Upper bounds on ground state energy of dilute Bose gases

Benjamin Schlein, University of Zurich

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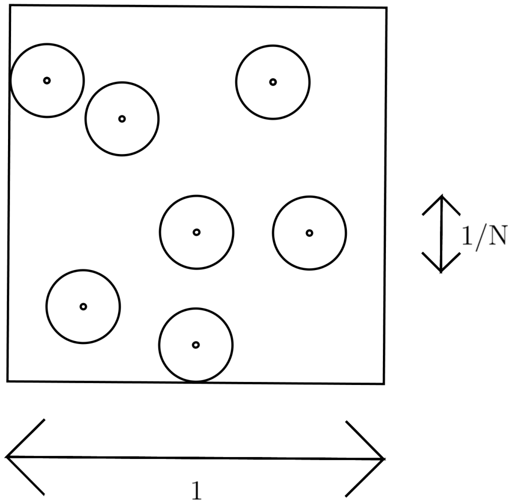
Gross-Pitaevskii regime: N bosons in $\Lambda = [0;1]^3$, interacting through potential with effective range of order N^{-1}, as $N \to \infty$.



Hamilton operator: has form

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \sum_{i<j}^{N} N^2 V(N(x_i - x_j))$$

on $L^2_s(\Lambda^N)$. $V \geq 0$ with **compact support**.

Scattering length: defined by zero-energy **scattering equation**

$$\left[-\Delta + \frac{1}{2} V\right] f = 0, \qquad \text{with} \qquad f \to 1 \quad \text{as } |x| \to \infty$$

$$\Rightarrow \qquad f(x) = 1 - \frac{\mathfrak{a}}{|x|}, \qquad \text{for large } |x|$$

Theorem [Boccato-Brennecke-Cenatiempo-S.]: for $V \in L^3(\mathbb{R}^3)$,

$$E_N = 4\pi\mathfrak{a}(N-1) + e_\Lambda \mathfrak{a}^2 - \frac{1}{2} \sum_{p \in 2\pi\mathbb{Z}^3 \setminus \{0\}} \left[p^2 + 8\pi\mathfrak{a} - \sqrt{|p|^4 + 16\pi\mathfrak{a}p^2} - \frac{(8\pi\mathfrak{a})^2}{2p^2} \right] + \mathcal{O}(N^{-1/4})$$

where

$$e_\Lambda = 2 - \lim_{M\to\infty} \sum_{|p_1|,|p_2|,|p_3|<M} \frac{\cos(|p|)}{p^2}$$

Moreover, **spectrum** of $H_N - E_N$ below $\zeta > 0$ consists of

$$\sum_{p \in 2\pi\mathbb{Z}^3 \setminus \{0\}} n_p \sqrt{|p|^4 + 16\pi\mathfrak{a}p^2} + \mathcal{O}(\zeta^3 N^{-1/4})$$

Remarks:

- Leading order estimates known since **[Lieb-Yngvason '98]**.

- Extensions in **[Nam-Triay '21]**, **[Brennecke-Schraven-S. '21]**, **[Boccato-Seiringer '22]**, **[Hainzl-S.-Triay '22]**

Thermodynamic limit: consider N particles in $\Lambda = [0; L]^3$. Let $N, L \to \infty$ with fixed density $\rho = N/L^3$.

Lee-Huang-Yang predicted:

$$\lim_{\substack{N,L\to\infty: \\ N/L^3=\rho}} \frac{E_{N,L}}{N} = 4\pi\rho\mathfrak{a}\left[1 + \frac{128}{15\sqrt{\pi}}(\rho\mathfrak{a}^3)^{1/2} + \ldots\right]$$

Remarks:

- Leading order by **[Dyson, '57]**, **[Lieb-Yngvason, '98]**.

- Upper bound by **[Yau-Yin, '09]**, **[Basti-Cenatiempo-S., '20]** for $V \in L^3$.

- Lower bound by **[Fournais-Solovej, '20-'21]**, also hard-sphere.

- LHY also derived by **[Carlen-Holzmann-Jauslin-Lieb, '20]**, assuming relations for reduced densities.

Ideas from proof: focus on upper bound.

Natural trial state is **Jastrow wave function**

$$\psi_N(x_1, \dots, x_N) = \prod_{i<j}^{N} f_\ell(x_i - x_j)$$

where f_ℓ describes correlations up to distance ℓ.

We choose f_ℓ as solution of **Neumann problem**

$$\Big(-\Delta + \frac{N^2}{2} V(N.) \Big) f_\ell = \lambda_\ell f_\ell \qquad \text{on } |x| \leq \ell$$

with $\partial_r f_\ell(x) = 0$, if $|x| = \ell$. We extend $f_\ell(x) = 1$, for $|x| \geq \ell$.

