Mathematical theory of Bose gases

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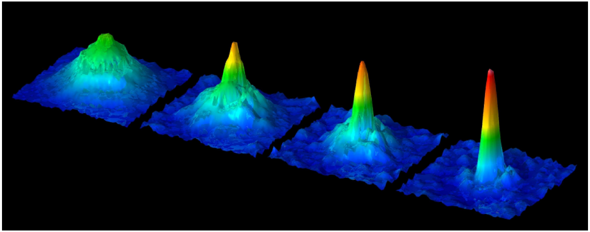
Motivation

In 1995, the **Bose-Einstein condensation** (BEC) was observed in experiments: many bosons occupy the same quantum state at a low temperature, leading to macroscopic quantum effects e.g. superfluidity, quantized vortices, ...



Cornell, Wieman, Ketterle (2001 Nobel Prize in Physics)

It was predicted by **Bose** and **Einstein** (1924-25) from the analysis of the **non-interacting** Bose gas

$$\frac{N_0}{N} = \left[1 - \left(\frac{T}{T_c}\right)^{3/2}\right]_+$$

Motivation

The Bose–Einstein condensate is closely related to the **superfluid**, a special state of matter which behaves like a fluid with **zero viscosity** at very low temperatures

- **Allen–Misener** & **Kapitsa** (1938): Superfluid ^{4}He (bosons) at below 2.17 K
- **London** (1938): Explanation via the Bose–Einstein condensation
- **Landau** (1941): Theoretical explanation (1962 Nobel Prize in Physics)
- **Lee – Osheroff–Richardson** (1972): ^{3}He (fermions) can form bosons by pairing and exhibit the superfluidity at 0.003 K (1996 Nobel Prize in Physics)

On mathematical side:

- **Bogoliubov** (1947): Microscopic explanation for Landau's criterion of superfluidity
- The fermionic of Bogoliubov theory is the **Bardeen–Cooper–Schrieffer (BCS) theory** (1957) for superconductivity (1972 Nobel Prize in Physics)

How to understand these properties from first principles?

J. F. Allen and A. D Misener, *Nature* 141, 75 (1938)
P. Kapitza, *Nature* 141, 74 (1938)
F. London, *Nature* 141, 643–644 (1938)
L.D. Landau, *Phys. Rev.* 60, 356 (1941)
N. N. Bogoliubov, *J. Phys. (USSR)*, 11, p. 23 (1947)
D. D. Osheroff, R. C. Richardson, and D. M. Lee, *Phys. Rev. Lett.* 28, 885–888 (1972)

Bosons and fermions

From first principles of quantum mechanics, N quantum particles in $\mathbb{R}^d$ is described by a (normalized) **wave function** $\Psi \in L^2(\mathbb{R}^{dN})$

- $|\Psi(x_1, ..., x_N)|^2 =$ probability density of positions of particles
- $|\widehat{\Psi}(p_1, ..., p_N)|^2 =$ probability density of momenta of particles

We will consider **identical** (indistinguishable) particles $\Rightarrow |\Psi|^2$ is symmetric

- **bosons:** Ψ symmetric (ex: photon, gluon, Higgs, Helium 4)

$$\Psi(x_{\sigma(1)}, ..., x_{\sigma(N)}) = \Psi(x_1, ..., x_N), \quad \forall \sigma \in S_N$$

- **fermions:** Ψ anti–symmetric (ex: electron, proton, neutron, Helium 3)

$$\Psi(x_{\sigma(1)}, ..., x_{\sigma(N)}) = (-1)^\sigma \Psi(x_1, ..., x_N), \quad \forall \sigma \in S_N$$

A typical example of N-body bosonic wave function is the **Hartree state**

$$\Psi(x_1, ..., x_N) = (u^{\otimes N})(x_1, ..., x_N) = u(x_1)...u(x_N), \quad \|u\|_{L^2(\mathbb{R}^d)} = 1$$

The fermionic analogue is the **Slater determinant** $u_1 \wedge u_2 \wedge ... \wedge u_N$

