The free energy of the Bose gas at low density

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July 26th 2024

Joint meeting AMS-UMI, Palermo

Finanziato dall'Unione europea NextGenerationEU
Ministero dell'Università e della Ricerca

Interacting Many-Body Systems

Many-body quantum mechanics:

Small scale: large number of particles described microscopically by the Schrödinger equation.

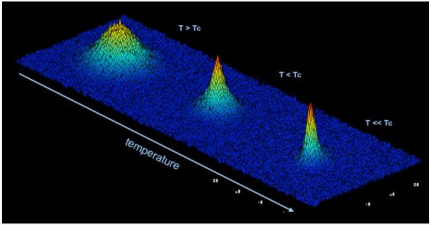
Large scale: we observe **emergent phenomena**, such as **phase transitions, universality, nonlinear effects**, macroscopic patterns, collective behavior.

The challenge

Derive **effective theories** from first principles of quantum mechanics, describing the emergent physics in terms of *few degrees of freedom*.

The Bose gas: a Many-Body Quantum Problem

Emergence of Bose-Einstein condensation in gas of bosonic particles at very low temperature.



Objects of study: BEC, excitation spectrum in scaling limits, **free energy at the critical temperature**

Zero temperature systems

Many-body bosonic system: noninteracting case

Consider N noninteracting bosons in a box $\Lambda = [-L/2, L/2]^3$ described by

$$H_N = -\sum_{i=1}^{N} \Delta_{x_i}$$

acting on $\Big(\underbrace{L^2(\Lambda) \otimes \cdots \otimes L^2(\Lambda)}_{N}\Big)_{\text{sym}} \cong L^2_s(\Lambda^N)$.

Bosonic statistics: permutation-symmetric wavefunctions $\psi \in L^2_s(\Lambda^N)$

$$\psi(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_N) = \psi(x_1, \ldots, x_j, \ldots, x_i, \ldots, x_N)$$

Bose-Einstein condensation[1]:

$$\psi(x_1, \ldots, x_N) = \varphi_0(x_1)\varphi_0(x_2) \ldots \varphi_0(x_N)$$

[1] Bose. *Z. Phys.* **26** (1924)
Einstein. *Sitzungsber. Preuss. Akad. Wiss.* (1924)

The interacting Bose gas

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

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

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

ψ is not factorized anymore!

$$\psi(x_1, \ldots, x_N) \neq \varphi_0(x_1)\varphi_0(x_2)\ldots\varphi_0(x_N)$$

Correlations

Interactions introduce **correlations:**
the many-body wave function ψ is far from a product (it is a linear combination of elementary tensors).

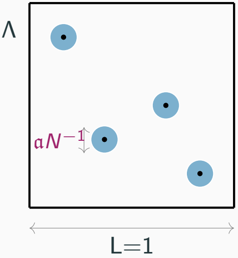
We need an efficient way to understand this.

Model for a dilute Bose gas: the Gross-Pitaevskii regime

N bosons in a box $\Lambda = [-L/2, L/2]^3$, described by

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

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



Dilute system: strong and short-range interactions for $N \to \infty$:

Range of the interaction $= N^{-1}$
Mean interparticle distance $= N^{-1/3}$

- It is a rescaling of lengths: $L \sim N$, $\rho \sim 1/N^2$. Simultaneous large volume and low density limit. (A spectral gap is introduced)

Ground state properties

We are interested in

- Ground state energy

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

- The **ground state vector** solves the eigenvalue problem (time independent Schrödinger equation)

$$H_N \psi_N = E_N \psi_N$$

- The **spectrum** $\sigma(H_N)$: excitation energies

Bose-Einstein Condensation

Consider the ground state vector ψ_N.

One-particle reduced density matrix (quantum marginal) associated to ψ_N:

$$\gamma_{\psi_N} := \mathrm{Tr}_{2,\ldots,N} |\psi_N\rangle\langle\psi_N|$$

$$\gamma_{\psi_N}(x,y) = \int dx_2 \ldots dx_N \psi_N(x, x_2, \ldots, x_N)\bar{\psi}_N(y, x_2, \ldots, x_N)$$

Definition: Bose-Einstein condensation

The one-particle reduced density matrix γ_{ψ_N} has a macroscopic eigenvalue.

