Lower bound for the free energy expansion of low temperature Bose gas

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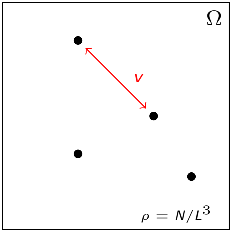
Math description of Bose gases: interacting particles

- N bosons in a volume

  $$\Omega = [-L/2, L/2]^3 \subseteq \mathbb{R}^3.$$



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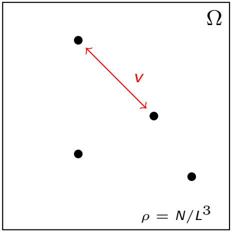

- Hamiltonian:

$$H_N = \sum_{j=1}^{N} -\Delta_j + \sum_{i<j}^{N} v(x_i - x_j), \quad \text{acting on } L^2_s(\Omega^N) \qquad \text{[Neumann b.c.]}.$$

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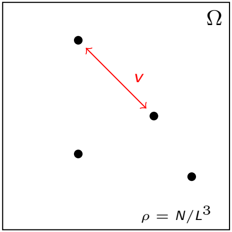

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- Potential:

$$v \geq 0, \quad \text{spherically symmetric, compactly supported, non-increasing}.$$

Free energy in thermodynamic limit

- Free energy at $T \geq 0$:

$$F_T(N,\Omega) = \inf_{\substack{\Gamma \in \mathscr{L}_1(L^2_s(\Omega^N)) \\ 0 \leq \Gamma \leq 1, \\ \mathrm{Tr}\Gamma = 1}} \mathrm{Tr}(H_N \Gamma) - TS(\Gamma),$$

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- energy density in thermodynamic regime

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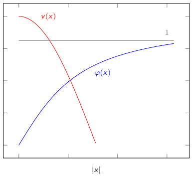

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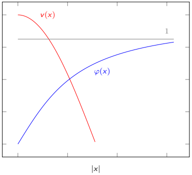

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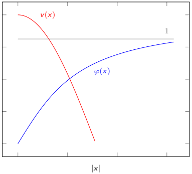

- We call $a > 0$ the scattering length of v.
- Important quantities:

$$g(x) := v(x)\varphi(x), \qquad \omega(x) := 1 - \varphi(x),$$

such that

$$\widehat{g}(0) = 8\pi a.$$

Main result

Theorem (Fournais, Girardot, Junge, Morin, O., Triay, '24)

There exists $C > 0$ such that, if $v \geq 0$, spherically symmetric, compactly supported, non-increasing, with scattering length $a > 0$ and if $0 \leq T \lesssim \rho a$, then for $\rho a^3 \leq C^{-1}$,

$$f_T(\rho) \geq 4\pi\rho^2 a\Big(1 + \frac{128}{15\sqrt{\pi}}(\rho a^3)^{1/2}\Big) + \frac{T^{5/2}}{(2\pi)^3}\int_{\mathbb{R}^3} \log\Big(1 - e^{-\sqrt{p^4 + 16\frac{\pi}{T}a\rho p^2}}\Big)\mathrm{d}p + o(\rho a)^{5/2}.$$

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$\frac{N(N-1)}{2}$ pairs, each pair with zero energy $\frac{8\pi a}{|\Omega|}$

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from the Bogoliubov integral

$$\frac{1}{2(2\pi)^3}\int_{\mathbb{R}^3}\mathrm{d}k\left(\sqrt{k^4+16k^2\pi\rho a}-k^2-8\pi\rho a+\frac{8\pi a\rho}{k^2}\right)$$

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from excitation spectrum

$$\sum_{\{n_p\}\subseteq\mathbb{N}} n_p\sqrt{p^4+16\pi\rho a p^2}$$

and Gibbs variational principle

$$F_T(N,\Omega) = -T\log\mathrm{Tr}(e^{-\frac{H_N}{T}}).$$

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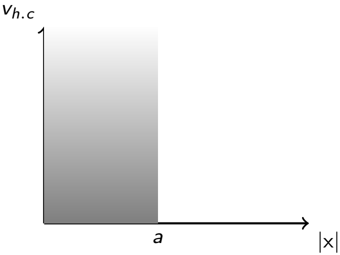
No restriction on the L^1 norm of the potential! **Hardcore potential** included



$$v_{h.c.}(x) = \begin{cases} +\infty, & \text{if } |x| \leq a, \\ 0, & \text{if } |x| > a. \end{cases}$$

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Haberberger, Hainzl, Nam, Seiringer, Triay, '24 : Lower bound, $v \in L^1$;

Haberberger, Hainzl, Schlein, Triay, '24 : Upper bound, $v \in L^1$.

