

A simplified approach to interacting Bose gases

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Interacting Bose gas

- State: symmetric wave functions in a finite box of volume V with periodic boundary conditions:

$$\psi(x_1, \dots, x_N), \quad x_i \in \Lambda_d := V^{\frac{1}{d}} \mathbb{T}^d$$

- Probability distribution: $|\psi(x_1, \dots, x_N)|^2$
- N -particle Hamiltonian:

$$H_N := -\frac{1}{2} \sum_{i=1}^N \Delta_i + \sum_{1 \leq i < j \leq N} v(x_i - x_j)$$

with $v(x - y) \geq 0$ and $v \in L_1 \cap L_{\frac{d}{2} + \epsilon}(\mathbb{R}^d)$.

Interacting Bose gas

- Ground state:

$$H_N \psi_0 = E_0 \psi_0, \quad E_0 = \min \text{spec}(H_N)$$

- Compute the ground state-energy per particle in the thermodynamic limit:

$$e_0 := \lim_{\substack{V, N \rightarrow \infty \\ \frac{N}{V} = \rho}} \frac{E_0}{N}$$

Energy

- Integrate $H_N \psi_0 = E_0 \psi_0$:

$$\frac{E_0}{N} = \frac{N-1}{2V} \int dx v(x) g_2(0, x)$$

- g_n : marginal of ψ_0

$$g_n(x_1, \dots, x_n) := \frac{V^n \int dx_{n+1} \dots dx_N \psi_0(x_1, \dots, x_N)}{\int dx_1 \dots dx_N \psi_0(x_1, \dots, x_N)}$$

- $\psi_0 \geq 0$, so it can be thought of as a probability distribution

Hierarchy

- Equation for g_2 : integrate $H_N\psi_0 = E_0\psi_0$ with respect to x_3, \dots, x_N :

$$-\frac{1}{2}(\Delta_x + \Delta_y)g_2(x, y) + \frac{N-2}{V} \int dz (v(x-z) + v(y-z))g_3(x, y, z) \\ + v(x-y)g_2(x, y) + \frac{(N-2)(N-3)}{2V^2} \int dz dt v(z-t)g_4(x, y, z, t) = E_0g_2(x, y)$$

- Factorization assumption:

$$g_3(x_1, x_2, x_3) = g_2(x_1, x_2)g_2(x_1, x_3)g_2(x_2, x_3)$$

$$g_4(x_1, x_2, x_3, x_4) = \prod_{i < j} (g_2(x_i, x_j) + O(V^{-1}))$$

Lieb's simple equation

- In the thermodynamic limit, after making a few additional assumptions, [Lieb, 1963]:

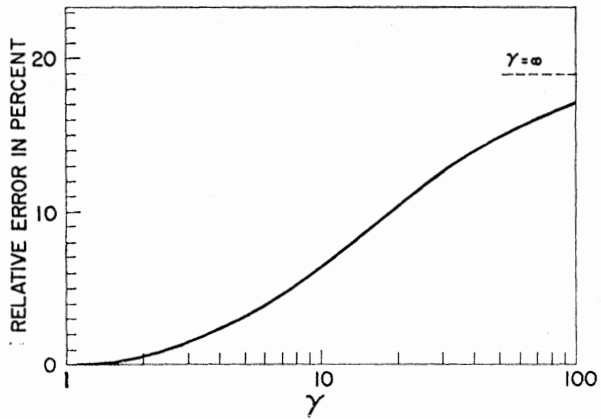
$$(-\Delta + v(x) + 4e)u(x) = v(x) + 2e\rho u * u(x)$$

$$e = \frac{\rho}{2} \int dx (1 - u(x))v(x)$$

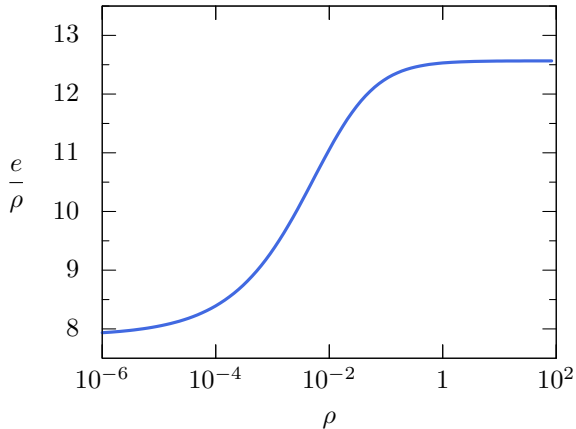
- with $\rho := \frac{N}{V}$

$$g_2(x, y) = 1 - u(x - y)$$

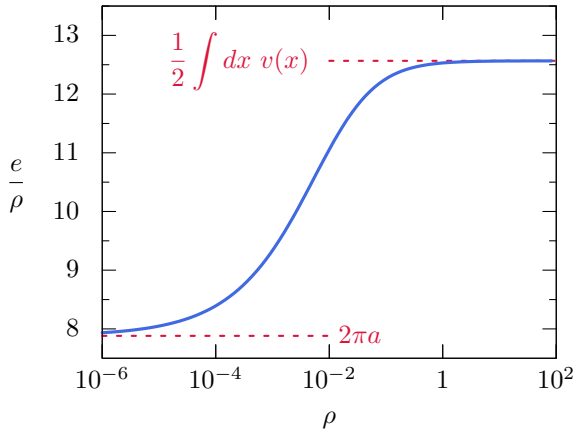
One dimension



Numerical solution for $v(x) = e^{-|x|}$ in 3 dimensions



Numerical solution for $v(x) = e^{-|x|}$ in 3 dimensions



Asymptotics for the Bose gas

- **Theorem** [Lieb, 1963]: if $\hat{v}(k) := \int dx e^{ikx} v(x) \geq 0$, then

$$\frac{e_0}{\rho} \xrightarrow{\rho \rightarrow \infty} \frac{1}{2} \int dx v(x)$$

