The Energy of the Interacting Bose Gas

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Introduction

The Bose gas: a Many-Body Quantum Problem

N **bosonic** particles in $\Lambda = [-L/2, L/2]^3$

$$H_N = -\sum_{i=1}^{N} \Delta_i + \kappa \sum_{i<j}^{N} V(x_i - x_j)$$

acting on $\psi \in L^2_s(\Lambda^N)$: symmetric tensor product $\Big(\underbrace{L^2(\Lambda) \otimes \cdots \otimes L^2(\Lambda)}_{N}\Big)_{\text{sym}}$

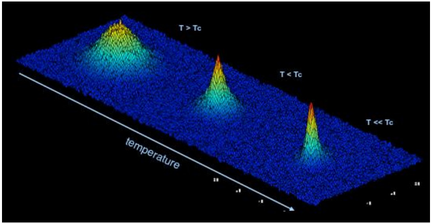
Bose-Einstein condensation

- $V = 0$ [Bose, Einstein 1924]
  The problem factorizes

$$\psi(x_1, x_2, \ldots, x_N) = \prod_{i=1} \varphi_0(x_i)$$

- $V \neq 0$: complicated linear combination of elementary tensors
  many-body correlations are crucial

  BEC proved only for lattice systems: [Dyson, Lieb, Simon 1978], [Kennedy, Lieb, Shastry 1988]

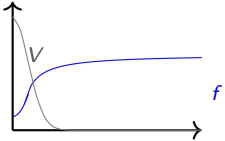


The Dilute Bose Gas

The dilute regime is the regime where $\rho\mathfrak{a}^3$ **small**.

$\rho = N/|\Lambda|$ is the density of the gas, $\mathfrak{a}$ **is the scattering length of** V

To define the scattering length, we consider the **two-body problem**



$$[-\Delta + \frac{1}{2}V]f_0 = 0$$

$$f_0(x) = 1 \quad \text{for} \quad |x| \to \infty$$

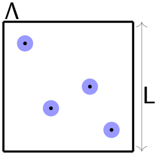
Outside the range of V, f is harmonic in the form:

$$f_0(x) = 1 - \frac{\mathfrak{a}}{|x|}$$

$\mathfrak{a}$ is the scattering length of V.

What We Know

The thermodynamic limit of the Bose gas



Thermodynamic limit:
$N \to \infty$, $L \to \infty$ with $\rho = N/|\Lambda|$ fixed.

We define the ground state energy of H_N

$$E(N, L) = \inf_{\psi \in L^2_s(\Lambda^N),\, ||\psi||=1} \langle \psi, H_N \psi \rangle .$$

The ground state energy per particle

$$e(\rho) = \lim_{\substack{N, L \to \infty \\ \rho = N/|\Lambda|}} \frac{E(N, L)}{N}$$

Lee-Huang-Yang formula: for $\rho \mathfrak{a}^3$ small

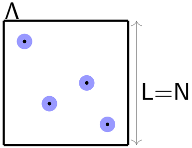
$$e(\rho) = 4\pi\rho\mathfrak{a}\left[1 + \frac{128}{15\sqrt{\pi}}(\rho\mathfrak{a}^3)^{1/2} + o((\rho\mathfrak{a}^3)^{1/2})\right]$$

[Yau, Yin 2009], [Fournais, Solovej 2020], [Basti, Cenatiempo, Schlein 2021]

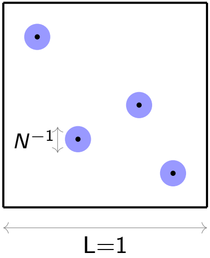
Remark. Universality: no dependence on details of V

Gross-Pitaevskii limit:
$N \to \infty$, $L = N$ with $\rho = 1/N^2$.

(Simultaneous large volume and low density limit)



Rescaling lengths: fixed box $\Lambda_1 = [-1/2, 1/2]^3$



the Hamiltonian takes the form

$$H_N = -\sum_{i=1}^{N} \Delta_{x_i} + \sum_{i<j}^{N} N^2 V\big(N(x_i - x_j)\big)$$

acting on $L^2_s(\Lambda^N)$.

Call

$$E_N = \inf_{\substack{\psi \in L^2_s(\Lambda^N),\\ \|\psi\|_2 = 1}} \langle \psi, H_N \psi \rangle$$

The Gross-Pitaevskii Limit, Periodic B.C.

- Ground state energy: $V \in L^3(\mathbb{R}^3)$ positive, spherically symmetric, compactly supported

$$E_N = 4\pi\mathfrak{a}(N-1) + e_\Lambda \mathfrak{a}^2 \\ -\frac{1}{2}\sum_{p\in\Lambda_+^*}\left[p^2 + 8\pi\mathfrak{a} - \sqrt{|p|^4 + 16\pi\mathfrak{a}p^2} - \frac{(8\pi\mathfrak{a})^2}{2p^2}\right] + \mathcal{O}(N^{-1/4})$$

where $\Lambda_+^* = 2\pi\mathbb{Z}^3\backslash\{0\}$ and $e_\Lambda \simeq 10.0912$.