Theorem

Let $V \in L^3(\mathbb{R}^3)$ positive, spherically symmetric and compactly supported. Then

$$1 - \langle \varphi_0, \gamma_{\psi_N} \varphi_0 \rangle \leq \frac{C}{N}$$

$\varphi_0 = 1$ *(for periodic b.c.) and represents the condensate wave function.*

The number of excitations over the condensate is bounded uniformly in N

Ground state energy and excitation spectrum [2]

Theorem

Let $V \in L^3(\mathbb{R}^3)$ positive, spherically symmetric and compactly supported. Then we have

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

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

The spectrum $\sigma(H_N - E_N)$ below a threshold ζ is given by

$$\sum_{p\in\Lambda_+^*} n_p\sqrt{|p|^4 + 16\pi\mathfrak{a}p^2} + \mathcal{O}(N^{-1/4}(1+\zeta^3))$$

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).

[2] Boccato, Brennecke, Cenatiempo, Schlein. *Acta Mathematica* **222** (2019)

Main idea of the proof

Idea: transform the interacting N-**body** Hamiltonian into N decoupled **one-body** Hamiltonians.

We construct 4 unitaries $\mathcal{U}_1\mathcal{U}_2\mathcal{U}_3\mathcal{U}_4 =: \mathcal{U}$ on different energy scales so that

$$\mathcal{U}^* H_N \mathcal{U} \simeq E_N + \mathbb{H}_\mathrm{B}$$

- The many-body Hamiltonian in second quantization is a quartic operator:

$$H_N = \sum_{p\in\Lambda_+^*} p^2 a_p^* a_p + \frac{1}{2N} \sum_{p,u,v\in\Lambda^*} \hat{V}(p/N)\, a_{u+p}^* a_{v-p}^* a_u a_v$$

- The effective Hamiltonian $\mathbb{H}_B$ instead is a one-body operator, i.e., quadratic in second quantization

$$\mathbb{H}_\mathrm{B} = \sum_{p\in\Lambda_+^*} \sqrt{|p|^4 + 16\pi\mathfrak{a}p^2}\, a_p^* a_p$$

Main idea of the proof: nonlinear theory

$\mathcal{U}_3$ extracts the contribution of terms higher than quadratic and renormalizes the quadratic part of the Hamiltonian. It implements a nonlinear transformation of creation and annihilation operators.

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

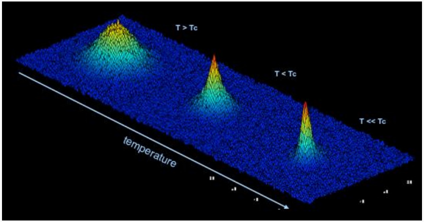
$$\left\|\psi_N - e^{i\omega}\mathcal{U}\Omega\right\|^2 \leq \frac{C}{\theta_2 - \theta_1} N^{-1/4}$$

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

Positive temperature systems

Positive temperature systems: the critical temperature

We need to consider temperature effects to be able to describe the phase transition.



Free energy with inverse temperature β:

$$F(N, \Lambda, \beta) = -\frac{1}{\beta} \ln \left(\mathrm{Tr}\, e^{-\beta H_N} \right).$$

- Analysis within the quasi-free approximation[3]
- Proof of condensation obtained in the Gross-Pitaevskii regime[4]

Remark: at the **critical temperature**, number of excited particles is order N

[3]Napiórkowski, Reuvers, Solovej. *Comm. Math. Phys.* **360** (2018)
[4]Deuchert, Seiringer. *Arch. Ration. Mech. Anal.* **236** (2020)

Grand canonical free energy

- Set of states

$$\mathcal{S}_N = \{\Gamma \in \mathcal{B}(\mathcal{F}) \mid \Gamma \geq 0, \mathrm{tr}\Gamma = 1, \mathrm{tr}[\mathcal{N}\Gamma] = N\},$$

- Free energy functional

$$\mathcal{F}(\Gamma) = \mathrm{tr}[\mathcal{H}_N\Gamma] - \frac{1}{\beta}S(\Gamma) \quad \text{with} \quad S(\Gamma) = -\mathrm{tr}[\Gamma \ln(\Gamma)]$$

- Free energy

$$F(\beta, N, L) = \min_{\Gamma \in \mathcal{S}_N} \mathcal{F}(\Gamma) = -\frac{1}{\beta} \ln\left(\mathrm{tr}[e^{-\beta(\mathcal{H}_N - \mu\mathcal{N})}]\right) + \mu N.$$

Chemical potential μ chosen so that the minimizer (Gibbs state)

$$G = \frac{e^{-\beta(\mathcal{H}_N - \mu\mathcal{N})}}{\mathrm{tr}[e^{-\beta(\mathcal{H}_N - \mu\mathcal{N})}]}$$

satisfies $\mathrm{Tr}[\mathcal{N}G] = N$.

