A simplified approach to interacting Bose gases

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joint with Eric Carlen, Elliott H. Lieb

Lieb’s simple equation

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

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

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

- with

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

- and

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

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

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

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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:

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

\[ \frac{N}{V} = \rho \]
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 $x_3, \cdots, x_N$:

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

\[
+ v(x - y)g_2(x, y) + \frac{(N - 2)(N - 3)}{2V^2} \int dzdt \ v(z - t)g_4(x, y, z, t) = E_0g_2(x, y)
\]

- 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]:

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

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

- 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
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
  \[
  \frac{e_0}{\rho} \xrightarrow{\rho \to \infty} \frac{1}{2} \int dx \ v(x)
  \]

- **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 $v \in L_1 \cap L_{d+e}^1(\mathbb{R}^d)$, 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,
  \[
  e = 2\pi \rho a \left(1 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3} + o(\sqrt{\rho})\right), \quad \frac{e}{\rho} \xrightarrow{\rho \to \infty} \frac{1}{2} \int dx \ v(x)
  \]

- 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: $u_0 = 0$,

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

- 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, $e$ 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 $\varphi$ 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

$$\frac{2e}{\rho} \delta(x)$$

and solving the equation in Fourier space.
Decay (sketch)

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

- \( u \) 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)