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

Johannes Agerskov

Based on joint work with Robin Reuvers and Jan Philip Solovej arXiv:2203.17183

QMATH University of Copenhagen

September 7th 2022



## Overview

- 1 Background
- 2 Main result
- 3 Examples
- 4 Upper bound
- **5** Lower bound
- **6** Fermions

# Background

## The scattering length

#### Theorem 1

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

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

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

$$f(r) = \begin{cases} (r-a)/(R-a) & \text{for } d = 1\\ \ln(r/a)/\ln(R/a) & \text{for } d = 2\\ (1-ar^{2-d})/(1-aR^{2-d}) & \text{for } d \ge 3, \end{cases}$$
 (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  $v=v_{\rm reg}+v_{\rm h.c.}$ 

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

The ground state energy is defined by

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

## 2d and 3d

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)

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

Theorem 3 (d=2 result, Fournais et al. 2022)

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

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



(4)

#### Main result

For the remainder of the talk, d = 1.

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

Consider a Bose gas with repulsive interaction  $v=v_{\rm reg}+v_{h.c.}$  as defined above. Define the denisty  $\rho=N/L$ . For  $\rho|a|$  and  $\rho R_0$  sufficiently small, the ground state energy can be expanded as

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

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.

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

Scattering length is a = R.

Lieb-Liniger model

Energy behaves asymptotically like

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

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



# Variational principle

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

$$E(N,L) \leq rac{\mathcal{E}(\Psi)}{\left\|\Psi
ight\|^2}, \quad ext{for any } \Psi \in \mathcal{D}(\mathcal{E}).$$

#### Trial state

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

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

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

# One-particle reduced density matrix

For the free Fermi gas we have

$$\gamma^{(1)}(x,y) = \frac{2}{L} \sum_{j=1}^{N} \sin\left(\frac{\pi}{L}jx\right) \sin\left(\frac{\pi}{L}jy\right)$$

$$= \frac{\pi}{L} \left( D_N \left(\pi \frac{x-y}{L}\right) + D_N \left(\pi \frac{x+y}{L}\right) \right), \tag{9}$$

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  $\rho$ .

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

#### Lemma 2

We have the following bounds

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



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

#### 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

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

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

$$E^{D}(N,L) \le N \frac{\pi^{2}}{3} \rho^{2} \left( 1 + 2\rho a + C_{U} \left( (\rho |a|)^{6/5} + (\rho R_{0})^{3/2} + N^{-1} \right) \right). \tag{12}$$



#### Lower bound

#### Proof of lower bound consists of the following steps:

- 1 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.
- 3 Use a known lower bound for the Lieb Liniger model.

# The Lieb-Liniger (LL) model

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

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



## Reducing to the LL model

## Lemma 4 (Dyson)

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

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

where a is the s-wave scattering length.

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

$$\int \sum_{i} |\partial_{i}\Psi|^{2} + \sum_{i \neq j} \frac{1}{2} v_{ij} |\Psi|^{2} \ge 
\int \sum_{i} |\partial_{i}\Psi|^{2} \chi_{\mathfrak{r}_{i}(x)>R} + \sum_{i} \frac{1}{R-a} \delta(\mathfrak{r}_{i}(x)-R) |\Psi|^{2}.$$
(16)

**₩**MATH

## 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

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

(17)



# Lower bound for mass of $\psi$

#### Lemma 5

Let  $\psi$  be defined as above, then

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

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

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

$$E^{N}(n,\ell) \ge n \frac{\pi^2}{3} \rho^2 \left( 1 + 2\rho a - \text{const. } \left( (\rho R)^{6/5} + (\rho R)^{7/5} \right) \right).$$
 (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  $\mu = \pi^2 \rho^2 (1 + \frac{8}{3} \rho a)$ , then

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

$$E^{N}(N,L) \ge N \frac{\pi^{2}}{3} \rho^{2} \left( 1 + 2\rho a - C_{L} \left( (\rho |a|)^{6/5} + (\rho R_{0})^{6/5} + N^{-2/3} \right) \right). \tag{23}$$

# 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 (spinless fermions)

Consider a 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  $\rho a_o$  and  $\rho R_0$  sufficiently small, the ground state energy can be expanded as

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

where  $a_o \ge 0$  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

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

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

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

Thanks for your attention!