Third order corrections to the ground state energy of a Bose gas in the Gross-Pitaevskii regime

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joint work with C. Caraci, A. Olgiati and B. Schlein

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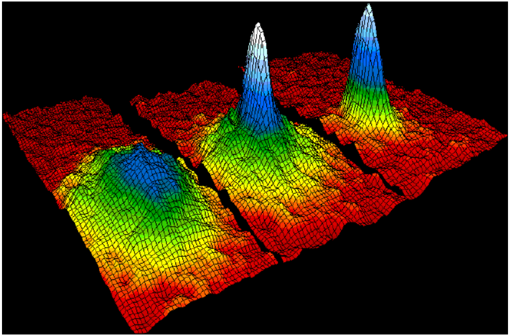
Bose-Einstein Condensate

- Predicted by Bose and Einstein (1924-25) for free systems
- Realised in 1995 for a gas of rubidium atoms at 170 nK



[Anderson-Ensher-Matthews-Wieman-Cornell '95]

Gross-Pitaevskii Regime

- N bosons in $\Lambda = [0,1]^3$ interacting through a repulsive potential, scaling with N

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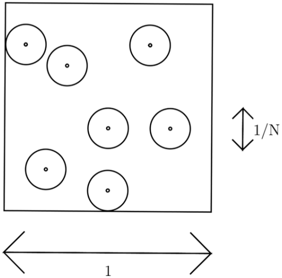
Hamiltonian:

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

on $L^2_s(\Lambda^N)$, $V \geq 0$, compact support, spherically symmetric



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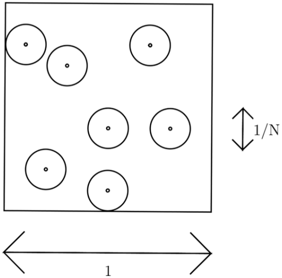

- Scattering length: $\mathfrak{a}$

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

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

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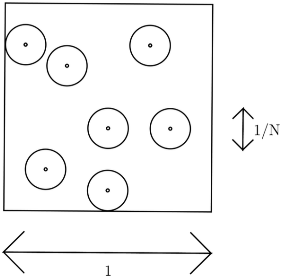

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- By scaling, $\mathfrak{a}_N = \frac{\mathfrak{a}}{N}$

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Ground State Energy

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- [Boccato, Brennecke, Cenatiempo, Schlein '18 -'20]: $V \in L^3(\mathbb{R}^3)$,

$$|E_N - 4\pi\mathfrak{a}N| \leq C$$

  For a sequence $\tilde{\psi}_N \in L^2_s(\Lambda^N)$; st $\langle\tilde{\psi}_N, H_N\tilde{\psi}_N\rangle \leq 4\pi aN + K$ with $K > 0$

$$1 - \langle\psi_0, \gamma_N\psi_0\rangle \leq \frac{C(K+1)}{N}$$

Ground State Energy

- Theorem [Boccato-Brennecke-Cenatiempo-Schlein '19]: $V \in L^3(\mathbb{R}^3)$

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

where

$$e_\Lambda = 2 - \lim_{M\to\infty} \sum_{\substack{p \in \mathbb{Z}^3 \setminus \{0\}: \\ |p_1|,|p_2|,|p_3| \leq M}} \frac{\cos|p|}{p^2}$$

- Also resolves the low-energy excitation spectrum

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- Also resolves the low-energy excitation spectrum
- Extensions: [Hainzl-Schlein-Triay '22], [Brooks '23], [Basti-Cenatiempo-Olgiati-Pasqualetti-Schlein '23], [Brennecke-Schlein-Schraven '22], [Nam-Triay '23]

Ground State Energy: Our Result

- Theorem [Caraci-Olgiati-S.A.-Schlein '23]: $V \in L^3(\mathbb{R}^3)$, $V \geq 0$, sph. sym., compact support

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

as $N \to \infty$.

Thermodynamic limit

- Lee-Huang-Yang formula '57:

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

for $\rho\mathfrak{a}^3 \to 0$.

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  for $\rho\mathfrak{a}^3 \to 0$.