Historical development for expansions in TD limit

	1st	2nd	3rd	free
UP	[1]			
LOW	[2]			

$$e(\rho) \simeq 4\pi\rho^2 a, \qquad \text{1st order, TD regime,}$$

[1] Dyson 1957: upper bound by trial state using Jastrow factors

[2] Lieb, Yngvason, 1998: lower bound, obtained by localization in small boxes

Historical development for expansions in TD limit

	1st	2nd	3rd	free
UP	[1]	[3,4]		
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$$e(\rho) \leq 4\pi\rho^2 a + O(\rho^2 a\sqrt{\rho a^3}),$$ 2nd order, TD regime,

[3] Erdos, Schlein, Yau 2008: upper bound for weak coupling, using quasi-free states,

[4] Basti, Cenatiempo, Giuliani, Olgiati, Pasqualetti, Schlein 2023: hardcore, upper bound, not right constant

Historical development for expansions in TD limit

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$$e(\rho) \simeq 4\pi\rho^2 a\left(1 + \frac{128}{15\sqrt{\pi}}(\rho a^3)^{1/2}\right)$$

[5] Yau, Yin 2009: upper bound using the soft pairs contribution in cubic interactions,

[6] Basti, Cenatiempo, Schlein, 2021: upper bound for larger class of potentials and better errors.

[7] Fournais, Solovej, 2020 + 2021 lower bound 2nd order, hardcore included.

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$$e(\rho) \simeq 4\pi\rho^2 a\Big(1 + \frac{128}{15\sqrt{\pi}}(\rho a^3)^{1/2} + 8\Big(\frac{4}{3}\pi - \sqrt{3}\Big)\rho a^3 \log(12\pi\rho a^3)\Big)$$

[8] Caraci, Olgiati, Saint Aubin, Schlein 2024: in GP regime, 3rd order correction.

Historical development for expansions in TD limit

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[9] Haberberger, Hainzl, Schlein, Triay, 2024: upper bound, $v \in L^1$.

[10] Haberberger, Hainzl, Nam, Seiringer, Triay, 2024: lower bound, $v \in L^1$;

[11] Fournais, Girardot, Junge, Morin, O., Triay 2024: lower bound, hardcore.

Strategy of the proof

- The second order is obtained from the Bogoliubov integral

$$\frac{\rho^2}{2}\left(\widehat{g}(0)+\widehat{g\omega}(0)\right)+\frac{1}{2(2\pi)^3}\int_{\mathbb{R}^3}\mathrm{d}k\left(k^2+\rho\widehat{g}(k)-\sqrt{k^4-2k^2\rho\widehat{g}(k)}\right)$$
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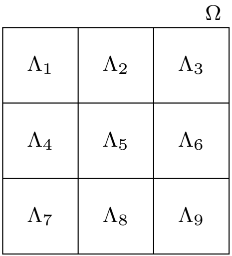
- The thermal contribution comes from the spectrum of an effective quadratic Hamiltonian

$$-T\log\mathrm{Tr}(e^{-\frac{1}{T}\sum_k\sqrt{k^4+2k^2\rho\widehat{g}(0)}\,b_k^*b_k})\simeq T\sum_{k\in\Lambda^*}\log(1-e^{-\frac{1}{T}\sqrt{k^4+2k^2\rho\widehat{g}(0)}})$$
$$\simeq\frac{T^{5/2}}{(2\pi)^3}\int_{\mathbb{R}^3}\log\left(1-e^{-\sqrt{p^4+16\frac{\pi}{T}a\rho p^2}}\right)\mathrm{d}p$$

