Upper bound on the ground state energy of a dilute gas of hard sphere bosons

Joint works with S. Cenatiempo, A. Giuliani, A. Olgiati, G. Pasqualetti and B. Schlein

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N bosons in the 3d box $\Lambda_L = \Big[-\frac{L}{2}, \frac{L}{2}\Big]^3$.

Hamiltonian on $L^2_{\mathrm{S}}(\Lambda_L^N)$:

$$H_{N,L} = -\sum_{i=1}^{N} \Delta_{x_i} + \sum_{1 \leq i < j \leq N} V(x_i - x_j),$$

$V \geq 0$, spherically symmetric, compact support.

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$V \ge 0$, spherically symmetric, compact support.

We are interested in the ground state energy per particle in the thermodynamic limit:

$$e(\rho) = \lim_{\substack{N,L \to +\infty \\ N/L^3 = \rho}} \frac{E_{N,L}}{N}, \qquad E_{N,L} = \inf_{\psi \neq 0} \frac{\langle \psi, H_{N,L} \psi \rangle}{\|\psi\|^2}$$

We are particularly interested in the case of hard sphere interaction:

$$V(x) = V^{\text{hs}}(x) = \begin{cases} +\infty, & |x| \leq a \\ 0, & |x| > a \end{cases}$$

In this case,

$$E^{\text{hs}}_{N,L} = \inf_{\psi \neq 0} \frac{\langle \psi, \sum_{i=1}^{N} -\Delta_{x_i} \psi \rangle}{\|\psi\|^2}$$

where the infimum is taken over ψ satisfying the hard sphere condition

$$\psi(x_1, \ldots, x_N) = 0 \ \text{ if } \ \exists\, i \neq j : |x_i - x_j| < a$$

Let

$$\begin{cases} \Big(-\Delta + \frac{1}{2}V \Big) f = 0 \\ f \to 1 \text{ for } |x| \to +\infty \end{cases}$$

Then

$$f(x) = 1 - \frac{a}{|x|} \qquad \text{outside the range of } V$$

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We consider the dilute regime: $\rho a^3 \ll 1$

Lee-Huang-Yang Formula

In [Bogolubov '47] and more explicitly in [Lee,Huang,Yang '57] it was predicted that in the dilute limit

$$e(\rho) = \lim_{\substack{N,L\to+\infty \\ N/L^3=\rho}} \frac{E_{N,L}}{N} = 4\pi a\rho \left[1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} + o(\sqrt{\rho a^3})\right].$$

Only dependence on V through its scattering length.

Lower bound:

[Lieb, Yngvason '98],. . . [Fournais, Solovej '20+'21], . . . (general V, also hard core)

Upper bound:

[Dyson '57], . . . [Yau, Yin '09], [B., Cenatiempo, Schlein '21], . . . ($V \in L^3$)

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$\rightsquigarrow$ upper bound for hard sphere still open.

An upper bound for hard-core bosons

Currently best available upper bound for hard sphere bosons:

Theorem [B., Cenatiempo, Giuliani, Olgiati, Pasqualetti, Schlein '23]

There exists $C > 0$ such that

$$\lim_{\substack{N,L\to\infty:\\ N/L^3=\rho}} \frac{E^{\mathrm{hc}}_{N,L}}{N} \leq 4\pi\rho a \left[1 + C(\rho a^3)^{1/2}\right]$$

- it captures the correct order but NOT the right constant
- we use a Bijl-Dingle-Jastrow factor similarly as in [Dyson '57]
- no box-method, differently from [Yau, Yin '09], [B., Cenatiempo, Schlein '21]
- fine cancellations among numerator and denominator

We look for a suitable trial state

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In the non-interacting case the (not normalized) ground state is

$$\psi^{V=0}(x_1, \ldots, x_N) = \varphi_0^{\otimes N}(x_1, \ldots, x_N) \quad \text{Bose-Einstein condensation}$$

with $\varphi_0(x) = 1$ condensate wave function.

