

# A simplified approach to interacting Bose gases

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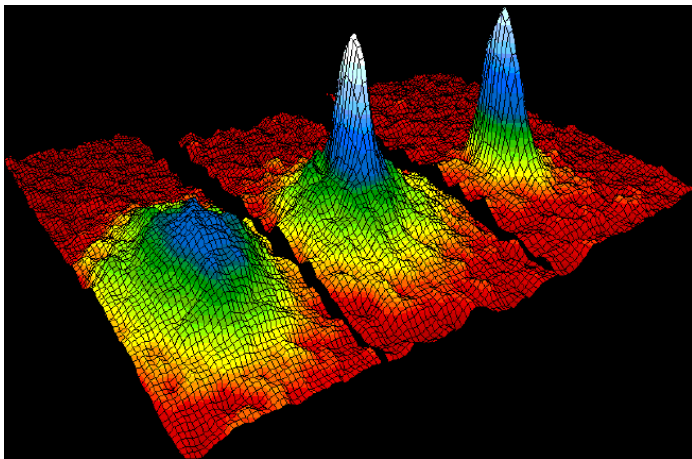
joint with **Eric Carlen, Elliott H. Lieb**

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# Bose gas

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# Interacting Bose gas

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

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

- $N$ -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

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- 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

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- 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  $\psi_0$

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

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

## Hierarchy

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- 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

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

$$(-\Delta + v(x) + 4e_0)u(x) = v(x) + 2e_0\rho u * u(x)$$

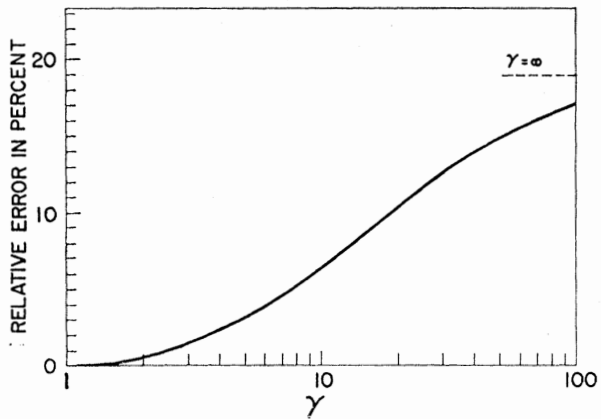
$$e_0 = \frac{\rho}{2} \int dx (1 - u(x))v(x)$$

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

$$g_2(x, y) = 1 - u(x - y), \quad u * u(x) := \int dy u(x - y)u(y)$$

# One dimension

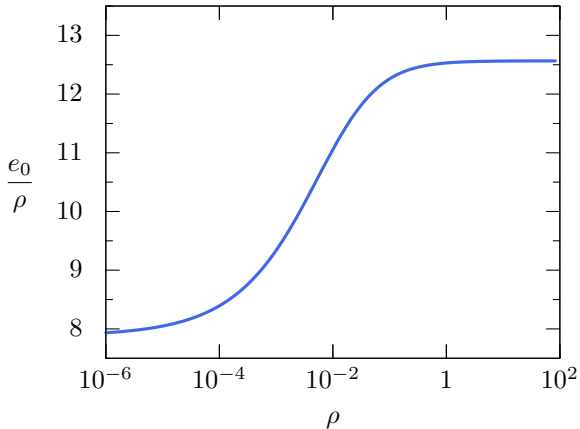
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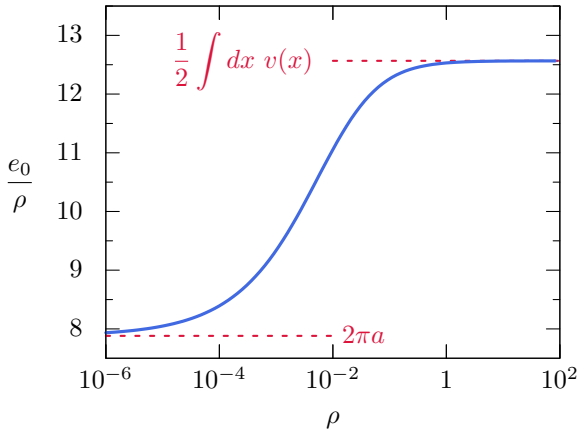
# Numerical solution for $v(x) = e^{-|x|}$ in 3 dimensions

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## Asymptotics for the Bose gas

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- **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)

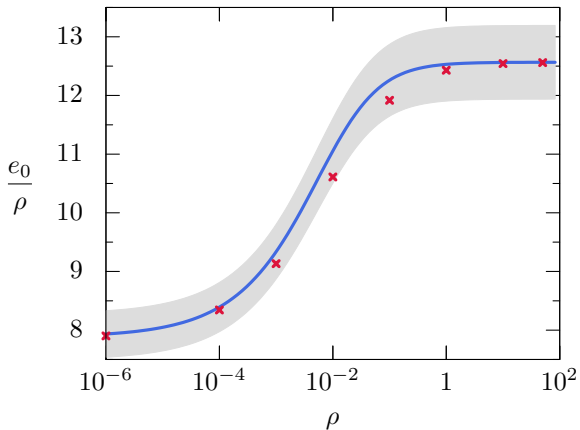
$$\frac{e_0}{\rho} \xrightarrow{\rho \rightarrow 0} 2\pi a$$

[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)

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Monte Carlo computation courtesy of M. Holzmann

## Main Theorem

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

$$(-\Delta + 4e_0 + v)u = v + 2e_0\rho u * u, \quad e_0 = \frac{\rho}{2} \int dx (1 - u(x))v(x)$$

has an integrable, non-negative solution (proved constructively).

- In 3 dimensions,

$$e_0 = 2\pi\rho a \left( 1 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3} + o(\sqrt{\rho}) \right), \quad \frac{e_0}{\rho} \xrightarrow{\rho \rightarrow \infty} \frac{1}{2} \int dx v(x)$$

- 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)

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- Change the point of view: fix  $e_0 > 0$ , and compute  $\rho$  and  $u$ .
- Iteration:  $u_0 = 0$ ,

$$(-\Delta + 4e_0 + v)u_n = v + 2e_0\rho_{n-1}u_{n-1} * u_{n-1}, \quad \rho_n := \frac{2e_0}{\int dx (1 - u_n(x))v(x)}.$$

- 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 non-negative solution of the equation with  $e_0$  fixed.
- In addition, we prove that  $e_0 \mapsto \rho(e_0)$  is continuous, and  $\rho(0) = 0$  and  $\rho(\infty) = \infty$ , which allows us to compute solutions for the problem at fixed  $\rho$ . This does not imply the uniqueness of the solution.

## Asymptotics (sketch)

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- When  $\rho$  is small,  $e_0$  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  $\varphi$  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

$$(1 - u(x))v(x) \approx \frac{2e_0}{\rho} \delta(x)$$

and solving the equation in Fourier space.

## Decay (sketch)

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$$(-\Delta + 4e_0 + v)u = v + 2e_0\rho u * u, \quad e_0 = \frac{\rho}{2} \int dx (1 - u(x))v(x)$$

- $u$  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

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- 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

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- Monotonicity of  $e_0 \mapsto \rho(e_0)$ , and concavity of  $e_0 \mapsto \frac{1}{\rho(e_0)}$  (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)