- Rigorous proofs for the L-H-Y correction:
  [Yau-Yin '09], [Basti-Cenatiempo-Schlein '21], [Fournais-Solovej '20-'23]

Thermodynamic limit

- [Wu '59], [Hugenholtz-Pines '59], [Sawada '59] predicted

$$e(\rho) = \lim_{\substack{N,L\to\infty \\ N/L^3=\rho}} \frac{E_{N,L}}{N} = 4\pi\mathfrak{a}\rho\Big[1 + \frac{128}{15\sqrt{\pi}}(\rho\mathfrak{a}^3)^{1/2} + 8\Big(\frac{4}{3}\pi - \sqrt{3}\Big)\rho\mathfrak{a}^3\log(12\pi\rho\mathfrak{a}^3) + \dots\Big]$$

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Proof...

- Switch to second quantization,

$$H_N = \sum_{p\in\Lambda^*} p^2 a_p^* a_p + \frac{1}{2N} \sum_{p,q,r\in\Lambda^*} \widehat{V}(r/N) a_{p+r}^* a_q^* a_{q+r} a_p$$

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- Factor out BEC: any $\psi_N \in L_s^2(\Lambda^N)$ can be uniquely written as

$$\psi_N = \sum_{n=0}^{N} \alpha_n \otimes_s \psi_0^{\otimes(N-n)}, \text{ with } \alpha_j \in L^2_{\perp \psi_0}(\Lambda)^{\otimes_s j} \text{ and } \psi_0 = 1$$

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- $U_N : L_s^2(\Lambda^N) \to \mathcal{F}_\perp^{\leq N} := \bigoplus_{n=0}^{N} L^2_{\perp \psi_0}(\Lambda)^{\otimes_s n}$

$$\begin{cases} U_N a_0^* a_0 U_N^* = N - \mathcal{N}_+ \\ U_N a_p^* a_0 U_N^* = \sqrt{N} b_p^* \\ U_N a_p^* a_q U_N^* = a_p^* a_q \end{cases}$$

$$b_p := (1 - N^{-1}\mathcal{N}_+)^{1/2} a_p$$

$$[b_p, b_q^*] = \left(1 - N^{-1}\mathcal{N}_+\right) \delta_{p,q} - N^{-1} a_q^* a_p$$

$$[b_p, b_q] = 0$$

Proof...

$$
\begin{aligned}
U_N H_N U_N^* =& \mathcal{K} + \mathcal{V}_N + \frac{\widehat{V}(0)}{2}(N-1) \\
&+ \sum_{p \in \Lambda_+^*} \widehat{V}(p/N) b_p^* b_p + \frac{1}{2} \sum_{p \in \Lambda_+^*} \widehat{V}(p/N)(b_p^* b_{-p}^* + b_p b_{-p}) \\
&+ \frac{1}{\sqrt{N}} \sum_{\substack{p,q \in \Lambda_+^* \\ p+q \neq 0}} \widehat{V}(p/N) \left(b_{p+q}^* a_{-p}^* a_q + a_q^* a_{-p} b_{p+q} \right) + \mathcal{O}(N^{-1})
\end{aligned}
$$

with

$$
\mathcal{K} = \sum_{p \in \Lambda_+^*} p^2 a_p^* a_p, \qquad \mathcal{V}_N = \frac{1}{2N} \sum_{\substack{r \in \Lambda^*, p,q \in \Lambda_+^* \\ r \neq -p,-q}} \widehat{V}(r/N) a_{p+r}^* a_q^* a_p a_{q+r}
$$

Proof...