We find

$$\lambda_\ell \simeq \frac{3\mathfrak{a}}{N\ell^3}\Big[1 + \frac{9\mathfrak{a}}{5N\ell}\Big], \qquad 0 \leq 1 - f_\ell(x) \lesssim \frac{\mathfrak{a}}{N|x|}\chi_\ell(x)$$

We compute

$$
\begin{aligned}
&-\Delta_{x_k} \prod_{i<j}^{N} f_\ell(x_i - x_j) \\
&\quad = \sum_{m\neq k} \frac{-\Delta f_\ell(x_k - x_m)}{f_\ell(x_k - x_m)} \prod_{i<j}^{N} f_\ell(x_i - x_j) \\
&\qquad - \sum_{n,m\neq k} \frac{\nabla f_\ell(x_k - x_n)}{f_\ell(x_k - x_n)} \cdot \frac{\nabla f_\ell(x_k - x_m)}{f_\ell(x_k - x_m)} \prod_{i<j}^{N} f_\ell(x_i - x_j)
\end{aligned}
$$

We find **energy**

$$
\begin{aligned}
\langle \psi_N, H_N \psi_N \rangle = 2\lambda_\ell \sum_{k<m}^{N} \int \chi_\ell(x_k - x_m) \prod_{i<j}^{N} f_\ell^2(x_i - x_j) \\
- \sum_{k,m,n} \int \frac{\nabla f_\ell(x_k - x_n)}{f_\ell(x_k - x_n)} \cdot \frac{\nabla f_\ell(x_k - x_m)}{f_\ell(x_k - x_m)} \prod_{i<j}^{N} f_\ell^2(x_i - x_j)
\end{aligned}
$$

With **notation** $\chi_{ij} = \chi_\ell(x_i - x_j)$, $f_{ij} = f_\ell(x_i - x_j)$, we obtain

$$\langle \psi_N, H_N \psi_N \rangle \simeq N^2 \lambda_\ell \int \chi_{12} \prod_{i<j}^N f_{ij}^2 - \frac{N^3}{6} \int \frac{\nabla f_{12}}{f_{12}} \cdot \frac{\nabla f_{13}}{f_{13}} \prod_{i<j}^N f_{ij}^2$$

Writing $f_\ell^2(x) = 1 - u(x)$, we observe that

$$\|\psi_N\|^2 = \int \prod_{i<j}^N f_{ij}^2 \geq 1 - \sum_{i<j}^N \int u_{i,j} \simeq 1 - CN\ell^2$$

Thus, we arrive at **upper bound**

$$\frac{\langle \psi_N, H_N \psi_N \rangle}{\|\psi_N\|^2} \leq N^2 \lambda_\ell \cdot \frac{4}{3}\pi \ell^3 \cdot (1 + CN\ell^2) \leq 4\pi \mathfrak{a} N \cdot \left(1 + \frac{C}{N\ell} + CN\ell^2\right)$$

Choosing $\ell = N^{-2/3}$, we obtain

$$\frac{\langle \psi_N, H_N \psi_N \rangle}{\|\psi_N\|^2} \leq 4\pi \mathfrak{a} N \cdot (1 + CN^{-1/3})$$

Bogoliubov approach: look for approximation of Jastrow.

For $p \in 2\pi\mathbb{Z}^3$, consider **creation** and **annihilation** ops a_p^*, a_p, satisfying canonical commutation relations

$$[a_p, a_q^*] = \delta_{pq}, \qquad [a_p, a_q] = [a_p^*, a_q^*] = 0$$

With $\varphi_0(x) = 1$ for all $x \in \Lambda$, we observe

$$\left[\frac{1}{2N} \sum_{p \neq 0} \eta_p a_p^* a_{-p}^* a_0 a_0\right] \varphi_0^{\otimes N} = \frac{1}{N} \sum_{i<j}^{N} \check{\eta}(x_i - x_j)$$

More generally

$$\left[\frac{1}{2N} \sum_{p \neq 0} \eta_p a_p^* a_{-p}^* a_0 a_0\right]^k \varphi_0^{\otimes N} = \frac{1}{N^k} \sum \check{\eta}(x_{i_1} - x_{j_1}) \dots \check{\eta}(x_{i_k} - x_{j_k})$$

For $k \ll N$, we find

$$\left[\frac{1}{2N} \sum_{p \neq 0} \eta_p a_p^* a_{-p}^* a_0 a_0\right]^k \varphi_0^{\otimes N} \simeq \left[\frac{1}{N} \sum_{i<j}^{N} \check{\eta}(x_i - x_j)\right]^k$$

Thus

$$\exp\left[\frac{1}{2N}\sum_{p\neq 0}\eta_p a_p^* a_{-p}^* a_0 a_0\right]\varphi_0^{\otimes N}$$

$$\simeq e^{\frac{1}{N}\sum_{i<j}^N \check{\eta}(x_i-x_j)} = \prod_{i<j}^N e^{\frac{1}{N}\check{\eta}(x_i-x_j)} \simeq \prod_{i<j}^N \left[1+\frac{1}{N}\check{\eta}(x_i-x_j)\right]$$

approximates Jastrow if $\check{\eta}(x) = N(f_\ell(x)-1)$.