A many–body quantum problem

A system of N bosons in $\mathbb{R}^d$ is described by the Hamiltonian

$$H_N = \sum_{i=1}^{N} (-\Delta_{x_i} + V(x_i)) + \lambda \sum_{i<j}^{N} w(x_i - x_j) \quad \text{on} \quad L^2_s(\mathbb{R}^{dN})$$

We are interested in the **ground state energy**

$$E_N = \inf_{\|\Psi\|_{L^2_s(\mathbb{R}^{dN})}=1} \langle \Psi, H_N \Psi \rangle$$

If a **ground state** Ψ exists, then it solves the **Schrödinger equation**

$$H_N \Psi = E_N \Psi$$

This is 'just' a **linear** equation, but not solvable even numerically when $N \geq 10$. For practical computation, we have to replace the **many-body linear** problem to **one-body nonlinear** problems

Hartree approximation

The idea goes back to **Pierre Curie** (1985) and **Pierre Weiss** (1907)

Mean–field theory: particles are treated as if they were **independent**

For bosons, MF theory suggests to restrict to the Hartree state $u^{\otimes N}$

$$\frac{\langle u^{\otimes N}, H_N u^{\otimes N}\rangle}{N} = \int |\nabla u|^2 + \int V|u|^2 + \frac{\lambda(N-1)}{2}\iint |u(x)|^2|u(y)|^2 w(x-y)\mathrm{d}x\mathrm{d}y$$

In the **mean–field regime** $\lambda = \frac{1}{N-1}$ we obtain the Hartree functional

$$\mathcal{E}_{\mathrm{H}}(u) = \int_{\mathbb{R}^d} |\nabla u|^2 + \int_{\mathbb{R}^d} V|u|^2 + \frac{1}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} |u(x)|^2|u(y)|^2 w(x-y)\mathrm{d}x\mathrm{d}y$$

Define the Hartree energy

$$e_{\mathrm{H}} = \inf_{\|u\|_{L^2(\mathbb{R}^d)}=1} \mathcal{E}_{\mathrm{H}}(u)$$

If a minimizer exists, it solves the Hartree equation for some $\varepsilon_0 \in \mathbb{R}$

$$-\Delta u + Vu + (w * |u|^2)u = \varepsilon_0 u$$

Bogoliubov theory

On a Hartree state $u^{\otimes N}$ we find the Hartree energy functional

$$\mathcal{E}_{\rm H}(u) = \int_{\mathbb{R}^d} |\nabla u|^2 + \int_{\mathbb{R}^d} V|u|^2 + \frac{1}{2} \iint_{\mathbb{R}^d\times\mathbb{R}^d} w(x-y)|u(x)|^2|u(y)|^2 \mathrm{d}x\mathrm{d}y$$

Assume $\exists$ unique minimizer u_0. Then $\forall v$ in $\{u_0\}^\perp$, we have Taylor's expansion

$$\mathcal{E}_{\rm H}\left(\frac{u_0+v}{\sqrt{1+\|v\|^2}}\right) = \mathcal{E}_{\rm H}(u_0) + \frac{1}{2}\text{Hess}\,\mathcal{E}_{\rm H}(u_0)(v,v) + o\left(\|v\|^2_{H^1}\right)$$

Bogoliubov theory (1947) can be formulated as

$$\lambda_k(H_N) = Ne_{\rm H} + \lambda_k(\mathbb{H}) + o(1)_{N\to\infty}, \quad \forall k\geq 1$$

where $\mathbb{H}$ = **second quantization** of $\frac{1}{2}\text{Hess}\,\mathcal{E}_{\rm H}(u_0)$ on **Fock space** $\mathcal{F}(\{u_0\}^\perp)$

$$\mathcal{F}(\mathfrak{H}) = \bigoplus_{n=0}^{\infty}\mathfrak{H}^n = \mathbb{C}\oplus\mathfrak{H}\oplus\mathfrak{H}^2\oplus\ldots, \quad \mathfrak{H}^n = \bigotimes_s^n \mathfrak{H}$$