- The spectrum of $H_N - E_N$ is given by

$$\sum_{p\in\Lambda_+^*} n_p\sqrt{|p|^4 + 16\pi\mathfrak{a}p^2} + \mathcal{O}(N^{-1/4})$$

with $n_p \in \mathbb{N}$ and $n_p \neq 0$ for finitely many $p \in \Lambda_+^*$ only (n_p is the number of excited states with momentum p).

[Boccato, Brennecke, Cenatiempo, Schlein 2019], [Hainzl, Schlein, Triay 2022]

The Gross-Pitaevskii Limit, Periodic B.C.

Ground state vector: $H_N \psi_N = E_N \psi_N$

One-particle reduced density matrix (quantum marginal): $\gamma^{(1)}_{\psi_N} := \mathrm{Tr}_{2,\dots,N} |\psi_N\rangle\langle\psi_N|$

- Bose-Einstein condensation in the ground state ψ_N means that

$$\lim_{N\to\infty} \langle \varphi_0, \gamma^{(1)}_{\psi_N} \varphi_0 \rangle = 1 \qquad \varphi_0 = 1$$

  Optimal rate (bound for the number of excitations) $1 - \langle \varphi_0, \gamma^{(1)}_{\psi_N} \varphi_0 \rangle \leq \frac{C}{N}$

- Approximation of eigenvectors
  If ψ_N denotes a ground state vector of H_N, and θ_1, θ_2 are the first two eigenvalues of H_N

$$\left\| \psi_N - e^{i\omega} U^* e^{B(\eta)} e^{A} e^{B(\tau)} \Omega \right\|^2 \leq \frac{C}{\theta_2 - \theta_1} N^{-1/4}$$

  for a phase $\omega \in [0; 2\pi)$

[Lieb, Seiringer 2002], [Boccato, C. Brennecke, S. Cenatiempo, B. Schlein 2020]

Systems in $\mathbb{R}^3$ trapped by an External Potential

Hamiltonian acting on $L^2_s(\mathbb{R}^{3N})$

$$H_N = \sum_{i=1}^{N} \big(-\Delta_{x_i} + V_{ext}(x_i) \big) + \sum_{i<j}^{N} N^2 V(N(x_i - x_j))$$

Bose-Einstein condensation, ground state energy and excitation spectrum obtained in [Lieb, Seiringer 2002],
[Nam, Napiórkowski, Ricaud, Triay 2020],
[Brennecke, Schlein, Schraven 2021,2022],
[Nam, Triay 2021]

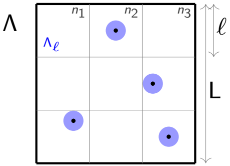
Main Result:
BEC with Neumann Boundary Conditions

Difficulty in the thermodynamic limit: absence of an energy gap!

Partition the volume in cells of side-length ℓ and study

$$H_{n,\ell} = -\sum_{i=1}^{n} \Delta_i + \kappa \sum_{i<j}^{n} \ell^2 V\big(\ell(x_i - x_j)\big)$$

acting on $L^2_s(\Lambda_1)$, with $\Lambda_1 = [-1/2, 1/2]$.



- ℓ to be chosen as a suitable function of ρ
- control of boundary effects needed!

For lower bounds, impose **Neumann boundary conditions** on Λ_1

$$E(N, L) \geq \frac{1}{\ell^2} \inf_{\{n_k\}:\sum_k n_k = N} \sum_k e_{n_k,\ell}$$

with

$$e_{n,\ell} = \inf_{\psi \in L^2_s(\Lambda_1),\, ||\psi||=1} \langle \psi, H_{n,\ell} \psi \rangle.$$

(n is the particle number in the small box)

Ground State Energy and BEC in the Neumann box

Theorem (B., Seiringer 2022)

Let $V > 0$ be compactly supported, spherically symmetric and bounded. Assume κ small enough and $n\ell^{-1} \leq 1$. Then

$$\Big| e_{n,\ell} - 4\pi\mathfrak{a}\frac{n^2}{\ell}\Big| \leq C\Big(\frac{n}{\ell} + \frac{n^2}{\ell^2}\ln(\ell)\Big)$$

for a constant $C > 0$.

Let $\psi_n \in L^2_s(\Lambda_1^n)$ be a normalized wave function, with

$$\langle \psi_n, H_{n,\ell}\psi_n\rangle \leq e_{n,\ell} + \zeta$$

for some $\zeta > 0$. Then there exists a constant $C > 0$ such that

$$1 - \langle \varphi_0, \gamma_n^{(1)}\varphi_0\rangle \leq C\Big(\frac{\zeta}{n} + \frac{1}{\ell}\Big)$$

where $\varphi_0(x) = 1$ for all $x \in \Lambda_1$.