Noninteracting Bose gas at positive temperature

N noninteracting bosons in a box $\Lambda = [-L/2, L/2]^3$

$$H_N = -\sum_{i=1}^{N} \Delta_{x_i} \qquad \text{acting on } L^2_s(\Lambda^N)$$

For large N, the asymptotic behavior of N_0, the number of particles in the condensate, is

$$\frac{N_0(N,\Lambda,\beta)}{N} \simeq \left[1 - \frac{\beta_c}{\beta}\right]_+ \qquad \text{with } \beta_c = \frac{1}{4\pi}\left(\frac{N}{L^3\zeta(3/2)}\right)^{-2/3}$$

Phase transition:

- for $\beta = \kappa\beta_c$, $\kappa \in (1,\infty)$, then $N_0 \sim N[1 - 1/\kappa]$
- for $\beta = \kappa\beta_c$, $\kappa \in (0,1)$, then $N_0 \sim 1$

The grand canonical free energy is

$$F_0(N,\Lambda,\beta) = \frac{1}{\beta}\sum_{p\in\Lambda^*} \ln\left(1 - e^{-\beta(p^2-\mu_0)}\right) + \mu_0 N = F_0^{\text{BEC}} + F_0^{+}$$

(by scaling $F_0(N,\Lambda,\beta) \sim \frac{1}{\beta^{5/2}} \sim N^{5/3}$)

Upper bound to the free energy,[5] interacting bosons

Theorem (B., Deuchert, Stocker, 2024)

Let $V \in L^3(\mathbb{R}^3)$ be positive, compactly supported, spherically symmetric.

Let μ_0 and $\rho_0(N,\Lambda,\beta)$ be the chemical potential and the expected condensate density of the ideal Bose gas. For $\beta = \kappa\beta_{\mathrm{c}}$ with $\kappa \in (1,\infty)$ we have

$$F(N,\Lambda,\beta) \leq F_0^+(N,\Lambda,\beta) + 4\pi\mathfrak{a}_N|\Lambda|\left(2\rho^2 - \rho_0^2(N,\Lambda,\beta)\right) + \frac{\ln(16\beta\mathfrak{a}_N/|\Lambda|)}{2\beta}$$

$$-\frac{1}{2\beta}\sum_{p\in\Lambda_+^*}\left[\frac{16\pi\mathfrak{a}_N\varrho_0(\beta,N,L)}{p^2} - \ln\left(1+\frac{16\pi\mathfrak{a}_N\varrho_0(\beta,N,L)}{p^2}\right)\right] + o\left(N^{2/3}L^{-2}\right),$$

where $\mathfrak{a}_N = \mathfrak{a}/N$ is the scattering length.

[5] Boccato, Deuchert, Stocker. *SIAM Journal on Mathematical Analysis* **56** (2024)

Remarks

- First two terms obtained in the canonical setting[6] and in the thermodynamic limit[7]
- $(2\beta)^{-1}\ln(16\beta\mathfrak{a}_N/|\Lambda|)$ related to particle number fluctuations in the BEC
- By restricting to quasi-free states: Bogoliubov free energy functional[8] predicts (by substituting $\int V$ with $8\pi\mathfrak{a}$):

$$f(\beta,\rho) = f_0(\beta,\rho) + 4\pi\mathfrak{a}(2\rho^2 - \rho_0^2) - \frac{16\sqrt{\pi}}{3\beta}(\mathfrak{a}\varrho_0)^{3/2} + o\big((\mathfrak{a}\varrho_0)^{3/2}\big)$$

- For very low temperatures ($T \sim \rho\mathfrak{a}$): correction to the Lee-Huang-Yang formula[9]

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[6] Deuchert, Seiringer. *Arch. Ration. Mech. Anal.* **236** (2020)
[7] Seiringer. *Commun. Math. Phys.* **279** (2008)
Yin. *J. Stat. Phys.* **141** (2010)
[8] Napiórkowski, Reuvers, Solovej. *Comm. Math. Phys.* **360** (2018)
[9] Haberberger, Hainzl, Nam, Seiringer, Triay. arXiv:2304.02405 (2023)
Haberberger, Hainzl, Schlein, Triay. arXiv:2405.03378 (2024)
Fournais, Girardot, Junge, Morin, Olivieri, Triay.

