The free energy of dilute Bose gases at low temperatures

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The Hamiltonian

- We consider N bosons in a box Ω

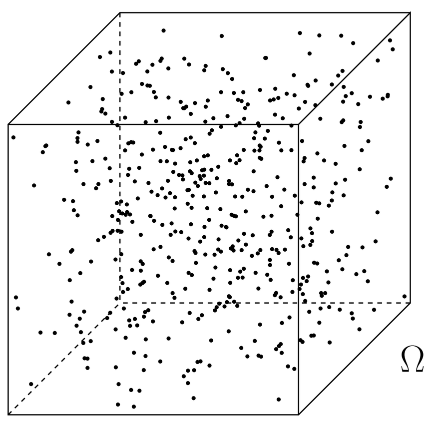
$$H_N = -\sum_{i=1}^{N} \Delta_i + \sum_{i<j}^{N} V(x_i - x_j)$$

with $0 \le V(|x|)$ compactly supported

- According to **[Lee-Huang-Yang '57]** at low temperatures and in the dilute regime $\rho\mathfrak{a}^3 \to 0$ the gas behaves as a collection of independent quantum oscialltors

$$H_N \simeq \sum_{p\in 2\pi\mathbb{Z}^3} \sqrt{p^4 + 16\pi\rho\mathfrak{a}p^2}\, a_p^\dagger a_p$$

where $\rho = N/|\Omega|$ and $\mathfrak{a}$ is the scattering length of V (radius for hard core potentials).



- We justify the LHY conjecture by computing the **Free energy** in the thermodynamic limit,

$$f(\rho, T) = \lim_{\substack{n,|\Omega|\to\infty:\\ N/|\Omega|=\rho}} \frac{F_\Omega(N,T)}{|\Omega|},$$

where $F_\Omega(N,T) = \inf\{\mathrm{Tr}\,(H_N\Gamma) + T\,\mathrm{Tr}(\Gamma\log\Gamma) \mid \Gamma \ge 0, \mathrm{Tr}(\Gamma) = 1\}$ with $T \ge 0$ the temperature

Main Result

$$f(\rho,T) = 4\pi\mathfrak{a}\rho^2\Big(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho\mathfrak{a}^3}\Big) + \frac{T^{5/2}}{(2\pi)^3}\int_{\mathbb{R}^3} \log\Big(1 - e^{-\sqrt{|p|^4 + \frac{16\pi\rho\mathfrak{a}}{T}p^2}}\Big)\,\mathrm{d}p + o\big((\rho\mathfrak{a})^{5/2}\big)_{\rho\mathfrak{a}^3\to 0}$$

- The first order is governed by two body collisions

$$4\pi\mathfrak{a} := \inf\Big\{\int_{\mathbb{R}^3} |\nabla f|^2 + \frac{1}{2}V|f|^2 : \lim_{|x|\to\infty} f(x) = 1\Big\}$$

- The LHY correction at $T=0$ is the total (renormalized) ground state energy of the quantum oscillators

$$4\pi\frac{128}{15\sqrt{\pi}}(\rho a)^{5/2} \simeq \frac{1}{2}\sum_{p\in 2\pi\mathbb{Z}^3} \sqrt{p^4 + 16\pi\rho a p^2} - p^2 - 8\pi\rho a + \frac{(8\pi\rho a)^2}{2p^2}$$

- The thermal contributions come from the elementary excitations above the condensate

$$-T\log\mathrm{Tr}\, e^{-T^{-1}\sum_p \sqrt{p^4+16\pi\rho a p^2}\,a_p^\dagger a_p} \simeq \frac{T^{5/2}}{(2\pi)^3}\int_{\mathbb{R}^3}\log\Big(1 - e^{-\sqrt{|p|^4 + \frac{16\pi\rho a}{T}p^2}}\Big)\,\mathrm{d}p$$

- Correlation length (aka Healing length or Gross—Pitaevskii length) $\ell_{\mathrm{GP}} = (\rho\mathfrak{a})^{-1/2}$
- Small temperatures $0 \le T \le \rho\mathfrak{a} \quad (\simeq \ell_{\mathrm{GP}}^{-2})$

Previous works:

