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:

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

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

- $N$-particle Hamiltonian:

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

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

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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:

\[ e_0 := \lim_{V,N \to \infty} \frac{E_0}{N} \quad \frac{N}{V} = \rho \]
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 $\psi_0$

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

- $\psi_0 \geq 0$, 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 $x_3, \cdots, x_N$:
\[
-\frac{1}{2}(\Delta_x + \Delta_y)g_2(x, y) + \frac{N - 2}{V} \int dz \left( v(x - z) + v(y - z) \right)g_3(x, y, z)
\]
\[
+ v(x - y)g_2(x, y) + \frac{(N - 2)(N - 3)}{2V^2} \int dz dt \, v(z - t)g_4(x, y, z, t) = E_0 g_2(x, y)
\]

- 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]:

\[ (-\Delta + v(x) + 4e)u(x) = v(x) + 2e\rho \ u \ast u(x) \]

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

• 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 $\hat{v}(k) := \int dx \ e^{ikx}v(x) \geq 0$, then
  \[
  \frac{e_0}{\rho} \xrightarrow{\rho \to \infty} \frac{1}{2} \int dx \ v(x)
  \]

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

[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
  \[
  (-\Delta + 4e + v)u = v + 2e \rho u \ast u, \quad e = \frac{\rho}{2} \int dx \ (1 - u(x))v(x)
  \]
  has an integrable solution (proved constructively), with $0 \leq u \leq 1$.

- In 3 dimensions,
  \[
  e = 2\pi \rho a \left( 1 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3} + o(\sqrt{\rho}) \right), \quad \frac{e}{\rho} \xrightarrow{\rho \to \infty} \frac{1}{2} \int dx \ v(x)
  \]

- If $v(x) \equiv v(|x|)$ is radially symmetric and decays exponentially,
  \[
  u(|x|) \xrightarrow{|x| \to \infty} \frac{\alpha}{|x|^4}
  \]
Existence of a solution (sketch)

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

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

- 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 $\rho$. This does not imply the uniqueness of the solution.
Asymptotics (sketch)

- When $\rho$ is small, $\epsilon$ 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
  \[(1 - u(x))v(x) \approx \frac{2\epsilon}{\rho}\delta(x)\]
  and solving the equation in Fourier space.
Decay (sketch)

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

- \(u\) and \(u \ast u\) have to decay at the same rate. This is a property of algebraically decaying functions.
- (Remark: if \(f(x) \geq f \ast f(x)\) 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)
Teaser: Full equation