For dilute interacting Bose gas condensation is expected BUT $\psi \not\simeq \varphi_0^{\otimes N}$
(a product state doesn't respect the hard sphere condition)

The trial state in [B., Cenatiempo, Schlein '21] is not well suited for hard sphere (Bogoliubov approach)

⇝ We have to describe correlations:

$$\psi(x_1, \ldots x_N) = \prod_{i<j} f_\ell(x_i - x_j), \qquad \text{Bijl-Dingle-Jastrow factor}$$

with $0 \leq f_\ell \leq 1$ solution of

$$\begin{cases} -\Delta f_\ell = \lambda_\ell f_\ell \chi_\ell \\ f_\ell(x) = 0 & \text{if } |x| \leq a \;, \\ \partial_r f_\ell(x) = 0 & \text{if } |x| = \ell \end{cases} \qquad a \leq \ell \leq L$$

normalized so that $f_\ell(x) = 1$ if $|x| = \ell$.

Then,

$$\lambda_\ell = \frac{3a}{\ell^3}\left(1 + \mathcal{O}\left(\frac{a}{\ell}\right)\right), \qquad 0 \leq \underbrace{1 - f_\ell^2(x)}_{u_\ell(x)} \leq C\frac{a}{|x|}\chi_\ell(x)$$

The Bijl-Dingle-Jastrow factor [Bijl '40, Dingle '49, Jastrow '55]

We try to expand the Bijl-Dingle-Jastrow factor:

$$\begin{aligned}\int \prod_{i<j}^{N} f_\ell^2(x_i - x_j) d\mathbf{x} &= \int \prod_{i<j}^{N} \left[1 - u_\ell(x_i - x_j)\right] d\mathbf{x} \\ &= |\Lambda_L|^N - N^2 |\Lambda_L|^{(N-1)} \int u_\ell(x) dx + \dots \\ &= |\Lambda_L|^N \left[1 - N\rho a \ell^2 + \dots\right]\end{aligned}$$

$\rightsquigarrow$ for any $\ell \geq a$, the expansion diverges.

Nevertheless we can expand in one variable:

$$\begin{aligned}\int \prod_{i<j}^{N} f_\ell^2(x_i - x_j) d\mathbf{x} &= \int \prod_{j=2}^{N} \left[1 - u_\ell(x_1 - x_j)\right] \prod_{2\le i<j}^{N} f_\ell^2(x_i - x_j)\, d\mathbf{x} \\ &= \int \left[1 - \sum_{j=2}^{N} u_\ell(x_1 - x_j) + \dots\right] \prod_{2\le i<j}^{N} f_\ell^2(x_i - x_j)\, d\mathbf{x} \\ &= |\Lambda_L|[1 - C\underbrace{\rho a \ell^2}_{\ll 1} + \dots] \int \prod_{2\le i<j}^{N} f_\ell^2(x_i - x_j)\, dx_2 \dots dx_N\end{aligned}$$

$\rightsquigarrow$ converges assuming $\rho a \ell^2 \ll 1$. We choose $\ell = c(\rho a)^{-1/2}$, $c \ll 1$.

We set $f_{ij} = f_\ell(x_i - x_j)$ and $\chi_{ij} = \chi_\ell(x_i - x_j)$.

We compute

$$-\Delta_{x_k} \prod_{i<j}^{N} f_{ij} = \sum_{m \neq k}^{N} \frac{-\Delta f_{km}}{f_{km}} \prod_{i<j}^{N} f_{ij} - \sum_{n,m \neq k}^{N} \frac{\nabla f_{kn}}{f_{kn}} \cdot \frac{\nabla f_{km}}{f_{km}} \prod_{i<j}^{N} f_{ij}$$

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We compute

$$-\Delta_{x_k} \prod_{i<j}^{N} f_{ij} = \sum_{m \neq k}^{N} \frac{-\Delta f_{km}}{f_{km}} \prod_{i<j}^{N} f_{ij} + \text{three body term}$$

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Using the scattering equation

$$\langle \psi, \sum_{k=1}^{N} -\Delta_{x_k} \psi \rangle = \sum_{k<m}^{N} \int 2\lambda_\ell \chi_{km} \prod_{i<j}^{N} f_{ij}^2 d\mathbf{x} + \text{three body term}$$

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we obtain

$$\langle \psi, \sum_{k=1}^{N} -\Delta_{x_k} \psi \rangle \simeq N^2 \lambda_\ell \int \chi_{12} \prod_{i<j}^{N} f_{ij}^2 \, d\mathbf{x} + \text{three body term}$$

Expanding in the first variable and setting $u_{ij} = u_\ell(x_i - x_j)$.