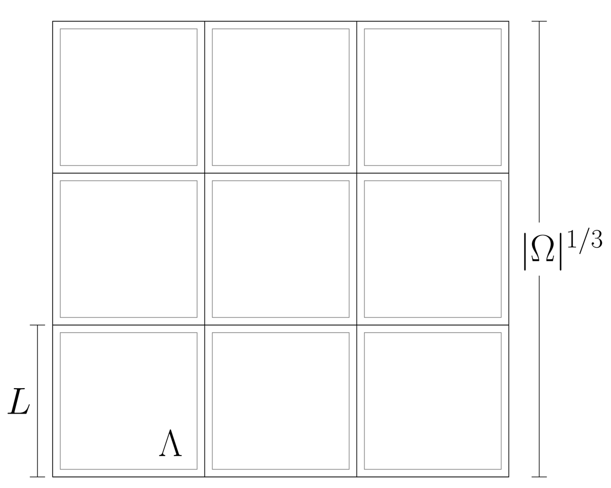
- $T=0$ Upper bound: Dyson (1957), Yau-Yin (2009), Basti-Cenatiempo-Schlein (2021),
- $T=0$ Lower bound: Lieb-Yngvason (1998), Fournais-Solovej (2020,2023)
- $T>0$ First order: Seiringer (2008), Yau-Yin (2009)
- Methods from Boccato-Brenneck-Cenatiempo-Schlein (2019), Basti-Cenatiempo-Schlein (2021), Nam-Triay (2023)

Division into Boxes

- Using Neumann — Dirichlet bracketing we prove the approximate additivity of the (free) energy

$$f(\rho,T) = \lim_{|\Omega|\to\infty} \frac{F_\Omega(N,T)}{|\Omega|} \approx \frac{F_\Lambda(\rho L^3, T)}{|\Lambda|}.$$

- To capture correlations $L \gg \ell_{\mathrm{GP}}$
- In large boxes the interaction potential dominates the kinetic energy (small gap) and the LHY computation are hard to carry out.



Bogoliubov's Theory

We rewrite H_N on Λ in second quantization:

$$H_N = \sum_p p^2 a_p^* a_p + \frac{1}{2}\sum_{m,n,p,q} \langle u_m \otimes u_n, V u_p \otimes u_q\rangle\, a_m^* a_n^* a_p a_q,$$

Bogoliubov's approximation: most particles are in the BEC $a_0^* \approx a_0 \approx \sqrt{N}$ + discard 3rd and 4th order in $a^\dagger, a$:

$$H_N \approx \frac{N\rho}{2}\hat{V}(0) + \sum_{p\ne 0}\big(p^2 + \rho\hat{V}(p)\big)a_p^* a_p + \frac{1}{2}\sum_{p\ne 0}\rho\hat{V}(p)(a_p^\dagger a_p^\dagger + a_p a_p)$$

This quadratic Hamiltonians is exactly diagonalizable but gives the LHY conjecture with the wrong constant: $8\pi\mathfrak{a}$ replaced by $\widehat{V}(p)$.

$\implies$ Higher order contributions are responsible for the renormalization

Renormalization at large momenta

The renormalization $\hat{V}(p) \mapsto 8\pi\mathfrak{a}$ is caused by the correlation structure at short length scale $\ell \ll \ell_{\mathrm{GP}}$

- it is encoded by the scattering solution

$$-\Delta f + \frac{1}{2}Vf = 0$$

- two main processes are taking place: hard and soft collisions. To extract the corresponding contributions, we conjugate the Hamiltonian with suitable unitary transformations $U_{\mathrm{hard}} = e^{\mathcal{B}_{\mathrm{hard}}}, U_{\mathrm{soft}} = e^{\mathcal{B}_{\mathrm{soft}}}$, where

$$\mathcal{B}_{\mathrm{hard}} = \frac{1}{2}\sum_{k\gg\ell_{\mathrm{GP}}} \widehat{f}(k)a_k^\dagger a_{-k}^\dagger - h.c.$$

$$\mathcal{B}_{\mathrm{soft}} = \frac{1}{2}\sum_{\substack{k\gg\ell_{\mathrm{GP}}\\ p\lesssim\ell_{\mathrm{GP}}^{-1}}} \widehat{f}(k)a_k^\dagger a_{-k+p}^\dagger a_p - h.c.$$

- This is a unitary implementation of the multiplication by a Jastrow type correlation factor $\prod_{i<j} f(x_i - x_j)$

