An effective equation to study Bose gasses at all densities

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arXiv:1912.04987 http://ian.jauslin.org

Repulsive Bose gas

- Potential: $v(r) \geqslant 0$ and $v \in L_1(\mathbb{R}^3)$, Hamiltonian:

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

- Ground state: ψ_0, energy E_0.
- Observables in the thermodynamic limit: ground state energy per particle and condensate fraction:

$$e_0 := \lim_{\substack{V,N\to\infty \\ \frac{N}{V}=\rho}} \frac{E_0}{N}, \quad \eta_0 := \lim_{\substack{V,N\to\infty \\ \frac{N}{V}=\rho}} \frac{1}{N} \left\langle\psi_0\right| \sum_{i=1}^{N} \int \frac{dx_i}{V} \left|\psi_0\right\rangle .$$

Low density

- Bogolubov theory: approximation scheme that reduces the problem to an effective 1-particle problem.
- Predictions [Lee, Huang, Yang, 1957]:
  - Energy:

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

  - Condensate fraction:

$$1 - \eta_0 \sim \frac{8\sqrt{\rho a^3}}{3\sqrt{\pi}}$$

Low density

- Energy asymptotics: proved: [Lieb, Yngvason, 1998], [Yau, Yin, 2009], [Fournais, Solovej, 2019]
- Condensate fraction: still open in the theormodynamic limit, but there are proofs of condensation in the Gross-Pitaevskii regime (ultra-dilute): [Lieb, Seiringer, 2002], [Boccato, Brennecke, Cenatiempo, Schlein, 2018].
- In Gross-Pitaevskii limit, can also compute excitation spectrum: [Boccato, Brennecke, Cenatiempo, Schlein, 2019].

High density

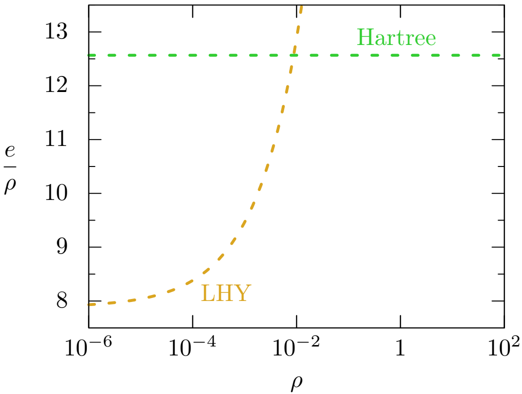
- [Bogolubov, 1947]: if $\hat{v} \geqslant 0$.

$$e_0 \sim \frac{\rho}{2} \int v$$

- Proved in [Lieb, 1963].
- The ultra-concentrated limit is the Hartree regime, in which the excitation spectrum can also be computed: [Seiringer, 2011].

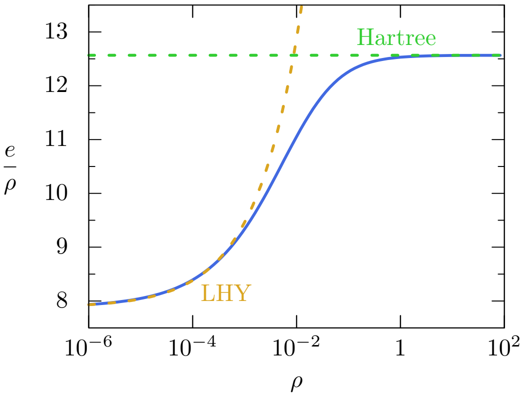
Energy as a function of density

For $v(x) = e^{-|x|}$:



Energy as a function of density

For $v(x) = e^{-|x|}$:



Derivation of the equation

- [Lieb, 1963].
- Integrate $H_N\psi_0 = E_0\psi_0$:

$$\int dx_1 \cdots dx_N \left(-\frac{1}{2}\sum_{i=1}^{N} \Delta_i \psi_0 + \sum_{1\leqslant i<j\leqslant N} v(x_i - x_j)\psi_0 \right) = E_0 \int dx_1 \cdots dx_N \ \psi_0$$

- Therefore,

$$\frac{N(N-1)}{2} \int dx_1 dx_2 \ v(x_1 - x_2) \frac{\int dx_3 \cdots dx_N \ \psi_0}{\int dx_1 \cdots dx_N \ \psi_0} = E_0$$