Let $M \in \mathbb{N}$ even

$$\int \chi_{12} \prod_{i<j}^{N} f_{ij}^2$$
$$\leq \int \chi_{12} f_{12}^2 \left[1 - \sum_{j_1} u_{1j_1} - \cdots + \sum_{j_1 < \cdots < j_M} u_{1j_1} \ldots u_{1j_M} \right] \prod_{2 \leq i < j \leq N} f_{ij}^2$$

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$$= \sum_{m_1=0}^{M} (-1)^{m_1} \binom{N-2}{m_1} \int \chi_{12} f_{12}^2 \, u_{13} \ldots u_{1m_1} \prod_{2 \leq i < j \leq N} f_{ij}^2$$

An upper bound for hard-core bosons - Sketch of the proof

Expanding in the first variable and setting $u_{ij} = u_\ell(x_i - x_j)$.

Let $M \in \mathbb{N}$ even

$$\begin{aligned}
&\int \chi_{12} \prod_{i<j}^{N} f_{ij}^2 \\
&\leq \int \chi_{12} f_{12}^2 \left[1 - \sum_{j_1} u_{1j_1} - \cdots + \sum_{j_1 < \cdots < j_M} u_{1j_1} \ldots u_{1j_M} \right] \prod_{2 \leq i < j \leq N} f_{ij}^2 \\
&= \sum_{m_1=0}^{M} (-1)^{m_1} \binom{N-2}{m_1} \int \chi_{12} f_{12}^2 \, u_{13} \ldots u_{1m_1} \prod_{2 \leq i < j \leq N} f_{ij}^2
\end{aligned}$$

Expand second variable:

$$\begin{aligned}
\int \chi_{12} \prod_{i<j}^{N} f_{ij}^2 \leq& \sum_{m_1=0}^{M} (-1)^{m_1} \binom{N-2}{m_1} \sum_{m_2=0}^{M-m_1} (-1)^{m_2} \\
&\times \sum_{3 < j_1 < \cdots < j_{m_2} \leq N} \int \chi_{12} f_{12}^2 \, u_{13} \ldots u_{1,m_1+2} u_{2j_1} \ldots u_{2j_{m_2}} \prod_{3 \leq i < j \leq N} f_{ij}^2
\end{aligned}$$

We distinguish 3 types of terms:

i) Tree terms, still entangled with Jastrow:

$$N^3 \lambda_\ell \int \chi_{12} f_{12}^2 u_{13} \prod_{3 \leq i < j \leq N} f_{ij}^2 \, d\mathbf{x}$$

ii) Terms with loops, like

$$N^3 \lambda_\ell \int \chi_{12} f_{12}^2 u_{13} u_{23} \prod_{3 \leq i < j \leq N} f_{ij}^2 \, d\mathbf{x}$$

iii) Tree terms, disentangled from Jastrow:

$$N^2 \lambda_\ell \int \chi_{12} f_{12}^2 \prod_{3 \leq i < j \leq N} f_{ij}^2 \, d\mathbf{x}$$

We distinguish 3 types of terms:

i) Tree terms, still entangled with Jastrow:

$$N^3\lambda_\ell \int \chi_{12} f_{12}^2 u_{13} \prod_{3\leq i<j\leq N} f_{ij}^2 \, d\mathbf{x}$$

$\rightsquigarrow$ these terms must be further expanded

ii) Terms with loops, like

$$N^3\lambda_\ell \int \chi_{12} f_{12}^2 u_{13} u_{23} \prod_{3\leq i<j\leq N} f_{ij}^2 \, d\mathbf{x}$$