We are led to normalized **Bogoliubov state** $e^B\varphi_0^{\otimes N}$, with

$$B = \frac{1}{2N}\sum_{p\neq 0}\eta_p\Big(a_p^* a_{-p}^* a_0 a_0 - a_0^* a_0^* a_p a_{-p}\Big)$$

Big advantage: with $2\widetilde{B} = \sum_{p\neq 0}\eta_p(a_p^* a_{-p}^* - a_p a_{-p})$, we have

$$e^{\widetilde{B}} a_q\, e^{-\widetilde{B}} = \cosh\eta_q\, a_q + \sinh\eta_q\, a_{-q}^*$$

Corrected Bogoliubov state $e^A e^B \varphi_0^{\otimes N}$ leads to right energy, with

$$A = \frac{1}{\sqrt{N}}\sum_{p,r}\eta_r\Big(a_{p+r}^* a_{-r}^* a_p a_0 - a_0^* a_p^* a_{-r} a_{p+r}\Big)$$

Hard sphere interaction: consider

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

More precisely, we are interested in **ground state energy**

$$E_N^{\text{hs}} = \min \frac{\langle \psi_N, \sum_{j=1}^N -\Delta_{x_j} \psi_N \rangle}{\|\psi_N\|^2}$$

with minimum taken over $\psi \in L_s^2(\Lambda^N)$ satisfying

$$\psi_N(x_1, \dots, x_N) = 0 \qquad \text{if } \exists\, i \neq j : \; |x_i - x_j| \leq \mathfrak{a}/N$$

Challenge: Bogoliubov states do not satisfy condition...

Idea: keep **Jastrow** on short length scales, approximate with **Bogoliubov** state on large scales.

$$\prod_{i<j}^{N} f_\ell(x_i - x_j) = \prod_{i<j}^{N} f_{\ell_1}(x_i - x_j) \cdot \prod_{i<j}^{N} \frac{f_\ell(x_i - x_j)}{f_{\ell_1}(x_i - x_j)}$$
$$= \prod_{i<j}^{N} f_{\ell_1}(x_i - x_j) \cdot \prod_{i<j}^{N} \left[1 + \frac{1}{N}\check{\eta}(x_i - x_j)\right]$$
$$\simeq \prod_{i<j}^{N} f_{\ell_1}(x_i - x_j)[e^{B}\varphi_0^{\otimes N}](x_1, \ldots, x_N)$$

Hard-sphere condition satisfied. If $N\ell_1^2 \ll 1$, we can still expand the Jastrow.

Theorem [Basti-Cenatiempo-Olgiati-Pasqualetti-S. '22]:

$$E_N^{\text{hs}} = 4\pi\mathfrak{a}(N-1) + e_\Lambda \mathfrak{a}^2 - \frac{1}{2}\sum_{p \in 2\pi\mathbb{Z}^3 \setminus \{0\}} \left[p^2 + 8\pi\mathfrak{a} - \sqrt{|p|^4 + 16\pi\mathfrak{a}p^2} - \frac{(8\pi\mathfrak{a})^2}{2p^2}\right] + \mathcal{O}(N^{-\varepsilon})$$

Natural question: is it possible to extend this upper bound to **thermodynamic limit**?

Interpolating between GP and TD: consider N hard spheres in $\Lambda = [0;1]^3$, with radius $\mathfrak{a}/N^{1-\kappa}$.

Then: $\kappa = 0$ is GP, $\kappa = 2/3$ is TD.

For $\kappa > 0$, we expect

$$E_N^{\text{hs}} = 4\pi\mathfrak{a}N^{1+\kappa} + 4\pi \cdot \frac{128}{15\sqrt{\pi}}\mathfrak{a}^{3/2}N^{5\kappa/2} + o(N^{5\kappa/2})$$

Remarks:

- To resolve LHY term, need **correlations** up to $\ell \simeq N^{-\kappa/2}$.
- For upper bound in TD limit, need to show it for $\kappa > 1/2$.

