Ground state energy of a dense Bose gas

Marcel Majocha

Faculty of Physics
University of Warsaw

Quantissima sur Oise, September 2025

Problem formulation

N particles Bose gas in $[0, L]^3$ with p.b.c.

$$H_N = -\sum_{j=1}^{N} \Delta_j + \sum_{i<j} w(x_i - x_j)$$

$w, \widehat{w} > 0$ and $w, \widehat{w} \in L^1(\mathbb{R}^3)$.

Ground state energy density in the thermodynamic limit

$$e(\rho) = \lim_{\substack{N,L\to\infty \\ \rho=\text{const}}} \inf_{\|\psi_N\|=1} \frac{\langle \psi_N, H_N \, \psi_N \rangle}{L^3},$$

where $\rho = N/L^3$

Theorem

For $\rho \gg 1$ we have

$$e(\rho) = \frac{1}{2}\widehat{w}(0)\rho^2 - \frac{1}{2}w(0)\rho + o(\rho),$$

Problem formulation

- First derived by Lieb [1963]
- Dilute gas is much more popular with many important results over the last decade (e.g. Fournais-Solovej proof of the Lee-Huang-Yang formula, 2020)
- Proof of the problem in the **grand canonical ensemble** is rather straightforward (e.g Mokrzański-Pałuba, 2024)
- The result in the canonical ensemble can be obtained using the equivalence of ensembles
- Goal of my bachelor project is to derive the result working directly in the **canonical ensemble**

Problem formulation

N particles Bose gas in $[0, L]^3$ with p.b.c.

$$H_N = -\sum_{j=1}^{N} \Delta_j + \sum_{i<j} w(x_i - x_j)$$

$w, \widehat{w} > 0$ and $w, \widehat{w} \in L^1(\mathbb{R}^3)$.

Ground state energy density in the thermodynamic limit

$$e(\rho) = \lim_{\substack{N,L\to\infty \\ \rho=\text{const}}} \inf_{\|\psi\|=1} \frac{\langle \psi_N, H_N \psi_N \rangle}{L^3},$$

where $\rho = N/L^3$

Theorem

For $\rho \gg 1$ we have

$$e(\rho) = \frac{1}{2}\widehat{w}(0)\rho^2 - \frac{1}{2}w(0)\rho + o(\rho),$$

Lower bound

Onsager Inequality

$$\sum_{1\leq i<j\leq N} w(x_i - x_j) \geq \frac{1}{2}\widehat{w}(0)\rho N - \frac{1}{2}w(0)N$$

Additionally $-\sum_i \Delta_i \geq 0$. Therefore

$$\frac{1}{L^3}H_N \geq \frac{1}{2}\widehat{w}(0)\rho^2 - \frac{1}{2}w(0)\rho$$

$$e(\rho) \geq \frac{1}{2}\widehat{w}(0)\rho^2 - \frac{1}{2}w(0)\rho$$

Upper bound

Variational method

$$E_0(N,\rho) \leq \frac{\langle H_N \rangle_{\varphi_N}}{\|\varphi_N\|^2}, \qquad \forall \varphi_N \in \mathfrak{H}_N.$$

Our trial state was inspired by the **Bogoliubov theory**

$$\varphi_N = U_N^* \mathbb{1}^{\leq N} U_\beta^* \Omega,$$

where

- $U_N : \mathfrak{H}_N \longrightarrow \mathcal{F}_+^{\leq N}$ $\left(\mathcal{F}_+ = \mathcal{F}(\text{span}\,\{u_0\}^\perp)\right)$ is an operator used for implementing Bogoliubov c-number substitution canonically (introduced by Lewin-Nam-Serfaty-Solovej, 2014)
- $\mathbb{1}^{\leq N}$ is a projection of the excited Fock space vector onto sectors with less or equal to N particles
- $U_\beta = \exp\left[\sum_{p\neq 0} \frac{1}{2}\beta(p)\left(a_p a_{-p} - a_p^* a_{-p}^*\right)\right]$ is a Bogoliubov transformation for β real, positive and continuous

Occuring problems

$$
\begin{aligned}
U_N H_N U_N^* =& \\
=& \frac{N-1}{2}\rho\widehat{w}(0) + \frac{\mathcal{N}_+(1-\mathcal{N}_+)}{2L^3}\widehat{w}(0) + \\
&+ \frac{\mathcal{N}_+(1-\mathcal{N}_+)}{2L^3}\widehat{w}(0) + \sum_{p\neq 0}\left(p^2 + \frac{N-\mathcal{N}_+}{L^3}\widehat{w}(p)\right) a_p^* a_p + \\
&+ \frac{1}{2}\sum_{p\neq 0}\left(\widehat{w}(p) a_p^* a_{-p}^* \frac{\sqrt{(N-\mathcal{N}_+)(N-\mathcal{N}_+-1)}}{L^3} \ + \ \text{h. c.}\right) + \\
&+ \sum_{\substack{p,q\neq 0\\ p+q\neq 0}}\left(\widehat{w}(p) a_{p+q}^* a_{-p}^* a_q \frac{\sqrt{N-\mathcal{N}_+}}{L^3} \ + \ \text{h. c.}\right) + \\
&+ \frac{1}{2L^3}\sum_{\substack{q,r\neq 0\\ p\notin\{-q,r\}}} \widehat{w}(p) a_{q+p}^* a_{r-p}^* a_q a_r
\end{aligned}
$$

Occuring problems

Estimating $a^*_{p+q}a^*_{-p}a_q\sqrt{N-\mathcal{N}_+}$ in a usual way (using Cauchy-Schwarz) gives us an upper bound that will diverge in the thermodynamic limit (always $\sim L^{3/2}$)

We introduce parity operator on the excited Fock space

$$\mathcal{V} = (-1)^{\mathcal{N}_+}$$

- $\mathbb{1}^{\leq N} U^*_\beta \Omega = \mathcal{V}\mathbb{1}^{\leq N} U^*_\beta \Omega$
- $\mathcal{V}\left[a^*_{p+q}a^*_{-p}a_q\sqrt{N-\mathcal{N}_+}\right]\mathcal{V} = -a^*_{p+q}a^*_{-p}a_q\sqrt{N-\mathcal{N}_+}$

$$\left\langle a^*_{p+q}a^*_{-p}a_q\sqrt{N-\mathcal{N}_+}\right\rangle_{\mathbb{1}^{\leq N} U^*_\beta \Omega} =$$
$$= -\left\langle a^*_{p+q}a^*_{-p}a_q\sqrt{N-\mathcal{N}_+}\right\rangle_{\mathbb{1}^{\leq N} U^*_\beta \Omega} = 0$$

Thank you for your attention!

Acknowledgements. I want to thank my supervisor Marcin Napiórkowski and Błażej Ruba for helpful insights and discussions.