Bogoliubov Hamiltonian $\mathbb{H}$ describes the fluctuations around the condensate

Bogoliubov theory

Write the Hamiltonian using $a_n = a(u_n)$, $\{u_n\}_{n=0}^{\infty}$ ONB for $L^2(\mathbb{R}^3)$

$$H_N = \sum_{m,n\geq 0} T_{mn} a_m^* a_n + \frac{1}{2} \sum_{m,n,p,q\geq 0} W_{mnpq} a_m^* a_n^* a_p a_q$$

1. Replace any a_0, a_0^* by $\sqrt{N}$ (**c-number substitution**);
2. Ignore all terms with 3 or 4 operators $a_n^\#$ with $n \neq 0$;
3. Diagonalize the resulting **quadratic Hamiltonian**
4. Anytime when you see $\int V$, replace it by b (**Landau's correction**)

All this leads to

$$H_N \approx N e_{\mathrm{GP}} + e_{\mathrm{Bog}} + \sum_{p,q\geq 1} e_p a_p^* a_p,$$

In the the mean–field regime, the first two steps are correct, so the last step (Landau's correction) is not needed

In the GP regime, **quartic terms have $O(N)$ contribution and cubic terms have $\mathcal{O}(1)$ contribution**. Thus without the last step, Bogoliubov theory is incorrect. How to implement the last step rigorously?

BEC in the thermodynamic limit: An open problem

Consider N bosons in a large torus $\Omega = [0, L]^3$ described by the Hamiltonian

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \sum_{i<j}^{N} W(x_i - x_j)$$

An outstanding open problem in mathematical physics is the proof of BEC in the **thermodynamic limit** $N \to \infty$, $L \to \infty$, $N/L^3 = \rho > 0$ fixed

Conjecture (BEC in the thermodynamic limit)

If $W \geq 0$, then the ground state Ψ_N of H_N **condensates** on $u_0(x) = L^{-3/2}\mathbb{1}_\Omega(x)$

$$\langle u_0, \gamma^{(1)}_{\Psi_N} u_0 \rangle = \frac{1}{|\Omega|^2} \iint_{\Omega\times\Omega} \gamma^{(1)}_{\Psi_N}(x, y)\mathrm{d}x\mathrm{d}y \geq c_0 > 0 \quad \text{independently of } \Omega$$

Best known: the **Lee–Huang–Yang formula** (1957), $a =$ scattering length of W

$$\lim_{\substack{N\to\infty \\ N/L^3=\rho}} \frac{E_N}{N} = 4\pi a\rho \left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} + o(\sqrt{\rho})_{\rho\to 0}\right)$$

proved by **Dyson** (57), **Lieb–Yngvason** (98), **Yau–Yin** (08), **Fournais–Solovej**

S. Fournais, J.P. Solovej. The energy of dilute Bose gases. *Annals of Math.* 192 (2020)

Intermediate regimes

- By rescaling, the thermodynamic limit is equivalently described by

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \sum_{i<j}^{N} N^{2/3} W(N^{1/3}(x_i - x_j)) \quad \text{on } L^2_s(([0,1]^3)^N)$$

- In the Gross–Pitaevskii limit

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \sum_{i<j}^{N} N^{2} W(N(x_i - x_j)) \quad \text{on } L^2_s(([0,1]^3)^N)$$

- We may consider an intermediate limit

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \sum_{i<j}^{N} N^{2\kappa} W(N^{\kappa}(x_i - x_j)) \quad \text{on } L^2_s(([0,1]^3)^N)$$

Theorem (BEC in intermediate regime, Fournais 2020)

If $W \geq 0$ and $1 > \kappa > 3/5$, then there is the **complete BEC** on $u_0(x) = 1$

$$\lim_{N\to\infty} \langle u_0, \gamma^{(1)}_{\Psi_N} u_0 \rangle = 1$$

S. Fournais. Length scales for BEC in the dilute Bose gas. arXiv:2011.00309