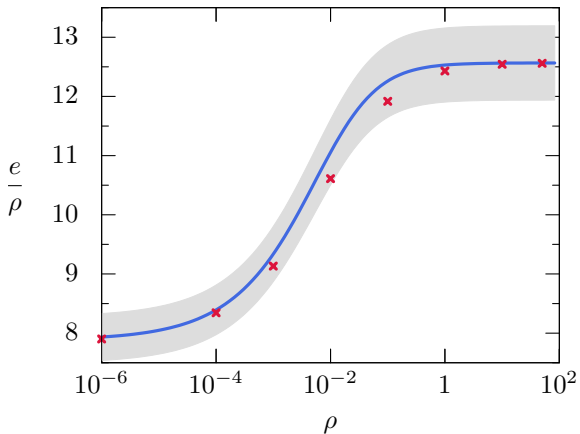
- **Theorem** [Lieb, Yngvason, 1998]: in 3 dimensions (a : scattering length)

$$\frac{e_0}{\rho} \xrightarrow{\rho \rightarrow 0} 2\pi a$$

[Lee, Huang, Yang, 1957], [Yau, Yin, 2009], [Fournais, Solovej, 2019]:

$$e_0 = 2\pi\rho a \left(1 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3} + o(\sqrt{\rho}) \right)$$

Comparison with Bose gas (Monte Carlo)



Monte Carlo computation courtesy of M. Holzmann

Main Theorem

- If $v(x) \geq 0$ and $v \in L_1 \cap L_{\frac{d}{2}+\epsilon}(\mathbb{R}^d)$, then Lieb's simple equation

$$(-\Delta + 4e + v)u = v + 2e\rho u * u, \quad e = \frac{\rho}{2} \int dx (1 - u(x))v(x)$$

has an integrable solution (proved constructively), with $0 \leq u \leq 1$.

- In 3 dimensions,

$$e = 2\pi\rho a \left(1 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3} + o(\sqrt{\rho}) \right), \quad \frac{e}{\rho} \xrightarrow{\rho \rightarrow \infty} \frac{1}{2} \int dx v(x)$$

- If $v(x) \equiv v(|x|)$ is radially symmetric and decays exponentially,

$$u(|x|) \underset{|x| \rightarrow \infty}{\sim} \frac{\alpha}{|x|^4}$$

Existence of a solution (sketch)

- Change the point of view: fix $e > 0$, and compute ρ and u .
- Iteration: $u_0 = 0$,

$$(-\Delta + 4e + v)u_n = v + 2e\rho_{n-1}u_{n-1} * u_{n-1}, \quad \rho_n := \frac{2e}{\int dx (1 - u_n(x))v(x)}.$$

- Prove by induction that $u_n(x)$ is an increasing sequence, and is bounded $u_n(x) \leq 1$. It therefore converges to a function u , which is the unique integrable solution of the equation with e fixed.
- In addition, we prove that $e \mapsto \rho(e)$ is continuous, and $\rho(0) = 0$ and $\rho(\infty) = \infty$, which allows us to compute solutions for the problem at fixed ρ . This does not imply the uniqueness of the solution.

Asymptotics (sketch)

- When ρ is small, e is small as well, so the solution u is *not too far from* the solution of the scattering equation

$$(-\Delta + v)\varphi = v.$$

- The energy of φ is

$$\frac{\rho}{2} \int dx (1 - \varphi(x))v(x) = 2\pi\rho a$$

which yields the first term in the expansion.

- The second term comes from approximating

$$(1 - u(x))v(x) \approx \frac{2e}{\rho}\delta(x)$$

and solving the equation in Fourier space.

Decay (sketch)

$$(-\Delta + 4e + v)u = v + 2e\rho u * u, \quad e = \frac{\rho}{2} \int dx (1 - u(x))v(x)$$

- u and $u * u$ have to decay at the same rate. This is a property of algebraically decaying functions.
- (Remark: if $f(x) \geq f * f(x)$ and $\int f = \frac{1}{2}$, then (morally) $f \sim |x|^{d+1}$.)
- (Remark: $u_n(x)$ decays exponentially).
- Proof is based on the Fourier transform and complex analysis.
- Remark: The truncated two-point correlation function of the Bose gas is also conjectured to decay like $|x|^{-4}$.

Conclusion

- Simple equation: correct asymptotics for the ground state energy at both high and low densities.
- Good approximation for intermediate densities (relative error of 5%).
- Intriguing non-linear PDE.
- Proved existence, asymptotics, and decay rate.

Open problems and conjectures

- Monotonicity of $e \mapsto \rho(e)$, and concavity of $e \mapsto \frac{1}{\rho(e)}$ (would imply uniqueness).
- Other observables? Condensate fraction? (in progress)
- Crystallization?
- *Lieb's simple equation* is actually a simplified version of a more complicated one: *Lieb's full equation*. Can it improve on the simple one? (in progress)