Derivation of the equation

- Thus,

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

- $\psi_0 \geqslant 0$, so it can be thought of as a probability distribution.
- g_n: correlation functions of $V^{-N}\psi_0$

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

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:

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

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

Big equation

- In the thermodynamic limit, if $u(x) := 1 - g_2(0,x)$,

$$-\Delta u(x) = (1-u(x))\left(v(x) - 2\rho K(x) + \rho^2 L(x)\right)$$

$$K := u * S, \quad S(y) := (1-u(y))v(y)$$

$$L := u * u * S - 2u * (u(u * S)) + \frac{1}{2}\int dydz\ u(y)u(z-x)u(z)u(y-x)S(z-y).$$

- "Big" equation:

$$L \approx u * u * S.$$

Simple equation

- Further approximate $S(x) \approx \frac{2e}{\rho}\delta(x)$ and $u \ll 1$.
- Simple equation

$$-\Delta u(x) = (1 - u(x))v(x) - 4eu(x) + 2e\rho\ u * u(x)$$

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

- **Theorem 1**: If $v(x) \geqslant 0$ and $v \in L_1 \cap L_2(\mathbb{R}^3)$, then the simple equation has an integrable solution (proved constructively), with $0 \leqslant u \leqslant 1$.

Energy for the simple equation

- **Theorem 2**:

$$\frac{e}{\rho} \underset{\rho\to\infty}{\longrightarrow} \frac{1}{2}\int dx\ v(x)$$

(note that there is no condition that $\hat v \geqslant 0$). This coincides with the Hartree energy.

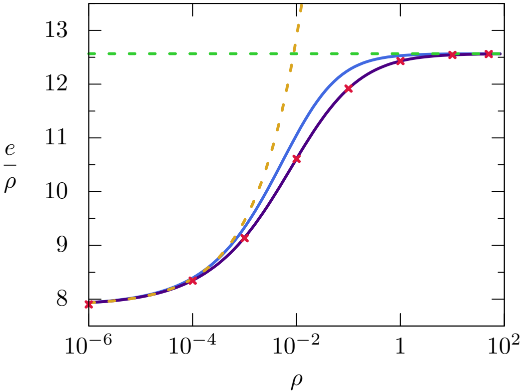
- **Theorem 3**:

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

This coincides with the Lee-Huang-Yang prediction.

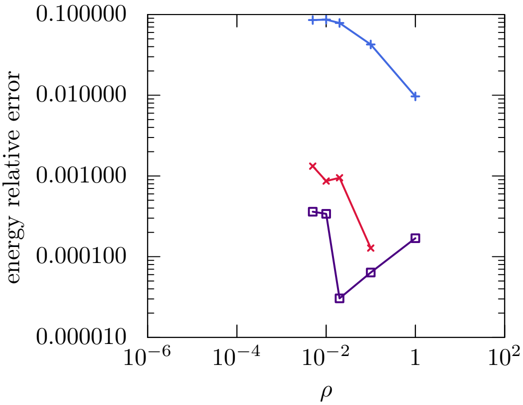
Energy

$v(x) = e^{-|x|}$, Blue: simple equation; purple: big equation; red: Monte Carlo



Energy

$v(x) = 2e^{-|x|}$, Blue: simple equation; red: Jastrow; purple: big equation



Condensate fraction

- Add a parameter μ to the Hamiltonian:

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

- Projection onto condensate wavefunction: $\sum_i \int \frac{dx_i}{V}$.
- Condensate fraction:

$$\eta_0 := \frac{1}{N}\left\langle\psi_0\right|\sum_{i=1}^{N}\int\frac{dx_i}{V}\left|\psi_0\right\rangle = -\frac{1}{N}\partial_\mu\left\langle\psi_0\right|H_N(\mu)\left|\psi_0\right\rangle|_{\mu_0} \equiv -\partial_\mu e_0(\mu)|_{\mu=0}$$