$\rightsquigarrow$ these terms give contributions of the LHY order

iii) Tree terms, disentangled from Jastrow:

$$N^2\lambda_\ell \int \chi_{12} f_{12}^2 \prod_{3\leq i<j\leq N} f_{ij}^2 \, d\mathbf{x}$$

$\rightsquigarrow$these terms cancel with the denominator

Beyond the Bijl-Dingle-Jastrow state

Partial expansion of the Bijl-Dingle-Jastrow state converges if

$$\ell \ll (\rho a)^{-1/2}$$

BUT to match the LHY term we expect correlations are needed up to

$$\ell > (\rho a)^{-1/2}$$

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Possible way out: trial state of the form

$$\psi(x_1, \ldots, x_N) = \underbrace{\prod_{i<j}^{N} f_\ell(x_i - x_j)}_{\text{hard sphere cond. \& correlation at short scale}} \quad \underbrace{\phi(x_1, \ldots, x_N)}_{\text{correlation at large scale}}$$

$\rightsquigarrow$ very difficult to use cancellations in the thermodynamic limit.

Trial states of this form on the other hand have been successfully used in

- [B., Cenatiempo, Olgiati, Pasqualetti, Schlein '23] dealing with the ultra dilute Gross-Pitaevskii regime.
  It corresponds to consider a box of side length $L \sim (\rho a)^{-1/2}$,
  Then,
  $$N\rho a\ell^2 = (\rho a^3)^{-1/2}\rho a\ell^2 \ll 1$$
  if $a \ll \ell \ll (\rho a)^{-1/2}(\rho a^3)^{1/4}$
  $\rightsquigarrow$ the Bijl-Dingle-Jastrow factor can be fully expanded
- [Fournais, Girardot, Junge, Morin, Olivieri '24] dealing with the thermodynamic limit in $2d$
  $\rightsquigarrow$ also in this case (by box-method) the Bijl-Dingle-Jastrow factor can be fully expanded

Thank you for your attention!

An upper bound for hard-core bosons - Sketch of the proof

Proceeding in this way we get

$$\frac{E_{N,L}^{\mathrm{hc}}}{N} \leq 4\pi a\rho\Big[1 + C(C\rho a\ell^2)^{M-1} + C\frac{a}{\ell}\sum_{j=2}^{M}(C\rho a\ell^2)^{j-2}\Big]$$

Choosing

$$\ell = c(\rho a)^{-1/2} \quad \text{s.t. } C\rho a\ell^2 \leq \frac{1}{2}$$

and

$$M \geq 1 + \log_2(\rho a^3)^{-1/2}$$

we conclude.

Choice of ϕ

$$\phi = U_N^* e^{B_\eta} e^{B_\tau} \Omega$$

where

- $U_N : L^2_S(\Lambda^N) \to \mathcal{F}_+^{\leq N} = \bigoplus_{n=0}^N L^2_\perp(\Lambda)^{\otimes_S n}$ factors out the condensate and allows to focus on orthogonal excitations
- B_η and B_τ are generalized Bogoliubov transformations: $B_\alpha = \frac{1}{2} \sum_{p \in 2\pi\mathbb{Z}^3} \alpha_p (b_p^* b_{-p}^* - b_p b_{-p})$,
- the kernel η is the Fourier transform of $\check{\eta} = -N(1-g)$, g being the solution of

$$\begin{cases} -\nabla(f_\ell^2 \nabla g) + \lambda_\ell \chi_\ell f_\ell^2 g = \lambda_{\ell_0} \chi_{\ell_0} f_\ell^2 g & \frac{a}{N} \leq |x| \leq \ell_0 \\ g(x) = 1 & |x| = \ell_0 \\ \partial_r g & |x| = \ell_0 \end{cases} \qquad \ell_0 = O(1).$$

$\rightsquigarrow g(x) = \frac{f_{\ell_0}(x)}{f_\ell(x)}$, and λ_{ℓ_0} as λ_ℓ with the replacement $\ell \to \ell_0$.