- Describe correlations: rescaled Neumann problem for $\ell > 0$,

$$\Big[-\Delta + \frac{N^2}{2} V(N\cdot) \Big] f_{N,\ell} = \lambda_\ell f_{N,\ell} \qquad |x| \leq \ell$$
$$\partial_r f_{N,\ell}(x) = 0 \qquad |x| = \ell$$

on $|x| \leq \ell$, with $f_\ell(x) = 1$ for $|x| \geq \ell$.

$$\Rightarrow \widehat{f}_{N,\ell}(p) = \delta_{p,0} + N^{-1}\eta_p \text{ and } \Big(\widehat{V}(\cdot/N) * \widehat{f}_{N,\ell} \Big)_0 = 8\pi\mathfrak{a} + \mathcal{O}(N^{-1})$$

verifying

$$p^2\eta_p + \frac{1}{2}\widehat{V}(p/N) + \frac{1}{2N} \sum_{q\in\Lambda^*} \widehat{V}((p-q)/N)\eta_q \simeq 0$$

$$\|\eta\|_2 \leq C, \qquad \textstyle\sum_{p\in\Lambda^*} p^2|\eta_p|^2 \leq CN$$

Proof... Strategy to extract contributions up to order 1

In [BBCS '19]:

1. Extract order N and 1 contributions with $B_\eta = \frac{1}{2}\sum_{p\in\Lambda_+^*} \eta_p \big(b_p^* b_{-p}^* - b_p b_{-p}\big)$:

$$e^{-B_\eta} U_N H_N U_N^* e^{B_\eta} \simeq 4\pi\mathfrak{a}N + \mathcal{Q}_B + \mathcal{C} + \mathcal{V}_N$$

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2. Cubic renormalization to extract order 1

$$e^{-A_1} e^{-B_\eta} U_N H_N U_N^* e^{B_\eta} e^{A_1} \simeq 4\pi\mathfrak{a}N + \mathcal{Q}_B + \mathcal{Q}_A + \mathcal{V}_N,$$

$$\text{with } \mathcal{Q}_B + \mathcal{Q}_A = \sum_{p\in\Lambda_+^*} \Big[F_p b_p^* b_p + \frac{1}{2} G_p\big(b_p^* b_{-p}^* + b_p b_{-p}\big) + C_p\Big]$$

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3. Diagonalize with B_τ, for $\tanh(2\tau_p) = -G_p/F_p$

$$e^{-B_\tau} e^{-A} e^{-B_\eta} U_N H_N U_N^* e^{B_\eta} e^{A} e^{B_\tau} \simeq 4\pi\mathfrak{a}N + E_{Bog} + \sum_{p\in\Lambda_+^*} \epsilon(p) a_p^* a_p + \mathcal{V}_N$$

with $\epsilon(p) = \sqrt{|p|^4 + 16\pi\mathfrak{a}p^2}$

Proof...Overview of our approach

Get to a precision of $o(N^{-1}\log N)$:

1. Single generalized Bogoliubov transformation $B_\mu = B_\eta + B_\tau$

$$e^{-B_\mu} U_N H_N U_N^* e^{B_\mu} \simeq 4\pi\mathfrak{a}N + E_{Bog} + \sum_{p\in\Lambda_+^*} \epsilon(p)\, a_p^* a_p - \mathcal{Q}_A + \mathcal{C} + \mathcal{V}_N$$

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2. Cubic renormalization A to extract order 1 and order $N^{-1}\log N$

$$e^{-A} e^{-B_\mu} U_N H_N U_N^* e^{B_\mu e^A} \simeq 4\pi\mathfrak{a}N + E_{Bog} + E_{log} + \sum_{p\in\Lambda_+^*} \epsilon(p)\, a_p^* a_p + \mathcal{V}_N$$

verifying $e^{-A}\mathcal{N}_+ e^A \lesssim \mathcal{N}_+$

Proof... Our approach

- Single generalized Bogoliubov transformation $B_\mu = B_\eta + B_\tau$

$$e^{-B_\mu} U_N H_N U_N^* e^{B_\mu} = 4\pi\mathfrak{a}N + E_{Bog} + \sum_{p\in\Lambda_+^*} \epsilon(p)\, a_p^* a_p - \mathcal{Q}_A + \mathcal{C} + \mathcal{V}_N + \mathcal{E}$$

- $\mathcal{C} = \frac{1}{\sqrt{N}} \sum_{\substack{p,q\in\Lambda_+^* \\ p+q\neq 0}} \widehat{V}(p/N)\, b_{p+q}^* b_{-p}^* (\gamma_q b_q + \sigma_q b_{-q}^*) + \mathrm{h.c.} = \mathcal{C}_\gamma + \mathcal{C}_\sigma$

  with $\gamma_q = \cosh(\mu_q)$ and $\sigma_q = \sinh(\mu_q)$.

