A simplified approach to interacting Bose gases

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Lieb's simple equation

- [Lieb, 1963]: $x \in \mathbb{R}^3$

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

- with

$$\rho > 0, \quad v(x) \geqslant 0, \quad v \in L_1 \cap L_2(\mathbb{R}^3)$$

- and

$$u(x) \geqslant 0, \quad u \in L_1(\mathbb{R}^3), \quad u * u(x) := \int dy\ u(x-y)u(y)$$

Interacting Bose gas

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

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

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

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

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

Interacting Bose gas

- Ground state:

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

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

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

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

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

- $\psi_0 \geqslant 0$, 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 $x_3, \cdots, x_N$:

$$-\frac{1}{2}(\Delta_x + \Delta_y)g_2(x,y) + \frac{N-2}{V}\int dz\ (v(x-z)+v(y-z))g_3(x,y,z)$$

$$+v(x-y)g_2(x,y) + \frac{(N-2)(N-3)}{2V^2}\int dzdt\ v(z-t)g_4(x,y,z,t) = E_0 g_2(x,y)$$

- 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]:

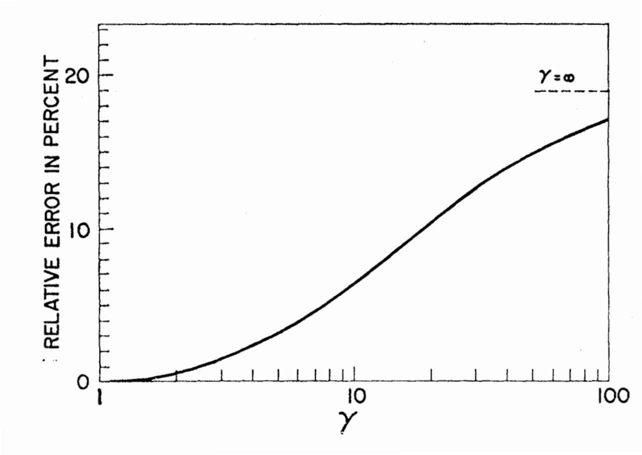
$$(-\Delta + v(x) + 4e)u(x) = v(x) + 2e\rho\ u * u(x)$$

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

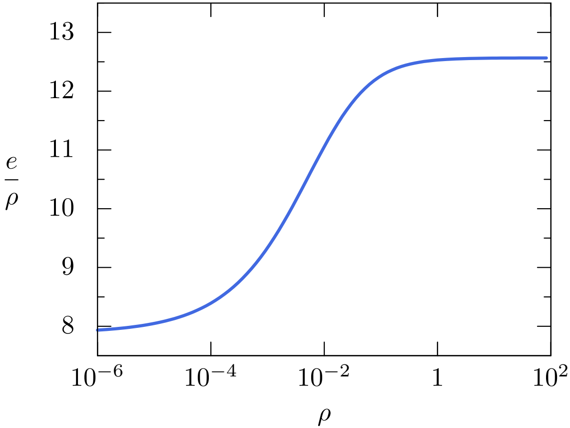
- with $\rho := \frac{N}{V}$

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

One dimension



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



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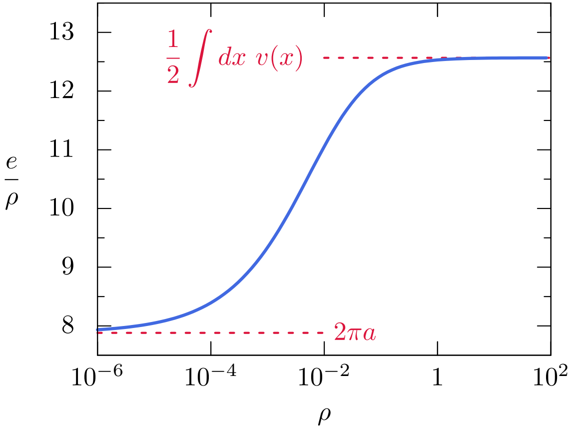


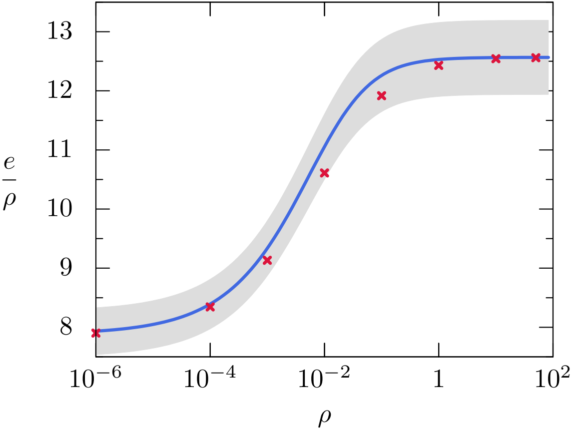
Asymptotics for the Bose gas

- **Theorem** [Lieb, 1963]: if $\hat{v}(k) := \int dx\ e^{ikx} v(x) \geqslant 0$, then
$$\frac{e_0}{\rho} \underset{\rho\to\infty}{\longrightarrow} \frac{1}{2}\int dx\ v(x)$$

- **Theorem** [Lieb, Yngvason, 1998]: in 3 dimensions (a: scattering length)
$$\frac{e_0}{\rho} \underset{\rho\to 0}{\longrightarrow} 2\pi a$$

  [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 $v(x) \geqslant 0$ 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, non-negative solution (proved constructively).

- In 3 dimensions,

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

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

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

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 $u_n(x) \leqslant 1$. It therefore converges to a function u, which is the unique integrable non-negative 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: $u_n(x)$ 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).
- Existence of solutions that are not non-negative? (seems unlikely)
- 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)