Idea of the proof

We define the quasi-free states with condensate

$$\Gamma_0 = \int_{\mathbb{C}} |z\rangle\langle z| \otimes G_{\mathrm{B}}(z) p(z) dz, \qquad \text{with} \quad G_{\mathrm{B}}(z) = \frac{\exp(-\beta \mathbb{H}^{\mathrm{Bog}})}{\mathrm{Tr}[\exp(-\beta \mathbb{H}^{\mathrm{Bog}})]}$$

- $\mathbb{H}^{\mathrm{Bog}}$ is the Bogoliubov Hamiltonian

$$\mathbb{H}^{\mathrm{Bog}} = \sum_{p \in \Lambda_+^*} p^2 a_p^* a_p + 4\pi \mathfrak{a}_N \varrho_0(\beta, N, L) \sum_{p \in \Lambda_+^*} \left[2 a_p^* a_p + (z/|z|)^2 a_p^* a_{-p}^* + (\bar{z}/|z|)^2 a_p a_{-p} \right]$$

- $|z\rangle = e^{z a_0^* - \bar{z} a_0} |\Omega\rangle$ is a coherent state and $p(z)$ is a probability distribution on $\mathbb{C}$

$$p(z) = \frac{\exp\left(-\beta\left(4\pi \mathfrak{a}_N L^{-3} |z|^4 - \widetilde{\mu} |z|^2\right)\right)}{\int_{\mathbb{C}} \exp\left(-\beta\left(4\pi \mathfrak{a}_N L^{-3} |z|^4 - \widetilde{\mu} |z|^2\right)\right) dz}$$

Γ_0 however does not describe correlations and justify universality

Idea of the proof

We write

$$\Gamma_0 = \sum_{\alpha=1}^{\infty} \lambda_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$$

Our trial state is

$$\Gamma = \sum_{\alpha=1}^{\infty} \lambda_\alpha |\phi_\alpha\rangle\langle\phi_\alpha|, \quad \text{where} \quad \phi_\alpha = \frac{(1+B)\psi_\alpha}{\|(1+B)\psi_\alpha\|}.$$

where correlations are described by the second-quantized operator

$$B = \frac{1}{2L^3} \sum_{p\in P_{\mathrm{H}},\ u,v\in P_{\mathrm{L}}} \eta_p\, a^*_{u+p} a^*_{v-p} a_u a_v$$

- particles with momenta in $P_{\mathrm{L}} = \{|p| \leq N^{1/3}\}$ are thermal excitations
- η_p, for $p \in P_{\mathrm{H}} = \{|p| \geq N^{1/2}\}$, describes two-body correlations

Correlations are not implemented unitarily. We need to estimate the entropy so to obtain[10]

$$S(\Gamma) = -\mathrm{tr}[\Gamma \ln(\Gamma)] \geq S(\Gamma_0) - \ln \mathrm{tr}\left(\sum_{\alpha'} |\phi_{\alpha'}\rangle\langle\phi_{\alpha'}| \; \Gamma\right)$$

and[11]

$$S(\Gamma) \geq \int_{\mathbb{C}} S(G_{\mathrm{B}}(z))p(z)dz + S(p) - CN^{-1+\delta},$$

where

$$S(p) = -\int_{\mathbb{C}} p(z)\ln(p(z))dz$$

[10] Seiringer: *The thermodynamic pressure of a dilute Fermi gas*, Commun. Math. Phys. **261** (2006)

[11] Berezin, *General concept of quantization*, Commun. Math. Phys. **40** (1975)
Lieb, *The classical limit of quantum spin systems*, Commun. Math. Phys. **31** (1973)

Lemma (Seiringer, 2006)