Neumann Localization



$$\Omega = [-L/2, L/2]^3 = \bigcup_{j=1}^{M} \Lambda_j$$

$$\Lambda = [-\ell/2, \ell/2]^3$$

Neumann Localization

Ω

Λ_1	Λ_2	Λ_3
Λ_4	Λ_5	Λ_6
Λ_7	Λ_8	Λ_9

$$\Omega = [-L/2, L/2]^3 = \bigcup_{j=1}^{M} \Lambda_j$$

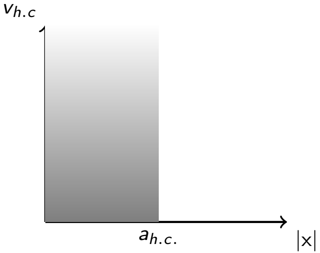
$$\Lambda = [-\ell/2, \ell/2]^3$$

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

$$F_T(N, \Omega) \geq -TM \log \sum_{n=0}^{N} e^{-\frac{1}{T} F(n,\Lambda)}$$

$F_T(n, \Lambda) =$ free energy for $\sum_{j=1}^{n} -\Delta_j + \sum_{i<j} v(x_i - x_j)$ on Λ with Neumann b.c.

Treatment of the hardcore potential



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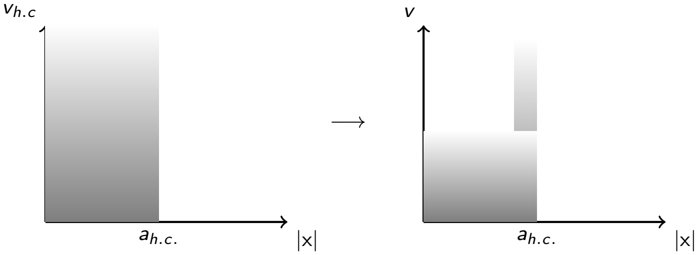

Lemma

There exists a positive, spherically symmetric potential $v < v_{h.c.}$ *with scattering length* $a_v > 0$ *such that*

$$0 < a_{h.c.} - a_v < \frac{a_{h.c.}}{\ell}, \qquad \|v\|_1 \leq C\ell, \qquad v \leq \frac{\ell^2}{a_{h.c.}^4},$$

such that

$$g_v(y) \leq v(x), \qquad \text{for } |y| \geq |x|.$$

Renormalization of the potential

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$$= \mathcal{Q}_0^{\text{ren}} + \mathcal{Q}_1^{\text{ren}} + \mathcal{Q}_2^{\text{ren}} + \mathcal{Q}_3^{\text{ren}} + \mathcal{Q}_4^{\text{ren}},$$

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$$\mathcal{Q}_1^{\text{ren}} := \sum_{i\neq j} \left(Q_i P_j (g + g\omega)(x_i - x_j) P_j P_i + h.c.\right),$$

$$\mathcal{Q}_2^{\text{ren}} := \sum_{i\neq j} P_i Q_j (g + g\omega)(x_i - x_j) P_j Q_i + \sum_{i\neq j} P_i Q_j (g + g\omega)(x_i - x_j) Q_j P_i + \frac{1}{2}\sum_{i\neq j} P_i P_j g(x_i - x_j) Q_j Q_i + h.c.,$$

$$\mathcal{Q}_3^{\text{ren}} := \sum_{i\neq j} P_i Q_j g(x_i - x_j) Q_j Q_i + h.c.,$$

$$\mathcal{Q}_4^{\text{ren}} := \frac{1}{2}\sum_{i\neq j} \Pi_{ij}^* v(x_i - x_j) \Pi_{ij} \geq 0, \qquad \Pi_{ij} := Q_j Q_i + \omega(x_i - x_j)\left(P_j P_i + P_j Q_i + Q_j P_i\right).$$

Thanks for your attention!