- Two kinds of errors $\mathcal{E} = \mathcal{E}_1 + \mathcal{E}_2$:
  - $\pm\mathcal{E}_1 \leq \varepsilon\mathcal{K} + \frac{C}{\varepsilon N}(\mathcal{H}_N + 1)(\mathcal{N}_+ + 1)^k$
  - $\pm\mathcal{E}_2 \leq \varepsilon\mathcal{N}_+ + \frac{C}{\varepsilon N}(\mathcal{H}_N + 1)(\mathcal{N}_+ + 1)^k$, for $\varepsilon > 0$ with $\mathcal{H}_N = \mathcal{K} + \mathcal{V}_N$

  For GS ψ_N: $\langle e^{-B_\mu} U_N\psi_N, (\mathcal{H}_N + 1)(\mathcal{N}_+ + 1)^k e^{-B_\mu} U_N\psi_N\rangle \leq C$, using [BBCS'19]

Proof...Our approach

- Cubic transformation:

$$A = \frac{1}{\sqrt{N}} \sum_{\substack{r,v \in \Lambda_+^* \\ r+v \neq 0}} b^*_{r+v} b^*_{-r} (\eta_r \gamma_v b_v + \nu_{r,v} b^*_{-v}) - \mathrm{h.c.} = A_\gamma + A_\nu$$

with $\nu_{r,v} = \eta_r(\sigma_v - \eta_v) + \eta_r \eta_v \frac{r^2+v^2}{|r+v|^2+r^2+v^2}$

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- $[\mathcal{K}, A_\gamma] \simeq \frac{2}{\sqrt{N}} \sum_{\substack{r,v \in \Lambda_+^* \\ r+v \neq 0}} r^2 \eta_r \gamma_v \, b^*_{r+v} b^*_{-r} b_v + \text{h.c.}$

$[\mathcal{V}_N, A_\gamma] \simeq \frac{1}{\sqrt{N}} \sum_{\substack{r,v \in \Lambda_+^* \\ r+v \neq 0}} (\widehat{V}(\cdot/N) * \eta)_r \gamma_v \, b^*_{r+v} b^*_{-r} b_v + \text{h.c.}$

$\rightarrow$ Use scattering equation to cancel $\mathcal{C}_\gamma$

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Proof...

- $e^{-A}\mathcal{C}e^{A} \simeq \mathcal{C} + [\mathcal{C}, A] \simeq \mathcal{C} + 2\mathcal{Q}_A + 2E_{\log,1}$
- $e^{-A}\mathcal{H}_N e^{A} \simeq \mathcal{H}_N + [\mathcal{H}_N, A] + \frac{1}{2}[[\mathcal{H}_N, A], A] \simeq \mathcal{H}_N - \mathcal{C} - \mathcal{Q}_A - E_{\log,1} + E_{\log,2}$

  using $[C_\sigma, A_\nu] \simeq 2E_{\log,1}$ and $[C_{log}, A_\nu] \simeq 2E_{\log,2}$

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- $e^{-A}\mathcal{H}_N e^{A} \simeq \mathcal{H}_N + [\mathcal{H}_N, A] + \frac{1}{2}[[\mathcal{H}_N, A], A] \simeq \mathcal{H}_N - \mathcal{C} - \mathcal{Q}_A - E_{\text{log},1} + E_{\text{log},2}$

  using $[C_\sigma, A_\nu] \simeq 2E_{\text{log},1}$ and $[C_{log}, A_\nu] \simeq 2E_{\text{log},2}$

$$\begin{aligned} E_{log} &= E_{log,1} + E_{log,2} \\ &= \frac{2}{N} \sum_{\substack{r,v\in\Lambda_+^* \\ r+v\neq 0}} \frac{1}{r^2+v^2+(r+v)^2} \Big[(r^2 + (r+v)^2) \big(\widehat{V}(\cdot/N) * \widehat{f}_{N,\ell}\big)_{r+v} \eta_r \eta_v \eta_{r+v} \\ &\qquad - (r\cdot v) \Big(\big(\widehat{V}(\cdot/N) * \widehat{f}_{N,\ell}\big)_{r+v} + \big(\widehat{V}(\cdot/N) * \widehat{f}_{N,\ell}\big)_{r} \Big) \eta_r \eta_v^2 \Big] + \mathcal{O}(N^{-1}) \end{aligned}$$

Proof...