Previous strategy: for $0 \leq \kappa \leq 2/3$, we have

$$0 \leq 1 - f_{\ell_1}(x) \lesssim \frac{\mathfrak{a}}{N^{1-\kappa}|x|}\chi_{\ell_1}(x)$$

To **fully expand** the Jastrow, we need (with $u = 1 - f_{\ell_1}^2$)

$$\int \prod_{i<j}^{N} f_{\ell_1}^2(x_i - x_j) \simeq 1 - \sum_{i<j}^{N} \int u(x_i - x_j) \simeq 1 - CN^2 N^{\kappa-1} {\ell_1}^2$$

Since $\ell_1 \geq N^{-1+\kappa}$, this can only work if

$$N^2 N^{-3+3\kappa} = N^{-1+3\kappa} \ll 1,$$

ie. for $\kappa < 1/3$.

Conclusion: need to use **cancellations**, avoiding overexpansion.

Model computation: observe that

$$\frac{\int h(x_1)\prod_{i<j}^N f_\ell^2(x_i-x_j)}{\int \prod_{i<j}^N f_\ell^2(x_i-x_j)}$$

$$\simeq \frac{\int h(x_1)\Big[1-\sum_{j\neq 1} u_{1j}\Big]\prod_{2\leq i<j}^N f_\ell^2(x_i-x_j)}{\int \Big[1-\sum_{j\neq 1} u_{1j}\Big]\prod_{2\leq i<j}^N f_\ell^2(x_i-x_j)}$$

$$\simeq \int h(x_1)\cdot\Big[1+CN^\kappa \ell^2\Big]$$

Need $N^\kappa \ell^2 \ll 1$, ie. $\ell \ll N^{-\kappa/2}$.

Theorem [Basti-Cenatiempo-Giuliani-Olgiati-Pasqualetti-S.]: fix $\kappa \in [0;2/3]$. For every $\varepsilon > 0$ there exists $C > 0$ such that

$$E_{N,\kappa}^{\text{hs}} \leq 4\pi\mathfrak{a}N^{1+\kappa} + CN^{5\kappa/2+\varepsilon}$$

Corollary: for every $\varepsilon > 0$ there exists $C > 0$ such that

$$\lim_{N,L\to\infty: N/L^3=\rho} \frac{E_{N,L}^{\text{hs}}}{N} \leq 4\pi\rho\mathfrak{a}\cdot\left(1+C(\rho\mathfrak{a}^3)^{1/2-\varepsilon}\right)$$

Proof: fix $\varepsilon > 0$ and let $\ell = N^{-\kappa/2-\varepsilon}$. Consider **Jastrow factor**

$$\psi_N(x_1, \dots, x_N) = \prod_{i<j}^N f_\ell(x_i - x_j)$$

Then

$$\langle \psi_N, H_N \psi_N \rangle = 2\lambda_\ell \sum_{k<m}^N \int \chi_\ell(x_k - x_m) \prod_{i<j}^N f_\ell^2(x_i - x_j)$$
$$- \sum_{k,m,n} \int \frac{\nabla f_\ell(x_k - x_n)}{f_\ell(x_k - x_n)} \cdot \frac{\nabla f_\ell(x_k - x_m)}{f_\ell(x_k - x_m)} \prod_{i<j}^N f_\ell^2(x_i - x_j)$$

Using **permutation symmetry**, we find

$$\langle \psi_N, H_N \psi_N \rangle \simeq N^2 \lambda_\ell \int \chi_{12} \prod_{i<j}^N f_{ij}^2 - \frac{N^3}{6} \int \frac{\nabla f_{12}}{f_{12}} \cdot \frac{\nabla f_{13}}{f_{13}} \prod_{i<j}^N f_{ij}^2$$

Expand particle 1, up to an even $M > \varepsilon^{-1}$:

$$N^2\lambda_\ell \int \chi_{12} \prod_{i<j}^{N} f_{ij}^2$$

$$\leq N^2\lambda_\ell \sum_{m_1=0}^{M} (-1)^{m_1} \binom{N-2}{m_1} \int \chi_{12}\, f_{12}^2\, u_{1,3} \cdots u_{1,m_1+2} \prod_{2\leq i<j}^{N} f_{ij}^2$$

Expand particle 2, and distinguish terms three contributions:

- Observable **disentangles** from Jastrow, ie.

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

- "**Tree**" contributions, proportional to

$$N^2\lambda_\ell \int \chi_{12} f_{12}^2\, u_{13} \cdots u_{1,m_1+2}\, u_{2,m_1+3} \cdots u_{2,m_1+m_2+2} \prod_{3\leq i<j\leq N} f_{ij}^2$$

- "**Loops**" contributions, for example

$$N^3\lambda_\ell \int \chi_{12} f_{12}^2\, u_{13}\, u_{23} \prod_{3\leq i<j}^{N} f_{ij}^2 \lesssim N^{3\kappa}\ell \int \prod_{4\leq i<j}^{N} f_{ij}^2 \lesssim N^{5\kappa/2-\varepsilon} \int \prod_{4\leq i<j}^{N} f_{ij}^2$$