Let Γ be a density matrix on some Hilbert space with eigenvalues $\{\lambda_\alpha\}_{\alpha\in\mathbb{N}}$, let $\{P_\alpha\}_{\alpha\in\mathbb{N}}$ be a family of one-dimensional orthogonal projection (for which $P_{\alpha_1}P_{\alpha_2} = \delta_{\alpha_1,\alpha_2}P_{\alpha_1}$ need not necessarily be true), and define $\hat{\Gamma} = \sum_\alpha \lambda_\alpha P_\alpha$. Then we have

$$S(\hat{\Gamma}) \geq S(\Gamma) - \ln \mathrm{Tr}\left(\sum_\alpha P_\alpha \hat{\Gamma}\right).$$

[11] Seiringer: *The thermodynamic pressure of a dilute Fermi gas*, Commun. Math. Phys. **261** (2006)

Lemma

Let $\{G(z)\}_{z\in\mathbb{C}}$ *be a family of states on a Hilbert space, let* $p:\mathbb{C}\to\mathbb{R}$ *be a probability distribution and define the state*

$$\Gamma = \int_{\mathbb{C}} |z\rangle\langle z| \otimes G(z)p(z)dz.$$

Then we have

$$S(\Gamma) \geq \int_{\mathbb{C}} S(G(z))p(z)dz + S(p) \quad \textit{with} \quad S(p) = -\int_{\mathbb{C}} p(z)\ln(p(z))dz.$$

[11] Berezin, *General concept of quantization*, Commun. Math. Phys. **40** (1975)
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Ground state energy

- Ground state energy

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

- At leading order (i.e., order N): Gross-Pitaevskii functional

$$\lim_{N\to\infty} \frac{E_N}{N} = \min_{\substack{\varphi \in L^2(\Lambda), \\ \|\varphi\|_2 = 1}} \mathcal{E}_{GP}(\varphi)$$

  with

$$\mathcal{E}_{GP}(\varphi) = \int dx \left[|\nabla \varphi(x)|^2 + 4\pi \mathfrak{a} \, |\varphi(x)|^4 \right]$$

  The minimizer φ_0 of $\mathcal{E}_{GP}(\varphi)$ represents the condensate wave function.

- For periodic boundary conditions: $E_N = 4\pi \mathfrak{a} N + o(N)$
- **Universality**: the ground state energy depends on the interaction potential only through its scattering length ($\mathfrak{a} > 0$)

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- For periodic boundary conditions: $E_N = 4\pi \mathfrak{a} N + o(N)$
- **Universality**: the ground state energy depends on the interaction potential only through its scattering length ($\mathfrak{a} > 0$)

Interactions may connect all particles, but two-particle correlations dominate.

Bose Gas at the Critical Temperature

To gain information on the phase transition, we study the free energy in the thermodynamic limit:

$$f(\beta,\rho) = \lim_{\substack{N,L\to\infty \\ \rho=N/|\Lambda|}} -\frac{1}{\beta|\Lambda|} \ln\left(\mathrm{Tr} e^{-\beta H_N}\right)$$

Within the quasi-free approximation: *Bogoliubov Free Energy functional* [12], containing information on the critical temperature of the interacting system.

Beyond the quasi-free approximation: we aim at computing the free energy from the original many-body problem[13]. We expect

$$f(\beta,\rho) = f_0(\beta,\rho) + 4\pi\mathfrak{a}(2\rho^2 - \rho_0^2) - \frac{16\sqrt{\pi}}{3\beta}(\mathfrak{a}\varrho_0)^{3/2} + o\big((\mathfrak{a}\varrho_0)^{3/2}\big)$$

Useful technique at zero temperature.[14]

Current projects:

→ Obtain upper and lower bounds for $f(\beta,\rho)$

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[12] Napiórkowski, Reuvers, Solovej. *Comm. Math. Phys.* **360** (2018)
[13] Seiringer. *Commun. Math. Phys.* **279** (2008)
Yin. *J. Stat. Phys.* **141** (2010)
[14] Basti, Cenatiempo, Schlein. *Forum Math. Sigma* **9**(2021)

Quadratic effective Hamiltonian

Naive approach (Bogoliubov theory, 1947):

- Expand around the condensate
- Drop terms higher than quadratic → completely solvable problem

$$H_{\mathrm{B}} \simeq \frac{N}{2}\widehat{V}(0) + \sum_{p\in\Lambda_+^*}\left[p^2 + \widehat{V}(p/N)\right] a_p^* a_p + \frac{1}{2}\sum_{p\in\Lambda_+^*}\widehat{V}(p/N)(a_p^* a_{-p}^* + a_p a_{-p})$$

- Diagonalize through linear transformation of creation and annihilation operators (Bogoliubov transformation)

This approach cannot yield the scattering length (at best its first Born approximation).