Second order upper bound for smooth potentials

For regular potentials the problem has been solved

Theorem (B., Cenatiempo, Schlein) Forum Math. Sigma, 9 (2021)

Let $V \in L^3(\mathbb{R}^3)$ non-negative, radially symmetric, with compact support in $B_R(0)$.
Then,

$$e(\rho) \leq 4\pi a\rho\left[1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3}\right] + C\rho^{\frac{3}{2}+\frac{1}{10}}$$

for some $C > 0$ and for ρ small enough.

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for some $C > 0$ and for ρ small enough.

- an upper bound for smooth potential was already obtained in [Yau,Yin '09]
- hard-core interaction is still open

Bogolubov-like trial state

The trial state is written in the grand-canonical setting.
Let $a^\sharp_p, p \in \frac{2\pi}{L^3}\mathbb{Z}^3$ the creation/annihilation operators, $\Omega \in \mathcal{F} = \oplus_{n\geq 0} L^2_s(\Lambda_L^n)$ the vaccum vector.
Inspired by [Bogolubov '47], we consider

$$e^B e^A W \Omega$$

where

$$W = \exp(\sqrt{N} a_0^* - \sqrt{N} a_0), \qquad \text{Weyl operator}$$

$$B = \frac{1}{2} \sum_{p \in \frac{2\pi}{L}\mathbb{Z}^3} \eta_p a_p^* a_{-p}^* - \text{h.c.}, \qquad \text{Bogolubov transformation}$$

$$A = \frac{1}{\sqrt{N}} \sum_{p,r \in \frac{2\pi}{L}\mathbb{Z}^3} \eta_r a_{p+r}^* a_{-r}^* a_p - \text{h.c.}, \qquad \text{cubic operator}$$

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Similar trial state already used in [Boccato,Brennecke,Cenatiempo,Schlein '19,'20] dealing with Gross-Pitaevskii regime.
Localization argument and suitable restrictions on the allowed momenta in the cubic operator allows to treat the thermodynamic limit.

Bogolubov-like trial state

Note that, setting $\check{\eta}(x) = -N(1 - f_\ell)$,

$$\prod_{i<j} f_\ell(x_i - x_j)\varphi_0^{\otimes N} \sim \prod_{i<j}\Big(1 + \frac{1}{N}\check{\eta}(x_i - x_j)\Big)\varphi_0^{\otimes N}$$

$$\sim \Big(1 + \frac{1}{N}\sum_{i<j}\check{\eta}(x_i - x_j) + \dots\Big)\varphi_0^{\otimes N}$$

$$\sim \Big(1 + \frac{1}{2}\sum_{p}\eta_p a_p^* a_{-p}^* \frac{a_0}{\sqrt{N}}\frac{a_0}{\sqrt{N}} + \dots\Big)\varphi_0^{\otimes N}$$

Bogolubov-like trial state

Note that, setting $\check{\eta}(x) = -N(1 - f_\ell)$,

$$\begin{aligned}\prod_{i<j} f_\ell(x_i - x_j)\varphi_0^{\otimes N} &\sim \prod_{i<j}\Big(1 + \frac{1}{N}\check{\eta}(x_i - x_j)\Big)\varphi_0^{\otimes N} \\ &\sim \Big(1 + \frac{1}{N}\sum_{i<j}\check{\eta}(x_i - x_j) + \dots\Big)\varphi_0^{\otimes N} \\ &\sim \Big(1 + \frac{1}{2}\sum_p \eta_p a_p^* a_{-p}^* \frac{a_0}{\sqrt{N}}\frac{a_0}{\sqrt{N}} + \dots\Big)\varphi_0^{\otimes N} \\ &\sim \exp\Big(\frac{1}{2}\sum_p \eta_p a_p^* a_{-p}^* - \text{h.c.}\Big)\varphi_0^{\otimes N}\end{aligned}$$

since we expect condensation we approximate $a_0^\sharp \sim \sqrt{N}$

Bogolubov-like trial state

- hence, $e^B W\Omega$ approximate the Jastrow factor.
  $\rightsquigarrow$ Big advantage: computations are easy

- to deal with the thermodynamic limit also the exponential of a cubic operator is needed $\rightsquigarrow$ more difficult to handle

- the trial state $e^B e^A W\Omega$ does not respect the hard-core condition
  $\rightsquigarrow$ hard-core case is still open