Wu's correction to the ground state energy of a Bose gas in the Gross-Pitaevskii regime

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Setting

Trapped Bose gas in the Gross-Pitaevskii regime

- N bosons on 3d unit torus $\Lambda = [0,1]^{\times 3}$ + periodic b.c..
- Scattering length of order N^{-1}.

Hamiltonian

For $V \geq 0$ and compactly supported

$$H_N = -\sum_{j=1}^{N} \Delta_{x_j} + N^2 \sum_{i<j}^{N} V(N(x_i - x_j)) \qquad \text{on} \quad L^2(\Lambda)^{\otimes_{\mathrm{sym}} N}.$$

Remark $\qquad \mathrm{scat}\big(N^2 V(N\cdot)\big) = \frac{1}{N}\mathrm{scat}(V) \equiv \frac{\mathfrak{a}}{N}.$

Ground state energy $\qquad E_N = \inf \sigma(H_N).$

Known results

(Upper/lower bounds, different assumptions on V, different $s > 0$)

Ground state energy

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

where $e_\Lambda := 2 - \lim_{M\to\infty}\sum_{0\neq p\in\mathbb{Z}^3}^{\leq|M|}\frac{\cos(|p|)}{p^2}$.

Low excited eigenvalues

$$E_N + \sum_{p\in 2\pi\mathbb{Z}^3} n_p\sqrt{p^4 + 16\pi\mathfrak{a}p^2} + O(N^{-s}),$$

where $n_p \in \mathbb{N}$ and $n_p \neq 0$ for finitely many $p \in 2\pi\mathbb{Z}^3$.

[Dyson'57, Lieb-Yngvason '98, Lieb-Seiringer-Yngvason '00, Lieb-Seiringer '06, Yau-Yin '09, Nam-Rougerie-Seiringer '16, Boccato-Brennecke-Cenatiempo-Schlein '19, Hainzl-Schlein-Triay '22, Basti-Cenatiempo-Olgiati-Pasqualetti-Schlein '23, Fournais-Solovej '23, Brooks '23,...]

Remarks

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

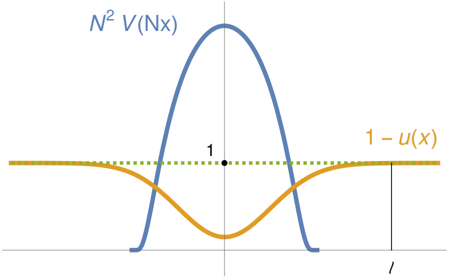
- Universality in terms of the scattering length.
- Best error estimate [Brooks '23]:
  - $O(N^{-1/2})$ for lower bound.
  - $O(N^{-1}\log N)$ for upper bound.

Heuristics

Trial state $\rightsquigarrow \psi_{\mathrm{trial}} = 1 - \sum_{i<j}^{N} u(x_i - x_j)$

Choose u by solving the scattering equation (with b.c. on radius ℓ small enough)

$$\begin{cases} \left(-\Delta + \frac{N^2 V(Nx)}{2}\right)(1 - u(x)) = 0 & \text{on } |x| \leq \ell \\ (1 - u(x)) = 1 & \text{on } |x| = \ell. \end{cases}$$



$$\langle \psi_{\mathrm{trial}}, H_N \, \psi_{\mathrm{trial}} \rangle \leq 4\pi \mathfrak{a} N + \frac{C}{\ell} + CN^2 \ell^2$$

$$\|\psi_{\mathrm{trial}}\|^2 \geq 1 - CN\ell^2$$

$$\Downarrow$$

$$E_N \leq 4\pi a N + \frac{C}{\ell} + CN^2 \ell^2$$

What is wrong with ψ_{trial}?

Unavoidable

- ℓ^{-1}-remainder requires $\ell \gtrsim O(1)$.
- u should be modified at lengths $\simeq O(1)$.
- Trial state not enough for lower bound
  $\hookrightarrow$ implement correlations e.g. with unitary transformations.

$N^2\ell^2 \gg 1$

- ψ_{trial} is not 'recursive' enough. QFT analogy:
  $\hookrightarrow$ no simplification of disconnected diagrams.

Better idea:

$$\psi_{2-\mathrm{body}} = 1 - \sum_{i<j}^{N} u(x_i - x_j)\left(1 - \sum_{\substack{m,n \\ m,n \neq i,j}}^{N} u(x_m - x_n)\left(1 - \ldots ...\right)\right).$$

$\rightsquigarrow$ Stronger simplification of the norm.

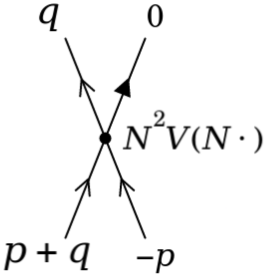
Still missing: three-body correlations.

Three-body correlations

Interactions of the type

$$\mathcal{C} = \frac{1}{N} \sum_{\substack{0 \neq p, q \in 2\pi\mathbb{Z}^3 \\ p+q \neq 0}} \widehat{V}\left(\frac{p}{N}\right) \left(a^*_{p+q} a^*_{-p} a_q a_0 + a^*_0 a_q a_{p+q} a_{-p} \right)$$

for $|q| \ll |p|$ matter for the $O(1)$-correction to E_N.