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MAIN IDEA OF OUR PROOF: NONLINEAR THEORY

Extract the contribution of terms higher than quadratic → use it to RENORMALIZE THE QUADRATIC PART OF THE HAMILTONIAN through a nonlinear transformation of creation and annihilation operators.

Successive unitary transformations

$$e^{-B(\tau)} e^{-A} e^{-B(\eta)} U H_N U^* e^{B(\eta)} e^{A} e^{B(\tau)} = E_N + \mathbb{H}_{\mathrm{B}} + o(1)$$

$$A = \frac{1}{\sqrt{N}} \sum_{r\in P_H, v\in P_L} \eta_r \left[\sinh(\eta_v) b_{r+v}^* b_{-r}^* b_{-v}^* + \cosh(\eta_v) b_{r+v}^* b_{-r}^* b_v - \text{h.c.}\right]$$

Idea of the proof

- Quasi-free states with condensate ($H_{\rm B}$ is the Bogoliubov Hamiltonian!)

$$\Gamma_0 = |W(N_0^{1/2})\Omega\rangle\langle W(N_0^{1/2})\Omega| \otimes \frac{e^{-\beta H_{\rm B}}}{\mathrm{Tr}[e^{-\beta H_{\rm B}}]} = \sum_{\alpha=1}^{\infty} \lambda_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$$

does not describe correlations and justify universality

- A more precise trial state is

$$\Gamma = \sum_{\alpha=1}^{\infty} \lambda_\alpha |\phi_\alpha\rangle\langle\phi_\alpha|, \qquad \text{where} \qquad \phi_\alpha = \frac{e^B \psi_\alpha}{\|e^B \psi_\alpha\|}.$$

where correlations are described by the second-quantized operator

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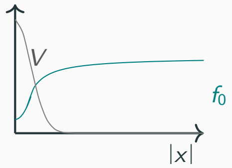
- η_p, for $p \in P_{\rm H} = \{|p| \geq N^{1/2}\}$, describes two-body correlations

Scattering length $\mathfrak{a}$: look at the two-body scattering process

Interactions may connect all particles, but two-particles correlations dominate.

Consider the **two-body problem** in the relative coordinates



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

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

Outside the range of V, f_0 is harmonic in the form:

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

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

To be interpreted as an effective range and strength of V.

Equivalently

$$\mathfrak{a} = \frac{1}{8\pi}\int_{\mathbb{R}^3} V(x)f_0(x)dx$$

Ground State Energy and BEC in the Neumann box[15]

Theorem (B., Seiringer 2022)

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

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

for a constant $C > 0$.

2. Every low-energy wave function exhibits Bose-Einstein condensation.

Corollary (Thermodynamic Limit)
Let V satisfy the same assumptions as above and λ small enough. Then there exists a constant $C > 0$ such that

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

[15] C. Boccato, S. Seiringer. *Ann. Henri Poincaré* **24** (2023)

The Thermodynamic Limit of the Bose gas

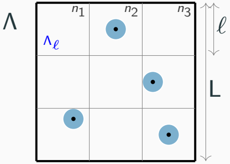
Mathematically harder, physically crucial model for the description of phase transitions: **thermodynamic limit**.

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

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

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

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 conditions needed

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

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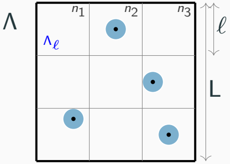
Difficulty in the thermodynamic limit: absence of an energy gap!

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

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

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 conditions needed

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

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

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

Ground State Energy and BEC in the Neumann box[16]

Theorem (B., Seiringer 2023)

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

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

for a constant $C > 0$.

