The ground state energy of 1D dilute many-body quantum systems

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Overview

Background

The scattering length

Theorem 1

For $B_R \subset \mathbb{R}^d$ with $R > R_0 :=$ 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 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***.*

Model

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

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

The ground state energy is defined by

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

Previous results

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

Theorem 2 ($d = 3$ result, Lee-Huang-Yang)

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

Theorem 3 ($d = 2$ result)

$$e(\rho) = 4\pi\rho^2 \left(\left|\ln(\rho a^2)\right|^{-1} + o(\left|\ln(\rho a^2)\right|^{-1})\right). \tag{5}$$

Main result

For the remaning of the talk, $d = 1$.

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

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

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

where a is the scattering length of v.

Examples

The hard core gas

Behaves like free fermi gas in volume $L - NR$, *i.e.*

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

Scattering length is $a = R$.

Lieb-Liniger model

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 $a = -\frac{2}{c}$.

Variational principle

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

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

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.

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

Lemma 2

We have the following bounds

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

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 $\|\Psi\|^2 \geq 1 -$ 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

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

Optimizing in M and 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

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

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

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

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 $\mathcal{I} \ni 0$

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

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

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

Lower bound for mass of ψ

Lemma 5

Let ψ be defined as above, then

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

Combining lemmas 4 and 5 we have the following lemma:

Lemma 6

Let C denote the constant in lemma 5. For $n(\rho R)^2 \leq \frac{3}{16\pi^2} C$, $\rho R \ll 1$ and $R > 2|a|$ we have

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

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-aligned 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 (spinless fermions)

Consider a Fermi gas with repulsive interaction $v = v_{reg} + v_{h.c.}$ *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 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 $a_e = -\frac{2}{c}$, $a_o = 0$.

A conjecture for spin-1/2 fermions

Based on the two solvable cases, we expect

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

Thanks for your attention!