$\rightsquigarrow$ Correlation structure needs terms [Yau-Yin '09, Boccato-Brennecke-Cenatiempo-Schlein '19,...]

$$u(x_1 - x_2) u(x_1 - x_3) + \mathrm{sym}.$$

Altogether: Jastrow function (cf. Giulia Basti's talk)

$$1 - \sum_{i<j}^{N} u(x_i - x_j)(1 - \dots) + \sum_{\substack{i,j,k \\ i \neq j,k,\, j<k}}^{N} u(x_i - x_j) u(x_i - x_k)(1 - \dots) \simeq \prod_{i<j}^{N} \big(1 - u(x_i - x_j)\big).$$

Correlation structure through unitaries

[following Boccato, Brennecke, Cenatiempo, Schlein '19]

Two-body correlations

In the space of excited modes ($a_0, a_0^* \rightsquigarrow \sqrt{N}$) define

$$\widetilde{B} = -\frac{1}{2} \sum_{0 \neq p \in 2\pi\mathbb{Z}^3} N \,\widehat{u}_p (a_p^* a_{-p}^* - \mathrm{h.c.}).$$

Then

- $e^{\widetilde{B}} |\Omega\rangle \overset{\text{morally}}{\simeq} \psi_{2-\mathrm{body}}$.
- $e^{-\widetilde{B}} H_N e^{\widetilde{B}}$ contains the two-body correlation structure up to lengths $\lesssim O(1)$.

Three-body correlations

$$e^{-\widetilde{B}} \mathcal{C} e^{\widetilde{B}} \simeq \frac{1}{\sqrt{N}} \sum_{\substack{0 \neq p,q \in 2\pi\mathbb{Z}^3 \\ p+q \neq 0}} \widehat{V}\Big(\frac{p}{N}\Big) a_{p+q}^* a_{-p}^* \big(\cosh(-N \,\widehat{u}_q) a_q + \sinh(-N \,\widehat{u}_q) a_{-q}^* \big) + \mathrm{h.c.}$$

Renormalized in [BBCS '19] through a cubic transformation $e^{-\widetilde{A}} e^{-\widetilde{B}} H_N e^{\widetilde{B}} e^{\widetilde{A}}$ with

$$\widetilde{A} \simeq -\frac{1}{\sqrt{N}} \sum_{\substack{0 \neq p,q \in 2\pi\mathbb{Z}^3 \\ |p| > N^{\varepsilon},\ |q| < N^{\varepsilon}}} N \,\widehat{u}_p \, a_{p+q}^* a_{-p}^* \big(\cosh(-N \,\widehat{u}_q) a_q + \sinh(-N \,\widehat{u}_q) a_{-q}^* \big) - \mathrm{h.c.}.$$

Towards our work

Questions

- Does universality w.r.t. $\mathfrak{a}$ break down after the $O(1)$-correction?
- How accurate is the 2-body + 3-body correlation structure?
- How large is the correction to the g.s. energy beyond $O(1)$?

Conjecture [Wu '59,...] in the thermodynamic limit and as $\rho\mathfrak{a}^3 \to 0$ the ground state energy per particle is

$$e(\rho) = 4\pi\mathfrak{a}\rho\left[1 + \frac{128}{15\sqrt{\pi}}(\rho\mathfrak{a}^3)^{1/2} + 8\left(\frac{4}{3}\pi - \sqrt{3}\right)\rho\mathfrak{a}^3\log(\rho\mathfrak{a}^3) + O(\rho\mathfrak{a}^3)\right].$$

Towards our work

Relevant clues

- [Brooks '23] upper bound to the g.s. energy in the GP regime with an error $\sim N^{-1}\log N$.
- Looking closely enough inside the Jastrow function

$$\frac{N(N-1)}{2}\left\langle \prod_{i<j}^{N}\big(1-u(x_i-x_j)\big),\, N^2V\big(N(x_1-x_2)\big)\prod_{i<j}^{N}\big(1-u(x_i-x_j)\big)\right\rangle$$
$$\simeq \cdots + \frac{N^3}{2}\int N^2V\big(N(x_1-x_2)\big)u(x_1-x_3)^2u(x_2-x_3)\,dx_1dx_2dx_3+\dots$$
$$\simeq \cdots + C\frac{\log N}{N}+\dots$$

Main result

Theorem

Let $V \in L^3(\mathbb{R}^3)$ be spherically symmetric, compactly supported, and satisfy $V \geq 0$. Let $E_N = \inf \sigma(H_N)$. Then

$$\begin{aligned} E_N = {} & 4\pi\mathfrak{a}(N-1) + e_\Lambda \mathfrak{a}^2 \\ & - \frac{1}{2} \sum_{0 \neq p \in 2\pi\mathbb{Z}^3} \left[p^2 + 8\pi\mathfrak{a} - \sqrt{p^4 + 16\pi\mathfrak{a}p^2} - \frac{(8\pi\mathfrak{a})^2}{2p^2} \right] \\ & - 64\pi \left(\frac{4}{3}\pi - \sqrt{3} \right) \mathfrak{a}^4 \frac{\log N}{N} + O(N^{-1} \log^{1/2} N). \end{aligned}$$