Condensate fraction

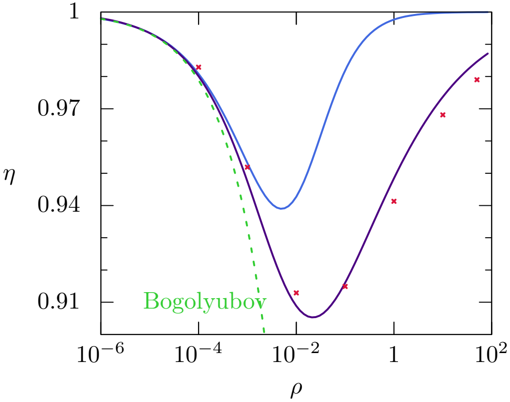
- **Theorem 4**: For the simple equation, as $\rho \to 0$

$$1 - \eta \sim \frac{8\sqrt{\rho a^3}}{3\sqrt{\pi}}$$

which coincides with Bogolubov's prediction.

Condensate fraction

$v(x) = e^{-|x|}$, Blue: simple equation; purple: big equation; red: Monte Carlo



Correlation function

- **Conjecture** [Lee, Huang, Yang, 1957]: Truncated two-point correlation function:

$$\sigma_0(x) \underset{|x|\to\infty}{\sim} \rho^2 \frac{\beta_0}{|x|^4}$$

- **Theorem 5**: If $|x|^4 v \in L_1(\mathbb{R}^3)$, then for the simple equation

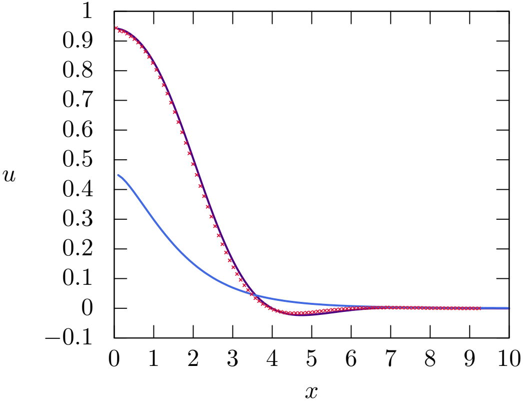
$$u(x) \underset{|x|\to\infty}{\sim} \frac{\alpha}{|x|^4}$$

and

$$\sigma(x) \underset{|x|\to\infty}{\sim} \rho^2 \frac{\beta}{|x|^4}.$$

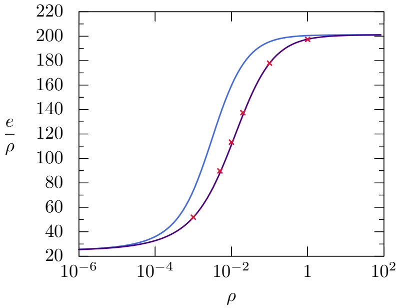
Linear correlation function

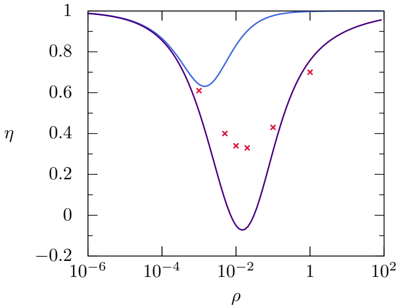
$v(x) = 16e^{-|x|}$, Blue: simple equation; purple: big equation; red: Jastrow



Limitations of the simple and big equations

- Only works at high densities for $\hat{v} \geqslant 0$.
- Less accurate for large potentials: for $v(x) = 16e^{-|x|}$,





Conclusions and outlooks

- Two effective equations: the big equation and the simple equation, which are non-linear 1-particle equations.
- Reproduce the known results for both small and large densities.
- Their derivation is different from Bogolubov theory, so they may give new insights onto studying the Bose gas in these asymptotic regimes.
- The big equation is quantitatively accurate at intermediate densities.
- This opens up the possibility of studying the physics of the Bose gas at intermediate densities.

Open problems

- Analysis of the simple equation: Monotonicity of $e(\rho)$, and convexity of $\rho e(\rho)$. (So far, we have proofs for small and large ρ.). Similarly, prove that $0 \leqslant \eta \leqslant 1$. (We have a proof for small ρ.)
- Analysis of the big equation: everything is still open.
- Relate these equations back to the many-body Bose gas.