Corollary (Thermodynamic Limit)

Let V satisfy the same assumptions as above and κ small enough. Then there exists a constant $C > 0$ such that

$$e(\rho) \geq 4\pi\mathfrak{a}\rho\Big(1 - C(\rho\mathfrak{a}^3)^{1/2}\ln(\rho)\Big)$$

Remarks.

- For $n = \ell = N$:
  – Condensate depletion rate N^{-1} as for periodic boundary conditions

  – Logarithmic behavior of the error bound for the ground state energy

$$\Big| e_{N,N} - 4\pi\mathfrak{a}N \Big| \leq C\Big(1 + \ln(N)\Big).$$

  Sharp and specific to the Neumann boundary conditions

- κ small needed for properties of the two-body Neumann problem

- Bound for $e(\rho)$ is not optimal (optimal in [Fournais Solovej 2021], different localization method, modified kinetic energy)

- We take $\ell \simeq \rho^{-1/2}$; larger lengths ℓ allow for a better precision but require a more precise study of $H_{n,\ell}$, with larger n/ℓ
  (with larger ℓ and periodic b.c.: [Adhikari, Brennecke, Schlein 2021], [Fournais 2021], [Brennecke, Caporaletti, Schlein 2021])

Proof: Control of Neumann Boundary Effects

Many-body analysis: conjugate the Hamiltonian with unitary transformations

$$e^{-B} U_n H_{n,\ell}\, U_n^* e^B$$

- $\mathcal{U}$ extracts the contribution of the factorized part of wave functions $U_n^* \Omega = \varphi^{\otimes n}$
  [Lewin, Nam, Serfaty, Solovej 2014]
- $e^B = \exp\left[\frac{1}{2}\int_{\Lambda_1 \times \Lambda_1} dxdy\, \eta(x,y)\, b_x^* b_y^* - \text{h.c.}\right]$ generalized Bogoliubov transformation implements correlations
  [Boccato, Brennecke, Cenatiempo, Schlein 2018]

With a suitable choice of $\eta(x,y)$

$$e_{n,\ell} \leq \langle \Omega, e^{-B} U_n^* H_{n,\ell}\, U_n e^B \Omega \rangle \leq C_{n,\ell} + C\kappa \frac{n}{\ell}$$

with $C_{n,\ell} = 4\pi\mathfrak{a}\frac{n^2}{\ell}\left(1 + \mathcal{O}\left(\frac{\mathfrak{a}}{\ell}\ln(\ell/\mathfrak{a})\right)\right)$

Use the energy gap $\mathcal{K} = \sum_{p \in \Lambda_{1,+}^*} p^2 a_p^* a_p \geq \pi^2 \sum_{p \in \Lambda_{1,+}^*} a_p^* a_p = \pi^2 \mathcal{N}_+$ for proving the lower bound and condensation.

Proof: Control of Neumann Boundary Effects

Neumann boundary conditions: choose $\eta(x,y) \simeq -n(1-\ell^3 f(\ell x, \ell y))$, f minimizer of

$$F[g] = \int_{\Lambda_\ell \times \Lambda_\ell} dxdy \left[\kappa V(x-y)|g(x,y)|^2 + |\nabla_x g(x,y)|^2 + |\nabla_y g(x,y)|^2 \right]$$

$g \in H^1(\Lambda_\ell \times \Lambda_\ell)$ with $\|g\|_{L^2(\Lambda_\ell \times \Lambda_\ell)} = 1$

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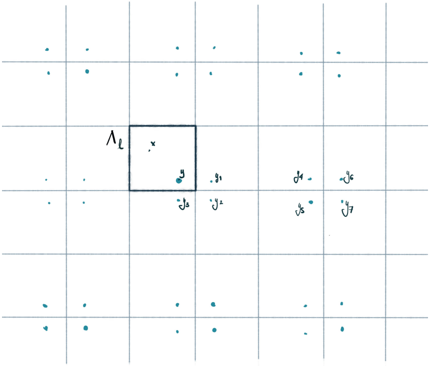
Pointwise estimates of the minimizer needed for the many-body analysis

- six-dimensional problem, f not explicitly known
- method of image charges to express Green functions

Remark. Very different from the trapped Bose gas: there the problem naturally decouples in relative coordinates and center of mass and
$\eta^{\mathrm{Trap}}(x,y) \simeq -n(1-f(x-y))\varphi_0^2(x+y)$



$(-\Delta+\varepsilon)G(x,y) = \delta_x(y)$

$G(x,y) = G_{\mathbb{R}^3}(x-y) + \sum_{n\in\mathbb{Z}^6\setminus\{0\}} G_{\mathbb{R}^3}(x-y_n)$