- $e^{-A}\mathcal{C}e^{A} \simeq \mathcal{C} + [\mathcal{C}, A] \simeq \mathcal{C} + 2\mathcal{Q}_A + 2E_{\log,1}$
- $e^{-A}\mathcal{H}_N e^{A} \simeq \mathcal{H}_N + [\mathcal{H}_N, A] + \frac{1}{2}[[\mathcal{H}_N, A], A] \simeq \mathcal{H}_N - \mathcal{C} - \mathcal{Q}_A - E_{\log,1} + E_{\log,2}$

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Proof...Our approach

$$e^{-A}e^{-B_\mu}U_N H_N U_N^* e^{B_\mu}e^{A} = 4\pi\mathfrak{a}N + E_{Bog} + E_{log} + \sum_{p\in\Lambda_+^*}\epsilon(p)\, a_p^* a_p + \mathcal{V}_N + \mathcal{E}$$

with $\pm\mathcal{E} \leq \varepsilon\mathcal{K} + \frac{C}{N}\left[(\log N)^{1/2} + \varepsilon^{-1}\right](\mathcal{K}+1)(\mathcal{N}_+ + 1)^4$, $\varepsilon > 0$

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- Lower bound:
  - $\mathcal{V}_N \geq 0$
  - $\varepsilon^{-1} = (\log N)^{1/2}$
  - $(1 - (\log N)^{-1/2})\sum_{p\in\Lambda_+^*}\epsilon(p)\, a_p^* a_p \geq 0$
  - For GS $\xi = e^{-A}e^{-B_\mu}U_N\psi_N$: $\quad\langle\xi, (\mathcal{H}_N + 1)(\mathcal{N}_+ + 1)^k\xi\rangle \leq C$

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Thank you for your attention!

Proof... details Quadratic

Lemma

For $s \in [0,1]$, *let* $\gamma_p^{(s)} = \cosh(s\mu_p)$ *and* $\sigma_p^{(s)} = \sinh(s\mu_p)$. *Then*

$$\begin{aligned} d_p = -\frac{1}{N}\int_0^1 ds\, e^{-(1-s)B_\mu}\Big[\gamma_p^{(s)}\Big(\mu_p\mathcal{N}_+ b_{-p}^* + \sum_{q\in\Lambda_+^*}\mu_q b_q^* a_{-q}^* a_p\Big) \\ + \sigma_p^{(s)}\Big(\mu_p\mathcal{N}_+ b_p + \sum_{q\in\Lambda_+^*}\mu_q a_{-p}^* a_{-q} b_q\Big)\Big] e^{(1-s)B_\mu}. \end{aligned} \tag{1}$$

Proof... details Cubic

- $e^{-A}(\mathcal{H}_N + 1)(\mathcal{N}_+ + 1)^k e^A \leq C(\mathcal{H}_N + 1)(\mathcal{N}_+ + 1)^k + C(\mathcal{N}_+ + 1)^{k+2}$
- $\pm e^{-A}\mathcal{E}_1 e^A \leq \varepsilon\mathcal{K} + \frac{C}{\varepsilon N}(\mathcal{H}_N + \mathcal{N}_+^2 + 1)$, for $\varepsilon > 0$
- $e^{-A}\left(\mathcal{K} - \sum_{p\in\Lambda_+^*} \epsilon(p)\, a_p^* a_p + \mathcal{Q}_A\right) e^A \simeq \mathcal{K} - \sum_{p\in\Lambda_+^*} \epsilon(p)\, a_p^* a_p + \mathcal{Q}_A$