Symmetrization of the potential

$$\frac{1}{2}\sum_{i\neq j} P_i P_j g(x_i - x_j) Q_j Q_i \xrightarrow{(*)} \frac{1}{2}\sum_{i\neq j} P_i P_j g_{\mathrm{sym}}(x_i, x_j) Q_j Q_i$$

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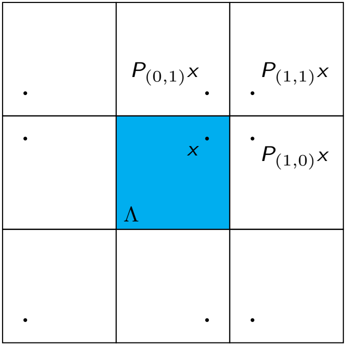

$$g_{\mathrm{sym}}(x,y) = \sum_{z\in\mathbb{Z}^3} g(P_z x - y)$$

We need to control error in $(*)$ via

$$g_v(y) \leq v(x), \qquad \text{for } |y| \geq |x|$$

Second quantization

- We switch to **momenta space**: $a_k^{\#} = a^{\#}(u_k), k \in \Lambda^*$, where

$$u_k(x) = \frac{1}{|\Lambda|^{1/2}} \prod_{j=1}^{3} c_{k_j} \cos(k_j x_j), \qquad c_{k_j} = \begin{cases} 1, & \text{if } p_j = 0, \\ \sqrt{2}, & \text{if } p_j \neq 0. \end{cases}$$

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we get, with $n_0 = a_0^\dagger a_0$ and $n_+ = \sum_{k \in \Lambda^*} a_k^\dagger a_k$,

$$\begin{aligned} H_\Lambda \simeq & \sum_{k \in \Lambda^*} k^2 a_k^\dagger a_k + \frac{1}{2|\Lambda|}(\widehat{g}_{\mathrm{sym}}(0) + \widehat{g\omega}_{\mathrm{sym}}(0)) a_0^\dagger a_0^\dagger a_0 a_0 \\ & + \frac{1}{|\Lambda|} \sum_{k \in \Lambda^*} \Big((\widehat{g}_{\mathrm{sym}}(k) + \widehat{g\omega}_{\mathrm{sym}}(k)) a_0^\dagger a_k^\dagger a_k a_0 + \frac{1}{2} \widehat{g}_{\mathrm{sym}}(k) (a_0^\dagger a_0^\dagger a_k a_k + h.c.) \Big) \\ & + (\widehat{g}_{\mathrm{sym}}(0) + \widehat{g\omega}_{\mathrm{sym}}(0)) \frac{n_0 n_+}{|\Lambda|} + \mathcal{Q}_3^{\mathrm{sym}} + \mathcal{Q}_4^{\mathrm{ren}}. \end{aligned}$$

Second quantization

- We switch to **momenta space**: $a_k^\# = a^\#(u_k)$, $k \in \Lambda^*$, where

$$u_k(x) = \frac{1}{|\Lambda|^{1/2}} \prod_{j=1}^{3} c_{k_j} \cos(k_j x_j), \qquad c_{k_j} = \begin{cases} 1, & \text{if } p_j = 0, \\ \sqrt{2}, & \text{if } p_j \neq 0. \end{cases}$$

we get, with $n_0 = a_0^\dagger a_0$ and $n_+ = \sum_{k\in\Lambda^*} a_k^\dagger a_k$,

$$\begin{aligned} H_\Lambda \simeq & \sum_{k\in\Lambda^*} k^2 a_k^\dagger a_k + \frac{1}{2|\Lambda|}(\widehat{g}_{\text{sym}}(0) + \widehat{g\omega}_{\text{sym}}(0)) a_0^\dagger a_0^\dagger a_0 a_0 \\ & + \frac{1}{|\Lambda|} \sum_{k\in\Lambda^*} \Big((\widehat{g}_{\text{sym}}(k) + \widehat{g\omega}_{\text{sym}}(k)) a_0^\dagger a_k^\dagger a_k a_0 + \frac{1}{2} \widehat{g}_{\text{sym}}(k)(a_0^\dagger a_0^\dagger a_k a_k + h.c.) \Big) \\ & + (\widehat{g}_{\text{sym}}(0) + \widehat{g\omega}_{\text{sym}}(0)) \frac{n_0 n_+}{|\Lambda|} + \mathcal{Q}_3^{\text{sym}} + \mathcal{Q}_4^{\text{ren}}. \end{aligned}$$