Remarks

- Correction equivalent to $8\left(\frac{4}{3}\pi - \sqrt{3}\right)\rho\mathfrak{a}^3 \log(\rho\mathfrak{a}^3)$ if $\rho \rightsquigarrow N$ and $\mathfrak{a} \rightsquigarrow \mathfrak{a}/N$.
- Error $O(N^{-1})$ with a slightly longer proof.
- Universality is preserved. Expected to break down at $O(N^{-1})$.
- From the proof: (modified) two- and three-body correlation are still enough. Expected to break down at $O(N^{-1})$.

Proof strategy

Two-body correlation structure [extension of Boccato, Brennecke, Cenatiempo, Schlein '19]

In the space of excited modes ($a_0, a_0^* \rightsquigarrow \sqrt{N}$) define

$$B = \frac{1}{2} \sum_{0 \neq p \in 2\pi\mathbb{Z}^3} \mu_p (a_p^* a_{-p}^* - \mathrm{h.c.}), \qquad \mu_p \simeq \begin{cases} -N\widehat{u}_p & |p| \geq N^\epsilon \\ \tau_p & |p| \simeq O(1), \end{cases}$$

and τ_p is the diagonalizing kernel for the Bogoliubov Hamiltonian.

Then

$$e^{-B} H_N e^B$$

contains the right two-body correlation structure to all lengths.

Proof strategy

Renormalized cubic operator

Extending the proof in [BBCS '19], $e^{-\widetilde{A}}e^{-B}H_N e^B e^{\widetilde{A}}$ would contain

$$\mathcal{C}_{\rm ren} \simeq \frac{8\pi\mathfrak{a}}{\sqrt{N}} \sum_{\substack{0\neq p,q\in 2\pi\mathbb{Z}^3\\ p+q\neq 0,\ |p|<N^{\varepsilon}}} a^*_{p+q}a^*_{-p}\big(\cosh(\mu_q)a_q + \sinh(\mu_q)a^*_{-q}\big) + \mathrm{h.c.}$$

Perturbation theory heuristics

At second order beyond $H_0 - E_0 \simeq \sum_{0\neq p\in 2\pi\mathbb{Z}^3} \sqrt{p^4 + 16\pi\mathfrak{a}p^2}\, a^*_p a_p$

$$\left\langle \Omega, \mathcal{C}_{\rm ren}\frac{1}{H_0 - E_0}\mathcal{C}_{\rm ren}\Omega\right\rangle \overset{\substack{\text{commuting and}\\ \text{contracting}}}{\simeq} \frac{c\mathfrak{a}^4}{N} \sum_{\substack{0\neq p,q\in 2\pi\mathbb{Z}^3\\ p+q\neq 0,\ |q|<N}} \frac{1}{p^2}\frac{1}{q^2}\frac{1}{|p+q|^2 + p^2 + q^2} + \dots$$

$$\simeq O\left(\frac{\log N}{N}\right).$$

Proof strategy

Our approach

Extract all contributions with a single cubic transformation

$$A = -\frac{1}{\sqrt{N}} \sum_{\substack{0\neq p+q\in 2\pi\mathbb{Z}^3 \\ p+q\neq 0}} N\,\widehat{u}_p a^*_{p+q} a^*_{-p}\Big(\cosh(\mu_q) a_q + \nu_{p,q}\sinh(\mu_q) a^*_{-q}\Big) - \mathrm{h.c.}$$

with

$$\nu_{p,q} = \frac{2p^2}{|p+q|^2 + p^2 + q^2}.$$

Overall

$$\begin{aligned} e^{-A}e^{-B}H_N e^B e^A = {} & 4\pi\mathfrak{a}(N-1) + e_\Lambda \mathfrak{a}^2 \\ & - \frac{1}{2}\sum_{0\neq p\in 2\pi\mathbb{Z}^3}\left[p^2 + 8\pi\mathfrak{a} - \sqrt{p^4 + 16\pi\mathfrak{a}p^2} - \frac{(8\pi\mathfrak{a})^2}{2p^2}\right] \\ & - 64\pi\left(\frac{4}{3}\pi - \sqrt{3}\right)\mathfrak{a}^4\frac{\log N}{N} + (1\pm\varepsilon)\sum_{0\neq p\in 2\pi\mathbb{Z}^3}\sqrt{p^4 + 16\pi\mathfrak{a}p^2}\,a^*_p a_p \\ & + \frac{1}{2N}\sum_{\substack{p,q,r\in 2\pi\mathbb{Z}^3 \\ p,q,r+p,r+q\neq 0}} \widehat{V}\left(\frac{p}{N}\right) a^*_{r+p} a^*_q a_p a_{r+q} + \mathrm{err} \end{aligned}$$

Thank you for your attention.