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

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Abstract

We study the ground state energy of a gas of 1D bosons with density ρ, interacting through a general, repulsive 2-body potential with scattering length a, in the dilute limit $\rho|a| \ll 1$. The first terms in the expansion of the thermodynamic energy density are $\pi^2\rho^3/3(1+2\rho a)$, where the leading order is the 1D free Fermi gas. This result covers the Tonks–Girardeau limit of the Lieb–Liniger model as a special case, but given the possibility that $a > 0$, it also applies to potentials that differ significantly from a delta function.

Set up and previous results

We consider the model

$$H = -\sum_{i=1}^{N} \Delta_{x_i} + \sum_{1\le i<j\le N} v(x_i - x_j), \tag{1}$$

where Δ_{x_i} is the d-dimension Laplacian w.r.t $x_i \in \mathbb{R}^d$, and v is a repulsive, spherically symmetry potential.
The corresponding bosonic energy functional is

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

with $v_{ij} = v(|x_i - x_j|)$, and the ground state energy is defined by

$$E(N,L) := \inf_{\psi \in \mathcal{D}(\mathcal{E}),\ \|\psi\|^2=1} \mathcal{E}(\psi). \tag{3}$$

Let $e(\rho) := \lim_{\substack{L\to\infty \\ N/L^d \to \rho}} E(N,L)/L^d$, then previously known result in $d = 2,3$ are

Theorem 1 ($d = 3$ result, Lee-Huang-Yang [4], [1, 2, 3, 6])

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

Theorem 2 ($d = 2$ result, [5])

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

The scattering length

Theorem 3 ([5])

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

$$-\Delta\phi + \frac{1}{2}v\phi = 0, \qquad \text{on } B_R, \tag{6}$$

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

$$f(r) = \begin{cases} (r-a)/(R-a) & \text{for } d = 1 \\ \ln(r/a)/\ln(R/a) & \text{for } d = 2 \\ (1 - ar^{2-d})/(1 - aR^{2-d}) & \text{for } d \ge 3, \end{cases} \tag{7}$$

with some constant a called the (s-wave, or even-wave in $d = 1$) ***scattering length***.

Similarly, one can define the p-wave, or odd-wave in $d = 1$, scattering length by having a p-wave boundary condition at $|x| = 1$.

Main result

Let $v = v_{\text{reg}} + v_{\text{h.c.}}$ with v_{reg} a finite measure, and $v_{\text{h.c.}}$ a positive linear combination of hard core potentials of the form

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

Then we have the result

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

Consider a one dimensional ($d = 1$) Bose gas with repulsive interaction $v = v_{reg} + v_{h.c.}$ as defined above. Write $\rho = N/L$. For $\rho|a|$ and ρR_0 sufficiently small, the ground state energy can be expanded as

$$E(N,L) = N\frac{\pi^2}{3}\rho^2 \left(1 + 2\rho a + \mathcal{O}\left((\rho|a|)^{6/5} + (\rho R_0)^{6/5} + N^{-2/3}\right)\right), \tag{8}$$

where a is the scattering length of v.

Since spinless (or spin-aligned) fermions are unitarily equivalent to impenetrable bosons, we have the following theorem as a corolarry

Theorem 5 (Spinless fermions [A., R. Reuvers, J. P. Solovej, 2022])

Consider a spinless 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

$$E_F(N,L) = N\frac{\pi^2}{3}\rho^2 \left(1 + 2\rho a_o + \mathcal{O}\left((\rho R_0)^{6/5} + N^{-2/3}\right)\right), \tag{9}$$

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

Upper bound proof sketch

Use Variational principle

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

Let $M = N(\rho b)^{3/2}$ and choose the trial state $\Psi = \prod_{i=1}^{M} \Psi_i$, where

$$\Psi_i(x) = \begin{cases} \omega(\mathcal{R}(x))\frac{\left|\Psi_F^i(x)\right|}{\mathcal{R}(x)} & \text{if } \mathcal{R}(x) < b \\ \left|\Psi_F^i(x)\right| & \text{if } \mathcal{R}(x) \ge b, \end{cases} \tag{10}$$

and ω is the (suitably normalized) solution to the two-body scattering equation, Ψ_F^i is the free Fermi ground state with N/M particles in the box $[(i-1)L/M, iL/M]$, and $\mathcal{R}(x) := \min_{i<j}(|x_i - x_j|)$ is uniquely defined a.e. Trial state energy computation amounts, after some manipulations and integration by parts, to computing integrals involving reduced densities and reduced density matrices of the free Fermi gas.