Upper Bound

- Trial state with Dirichlet boundary conditions
- To avoid pollution coming from the boundary effects we need boxes of size $L \gg a/(\rho a^3)$
- Problem: While the action of the quadratic unitary U_{hard} is exactly computable, the action of the cubic U_{soft} is not and $\mathcal{B}_{\mathrm{soft}} \gg 1$ in this regime, forbidding any naive perturbative argument.
- Solution: We decompose the U_{soft} into infinitesimal unitaries

$$U_{\mathrm{soft}} = \prod_k U_{\mathrm{soft}}^{(k)},$$

each parametrized by a low momentum $k \lesssim \ell_{\mathrm{GP}}^{-1}$. Generalizing some exclusion principle from [Basti-Cenatiempo-Schlein '21] for the ground state energy, we are able to compute exactly the action of each unitary transformation on an appropriate trial state

$$U_{\mathrm{soft}}^{(k)} = \cos X_k + \mathcal{B}_{\mathrm{soft},k}^\dagger \frac{\sin X_k}{X_k}$$

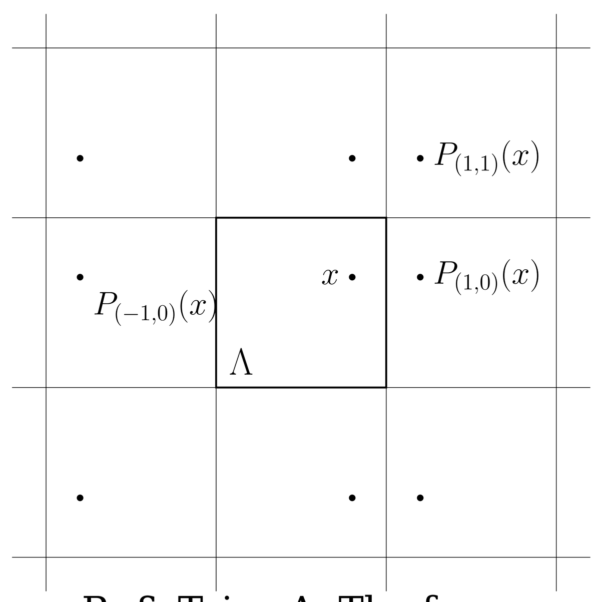
with $X_k = |\mathcal{B}_{\mathrm{soft},k}^\dagger| \ll 1$.

Preprint: Haberberger F., Hainzl C., Schlein B. & Triay A. Upper Bound for the Free Energy of Dilute Bose Gases at Low Temperature arXiv:2405.03378

Lower bound

- The subadditivity of the free energy leads to dealing with Neumann boundary conditions.
- Problem: Solving the scattering equation for the Neumann Laplacian is harder and its solution is not known explicitly [Boccato-Seiringer '23].
- Solution: Instead we take the scattering solution on the full space, add a spatial cut-off and use a mirroring technique to obtain a kernel in the domain of the Neumann Laplacian. This kernel is also diagonal in the Neumann basis, allowing us to diagonalize exactly the Bogoliubov Hamiltonian.

$$\widetilde{f}(x,y) = \sum_z f_{\mathrm{cut}}(P_z(x) - y) = \sum_p \widehat{f}_{\mathrm{cut}}(p)u_p(x)u_p(y)$$



Preprint: Haberberger F., Hainzl C., Nam P.T., Seiringer R. & Triay A. The free energy of dilute Bose gases at low temperatures arXiv:2304.02405

- For hard-sphere and potentials with large L^1 norm, a first renormalization has to be performed before following Bogliubov's strategy. The idea of [Fournais-Solovej '23] is to rewrite the interaction potential by completing the square

$$\sum_{i<j} V(x_i - x_j) = Q_0^{\mathrm{ren}} + Q_1^{\mathrm{ren}} + Q_2^{\mathrm{ren}} + Q_3^{\mathrm{ren}} + Q_4^{\mathrm{ren}}$$

where only Vf appears (which has a small L^1 norm), except in $Q_4^{\mathrm{ren}} \ge 0$ which is thrown away for a lower bound. In a combined effort, we merged the techniques of [Haberberger-Hainzl-Nam-Seiringer-Triay '23] and [Fournais-Solovej '20-'23] to deal with the hard core case.

Preprint: Fournais S., Junge L., Girardot T., Morin L, Olivieri M. & Triay A. The free energy of dilute Bose gases at low temperatures interacting via strong potentials arXiv:2408.14222