcal{O}(\rho^2 \max(|a_e|, a_o)^2) \right). \quad (27)$$

Spin-1/2 Fermions Main Result (Upper Bound)

Theorem 7

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

$$E \leq N \frac{\pi^2}{3} \rho^2 \left(1 + 2\rho (\ln(2)a_e + (1 - \ln(2))a_o) + \mathcal{O}\left((\rho R)^{6/5} + N^{-1}\right) \right), \quad (28)$$

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

Trial State

One the sector

$$\{1, 2, \dots, N\} = \{0 < x_1 < x_2 < \dots < x_N < L\}$$

we define the trial state by

$$\Psi_\chi = \begin{cases} \frac{\Psi_F}{\mathcal{R}} \left((\eta \omega_e^{\mathcal{R}} + (1 - \eta) \omega_o^{\mathcal{R}}) P_s^{\mathcal{R}} + \omega_o^{\mathcal{R}} P_t^{\mathcal{R}} \right) \chi, & \mathcal{R}(x) < b \\ \Psi_F \chi, & \mathcal{R}(x) \geq b \end{cases}, \quad (29)$$

where χ is some spin state, $b > R_0$, $\mathcal{R}(x) = \min_{i < j} |x_i - x_j|$,
 $\omega_{e/o}^{\mathcal{R}}(x) := \omega_{e/o}(\mathcal{R}(x)) = b f_{e/o}(\mathcal{R}(x))$ and

$$\eta(x) := \begin{cases} 0, & \text{if } \mathcal{R}_2(x) \leq b \\ \left(\frac{\mathcal{R}_2(x)}{b} - 1 \right), & \text{if } b < \mathcal{R}_2(x) < 2b \\ 1, & \text{if } \mathcal{R}_2(x) \geq 2b. \end{cases} \quad (30)$$

with $\mathcal{R}_2(x) = \min_{(i,j) \neq (k,l)} \max(|x_i - x_j|, |x_k - x_l|)$.

Antiferromagnetic Heisenberg Chain

The (periodic) antiferromagnetic Heisenberg chain

$$H = \sum_{i=1}^N S_i \cdot S_{i+1}, \text{ with } S_{N+1} := S_1$$

Ground state energy per site of the infinite chain is known due to Hulthén

Lemma 8

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

$$\lim_{N \rightarrow \infty} \left\langle \text{GS}_{\text{HAF}} \left| \frac{1}{N} \sum_{k=1}^N S_k \cdot S_{k+1} \right| \text{GS}_{\text{HAF}} \right\rangle = \frac{1}{4} - \ln(2) \quad (31)$$

Control of the error for a finite chain

Lemma 9

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

$$\left\langle \text{GS}_{\text{HAF}} \left| \frac{1}{N} \sum_{k=1}^N S_k \cdot S_{k+1} \right| \text{GS}_{\text{HAF}} \right\rangle = \frac{1}{4} - \ln(2) + \mathcal{O}(N^{-1}) \quad (32)$$

Proof.

Upper bound: Truncate longer of length $M > N$ chain at length N . Lower bound: Construct trial state for longer chain of length mN by m copies of length N chain. Use translation invariance and uniqueness of the ground state:

$$\frac{1}{mN}(E_{mN} - m) \leq \frac{1}{N}E_N \leq \frac{1}{M}E_M + 1/N.$$



Lower Bound in Terms of LLH Model

Lemma 10 (Dyson's lemma spin-1/2 fermions)

Let $R > R_0 = \text{range}(v)$ and

$\varphi \in \left(H_{\text{even}}^1(\mathbb{R}) \otimes P_s \left((\mathbb{C}^2)^2 \right) \right) \oplus \left(H_{\text{odd}}^1(\mathbb{R}) \otimes P_t \left((\mathbb{C}^2)^2 \right) \right)$, then for any interval $\mathcal{I} \ni 0$

$$\int_{\mathcal{I}} |\partial \varphi|^2 + \frac{1}{2} v |\varphi|^2 \geq \int_{\mathcal{I}} \bar{\varphi} \left(\frac{1}{R - a_e} P_s + \frac{1}{R - a_o} P_t \right) (\delta_R + \delta_{-R}) \varphi, \quad (33)$$

where $a_{e/o}$ is the even/odd-wave scattering length.

The Lieb-Liniger-Heisenberg model:

$$H_{LLH} = - \sum_i \partial_i^2 + 2 \sum_{i < j} \left(c' \tilde{P}_s^{i,j} + c \tilde{P}_t^{i,j} \right) \delta(x_i - x_j), \quad (34)$$

where the spin projectors, $\tilde{P}_{s/t}$ are defined on the sector $\{\sigma\}$ to be

$$\tilde{P}_{s/t}^{ij} = P_{s/t}^{\sigma^{-1}(i)\sigma^{-1}(j)}.$$

Proposition 5

For $n(\rho R)^2 \leq \frac{3}{16\pi^2} \frac{1}{8}$, $\rho R \leq \frac{1}{2}$ and $R > 2 \max(|a_e|, a_o, R_0)$ we have

$$E^N(N, L) \geq E_{LLH}^N \left(N, \tilde{L}, \frac{2}{R - a_e}, \frac{2}{R - a_o} \right) \times \left(1 - \text{const.} \left(n(\rho R)^3 + n^{1/3}(\rho R)^2 \right) \right). \quad (35)$$

Remark 1

The Lieb-Liniger-Heisenberg model is not exactly solvable. Thus no available good lower bound.

Thanks for your attention!