- **C-number substitution**: due to BEC, $n_+ \ll N \Rightarrow n_0 \simeq N$, we can substitute

$$a_0^\dagger, a_0 \quad \longrightarrow \quad \sqrt{N}.$$

Quadratic Hamiltonian

$$\mathcal{K}^{\text{Bog}} := \sum_{k\in\Lambda^*} (k^2 + \rho\widehat{g}(k))a_k^\dagger a_k + \frac{1}{2}\rho\widehat{g}(k)(a_k a_k + h.c.),$$

$$\mathcal{Q}_2^{\text{ex}} := \rho \sum_{k\in\Lambda^*} \big(\widehat{g\omega}(k) + \widehat{g\omega}(0)\big) a_k^\dagger a_k.$$

- **Diagonalization** of the quadratic Hamiltonian: introducing $b_k = \dfrac{a_k + \alpha_k a_k^\dagger}{\sqrt{1-\alpha_k^2}}$

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- **Diagonalization** of the quadratic Hamiltonian: introducing $b_k = \dfrac{a_k + \alpha_k a_k^\dagger}{\sqrt{1-\alpha_k^2}}$

  we can define

$$\mathcal{K}^{\text{diag}} = \frac{1}{2}\sum_{k\in\Lambda^*}\left(k^2 + \rho\widehat{g}(k) + \sqrt{k^4 + 2\rho\widehat{g}(k)k^2}\right) b_k^\dagger b_k = \mathcal{K}_L^{\text{diag}} + \mathcal{K}_H^{\text{diag}}$$

  with $\mathcal{K}^{\text{diag}} \geq 0$, diagonal and quadratic in creation/annihilation of excitations, such that

$$\boxed{\mathcal{K}^{\text{Bog}} \geq \mathcal{K}^{\text{diag}} - \frac{|\Lambda|}{2(2\pi)^2}\int_{\mathbb{R}^3}\left(k^2 + \rho\widehat{g}(k) - \sqrt{k^4 + 2\rho\widehat{g}(k)k^2}\right)\mathrm{d}k.}$$

Soft pairs

- The **soft pairs** action: we define two separated momenta scales, for $K_H \gg 1$

$$\mathcal{P}_L := \{|p| \leq K_H \ell^{-1}\}; \qquad \mathcal{P}_H := \{|k| \geq K_H \ell^{-1}\};$$

We consider $\mathcal{Q}_3^{\text{soft}}$ where $k \in \mathcal{P}_H$ and $p - k \in \mathcal{P}_H$ interact to give

$$k + (p - k) \to p \in \mathcal{P}_L$$

so that

$$\boxed{\mathcal{Q}_3^{\text{soft}} + \mathcal{Q}_2^{\text{ex}} + (1 - \varepsilon)\mathcal{K}_H^{\text{diag}} \geq 0.}$$

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- **Conclusion**:

$$\begin{aligned} H_N \geq{}& \frac{\rho}{2}(\widehat{g}(0) + \widehat{g\omega}(0)) + \mathcal{K}_L^{\text{diag}} + \varepsilon \mathcal{K}_H^{\text{diag}} \\ &- \frac{|\Lambda|}{2(2\pi)^2} \int_{\mathbb{R}^3} \Big(k^2 + \rho \widehat{g}(k) - \sqrt{k^4 + 2\rho \widehat{g}(k) k^2}\Big) \mathrm{d}k \end{aligned}$$

□

Last but not least

Neumann loc.

- Boccato, Seiringer 2022: The Bose gas in a box with Neumann boundary conditions.

$2D$ results

- Fournais, Girardot, Junge, Morin, Olivieri, 2023: The ground state energy of a two-dimensional Bose gas;
- Deuchert, Mayer, Seiringer 2020: The free energy of the two dimensional dilute Bose gas. I. Lower bound;
- Mayer, Seiringer 2020: The free energy of the two-dimensional dilute Bose gas. II. Upper bound.