One-dimensional Dilute Quantum Gases and Their Ground State Energies

Johannes Agerskov

Department of Mathematical Sciences
University of Copenhagen

PhD defense
June 6, 2023

Overview

QMATH

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 is suggest that the 1D dilute bose gas shares features with the Fermi gas.

Motivation (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

content...

The Scattering Length

Theorem 1

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*

$$-\Delta\phi + \frac{1}{2}v\phi = 0, \qquad \text{on } B_R, \tag{1}$$

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

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

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

QMATH

Model

We consider a many-body system of bosons that interacts via a repulsive pair potential $v_{ij} = v(|x_i - x_j|)$, with $v = v_{\text{reg}} + v_{\text{h.c.}}$

$$\mathcal{E}(\psi) = \int_{\Lambda_L} \left(\sum_{i=1}^{N} |\nabla_i \psi|^2 + \sum_{i<j} v_{ij} |\psi|^2 \right) \quad \text{on } L^2(\Lambda_L)^{\otimes_{\text{sym}} N}. \quad (3)$$

The ground state energy is defined by

$$E(N, L) := \inf_{\psi \in \mathcal{D}(\mathcal{E}),\ \|\psi\|^2 = 1} \mathcal{E}(\psi).$$

QMATH

2D and 3D

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

Theorem 2 ($d = 3$ result, Lee-Huang-Yang 1957[1])

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

Theorem 3 ($d = 2$ result[2])

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

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

[a] Upper bound: Yau-Yin 2009, Basti-Cenatiempo-Schlein 2021. Lower bound: Fournais-Solovej 2021

[b] Fournais-Girardot-Junge-Morin-Olivieri 2022

Bosons Main Result

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

Theorem 4 (A., R. Reuvers, J. P. Solovej, 2022)

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

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

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.*

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

Scattering length is $a = R$.

Lieb-Liniger model

Energy behaves asymptotically like

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

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

QMATH

Variational Srinciple

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

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

QMATH

Trial State

Trial state has to encapture 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 $D_N(x) = \frac{1}{2\pi}\sum_{k=-N}^{N} \mathrm{e}^{ikx} = \frac{\sin((N+1/2)x)}{2\pi\sin(x/2)}$ 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.

QMATH

Some Useful Bounds

Lemma 1

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

with $\int f(x_2)\,\mathrm{d}x_2 \le$ const. $\rho^3\log(N)$.

Lemma 2

We have the following bounds

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

QMATH

Collecting Everything

Upper bound

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

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

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

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

Proposition 1 (Upper bound Theorem 4)

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

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

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

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

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

with $\gamma = c/\rho$.

Lemma 3 (Lieb-Liniger lower bound)

Let $\gamma > 0$, *then*

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

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 $\mathcal{I} \ni 0$

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

where a is the s-wave scattering length.

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

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

Reducing to the LL Model

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

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

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

Then

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

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

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

QMATH

Lower Bound

By the reduction to the LL model we find

Proposition 2

For assumptions as in lemma 6 we have

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

Corollary 1

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

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

Lower Bound Localization

To prove the lower bound, we localize, as in the upper bound, to smaller boxes.

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* $\rho R \ll 1$ *and let* $\mu = \pi^2\rho^2\left(1 + \frac{8}{3}\rho a\right)$, *then*

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

Proposition 3 (Lower bound Theorem 4)

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

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

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 5 (Spin-polarized fermions)

Consider a Fermi gas with repulsive interaction $v = v_{\mathit{reg}} + v_{\mathit{h.c.}}$ 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 $a_o \geq 0$.

A conjecture for spin-1/2 fermions

Two solvable model for spin-1/2 fermion:

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

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

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

MATH

A Conjecture for Spin-1/2 Fermions

Based on the two solvable cases, we expect

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

Spin–$1/2$ Fermions Main Result (Upper Bound)

Theorem 6

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

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

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

QMATH

Trial State

One the sector

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

we define the trial state by

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

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

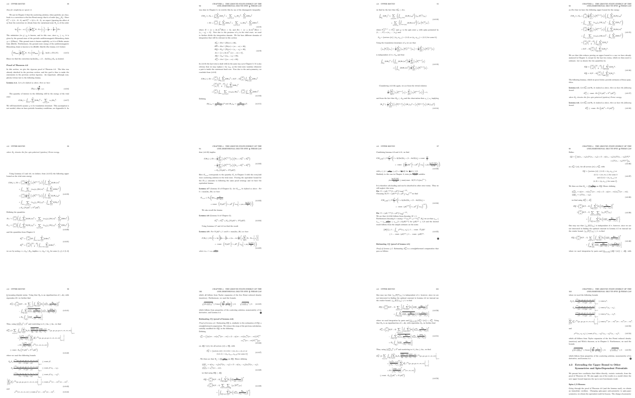
$$\eta(x) := \begin{cases} 0, & \text{if } \mathcal{R}_2(x) \leq b \\ \left(\frac{\mathcal{R}_2(x)}{b} - 1 \right), & \text{if } b < \mathcal{R}_2(x) < 2b \\ 1, & \text{if } \mathcal{R}_2(x) \geq 2b. \end{cases} \tag{30}$$

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

Trial state energy is the free Fermi energy with a correction of the form

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

proof:



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 know due to Hulthen

Lemma 7

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

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

Control of the error for a finite chain

Lemma 8

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

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

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

QMATH

Lower Bound in Terms of LLH Model

Lemma 9 (Dyson's lemma spin–$1/2$ fermions)

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

$$\int_{\mathcal{I}} |\partial\varphi|^2 + \frac{1}{2} v\,|\varphi|^2 \geq \int_{\mathcal{I}} \overline{\varphi}\left(\frac{1}{R-a_e}\,\mathrm{P}_s + \frac{1}{R-a_o}\,\mathrm{P}_t\right)(\delta_R + \delta_{-R})\,\varphi, \tag{33}$$

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

The Lieb-Liniger-Heisenberg model:

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

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

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

Proposition 4

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*

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

Remark 1

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

Conclusion and Outlook

Thanks for your attention!