Upper bound proof sketch

For the free Fermi gas, then one-particle reduced density matrix is known

$$\begin{aligned} \gamma^{(1)}(x,y) &= \frac{2}{l}\sum_{j=1}^{N} \sin\left(\frac{\pi}{l}jx\right)\sin\left(\frac{\pi}{l}jy\right) \\ &= \frac{\pi}{l}\left(D_N\left(\pi\frac{x-y}{l}\right) + D_N\left(\pi\frac{x+y}{l}\right)\right), \end{aligned} \tag{11}$$

where $l = L/M$ and $D_N(x) = \frac{1}{2\pi}\sum_{k=-N}^{N} e^{ikx} = \frac{\sin((N+1/2)x)}{2\pi\sin(x/2)}$ is the Dirichlet kernel. Bounds on k-particle reduced density matrices are provided by Wick's theorem, *e.g.* :

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. $\rho^3\log(N)$.

Collecting everything 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 $\rho|a|$, $\rho R_0 \le C_U^{-1}$, the ground state energy $E^D(N,L)$ satisfies

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

Lower bound proof sketch

Proof of lower bound consists of the following steps:

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

Lemma 2 (Dyson)

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

$$\int_{\mathcal{I}} |\partial\varphi|^2 + \frac{1}{2}v|\varphi|^2 \ge \int_{\mathcal{I}} \frac{1}{R-a}(\delta_R + \delta_{-R})|\varphi|^2, \tag{13}$$

where a is the s-wave scattering length.

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 $x_1 \le x_2 \le ... \le x_n$ and symmetrically extended.
Then by Lemma 2

$$\begin{aligned} \mathcal{E}(\Psi) &\ge E^N_{LL}(n, \ell - (n-1)R, 2/(R-a))\langle\psi|\psi\rangle \\ &\ge n\frac{\pi^2}{3}\rho^2\left(1 + 2\rho(a - \cancel{R}) + \cancel{2\rho R} - \text{const.}\ \frac{1}{N^{2/3}}\right)\langle\psi|\psi\rangle. \end{aligned} \tag{14}$$

Mass of ψ can be bounded by

Lemma 3

For some constant $C > 0$ and for $n(\rho R)^2 \le \frac{3}{16\pi^2}C$, $\rho R \ll 1$ and $R > 2|a|$ we have

$$\langle\psi|\psi\rangle \ge 1 - \text{const.}\ \left(n(\rho R)^3 + n^{1/3}(\rho R)^2\right). \tag{15}$$

and we find

Proposition 2

For assumptions as in lemma 3 we have

$$E^N(n,\ell) \ge n\frac{\pi^2}{3}\rho^2\left(1 + 2\rho a + \text{const.}\ \left(\frac{1}{n^{2/3}} + n(\rho R)^3 + n^{1/3}(\rho R)^2\right)\right). \tag{16}$$

Error grows with n, so localization is needed. Localization is justified by going to the grand canonical ensemble. We localize to boxes with $n = (\rho R)^{-9/5}$ giving

Proposition 3 (Lower bound Theorem 4)

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

$$E^N(N,L) \ge N\frac{\pi^2}{3}\rho^2\left(1 + 2\rho a - C_L\left((\rho|a|)^{6/5} + (\rho R_0)^{6/5} + N^{-2/3}\right)\right). \tag{17}$$

Spin-1/2 conjecture

For the spin-1/2 case, there are two solvable models. The Yang-Gaudin model, and the hard core model. Based on the ground state energies of these, one migth conjecture

Conjecture 1

For assumptions as in Theorem 4, the spin-1/2 Fermi ground state energy can be expanded as

$$\begin{aligned} E(N,L) = N\frac{\pi^2}{3}\rho^2\Big(&1 + 2\ln(2)\rho a_e + 2(1 - \ln(2))\rho a_o \\ &+ \mathcal{O}\left((\rho\max(|a_e|, a_o))^2\right)\Big). \end{aligned} \tag{18}$$

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