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

$$\langle \psi_n, H_{n,\ell}\psi_n \rangle \leq E^{Neu}(n,\ell) + \zeta$$

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

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

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

[16] Boccato, Seiringer. *Ann. Henri Poincaré* **24** (2023)

Ground State Energy and BEC in the Neumann box[17]

Theorem (B., Seiringer 2022)

1. 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 $C > 0$.

2. Every low-energy wave function exhibits Bose-Einstein condensation.

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

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

[17] C. Boccato, S. Seiringer. *Ann. Henri Poincaré* **24** (2023)

The Thermodynamic limit

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

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Remarks:

- Result for condensation and $E^{\mathrm{Neu}}(n,\ell)$ is optimal: logarithmic error term is specific of Neumann boundary conditions
- Bound for $e(\rho)$ is not optimal. 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
- Optimality reached with different localization method, modified kinetic energy[18], leading to the Lee-Huang-Yang formula:
  $e(\rho) = 4\pi\rho\mathfrak{a}\left[1 + \frac{128}{15\sqrt{\pi}}(\rho\mathfrak{a}^3)^{1/2} + o((\rho\mathfrak{a}^3)^{1/2})\right]$
- Reaching the precision of the spectrum allows[19] to compute a correction to the LHY formula for very low temperature ($T \leq \rho\mathfrak{a}(\rho\mathfrak{a}^3)^{-\varepsilon}$)

[18] Fournais, Solovej. *Invent. math.* **232** (2021)
[19] Haberberger, Hainzl, Nam, Seiringer, Triay. Preprint (2023)

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
  $$\left| e_{N,N} - 4\pi\mathfrak{a}N \right| \leq C\Big(1 + \ln(N)\Big).$$
  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
  ([Fournais21],
  periodic b.c.: [Adhikari,Brennecke,Schlein21],[Brennecke,Caporaletti,Schlein21])
  In particular, reaching the precision of the spectrum allows to compute a correction to the LHY formula for very low temperature ($T \leq \rho\mathfrak{a}(\rho\mathfrak{a}^3)^{-\varepsilon}$)
  [Haberberger,Hainzl,Nam,Seiringer,Triay23]

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]
- $e^B = \exp\left[\frac{1}{2}\int_{\Lambda_1\times\Lambda_1} dxdy\, \eta(x,y)\, a_x^* a_y^* - \text{h.c.}\right]$ 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 $C_{n,\ell} = 4\pi\mathfrak{a}\frac{n^2}{\ell}\Big(1 + \mathcal{O}\Big(\frac{\mathfrak{a}}{\ell}\ln(\ell/\mathfrak{a})\Big)\Big)$

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

- We need information on the minimizer to be used in the many-body analysis.

Remark. For periodic boundary conditions and for $\mathbb{R}^3$ with trapping potential: the problem naturally decouples in relative coordinates and center of mass and $\eta^{\text{Trap}}(x,y) \simeq -n(1-f_0(x-y))\varphi_0^2(x+y)$

Proof: Control of Neumann Boundary Effects

Now:

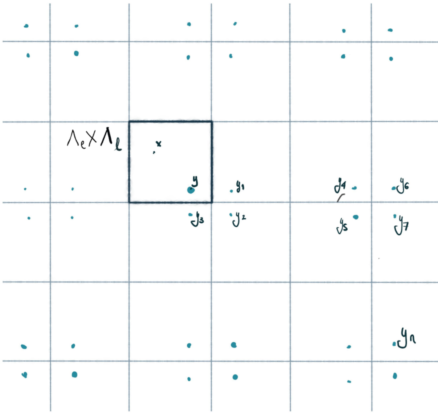
- six-dimensional problem, the minimizer f not explicitly known
- method of image charges to express Green functions

$$\big(-\Delta_x + \varepsilon\big) G_\varepsilon(x,y) = \delta_y(x)$$

for $x, y \in \Lambda_\ell \times \Lambda_\ell$

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

$$f(x) = \int_\Omega dy\, G_\varepsilon(x,y)\big(\lambda_\ell + \varepsilon - \kappa V(y)\big) f(y)$$



Proof: Control of Neumann Boundary Effects

Some properties of the minimizer:

$$\lambda_\ell := \inf_{\substack{g \in H^1(\Lambda_\ell \times \Lambda_\ell) \\ \|g\|_2 = 1}} F[g] = \frac{8\pi\mathfrak{a}}{\ell^3}\Big(1 + \mathcal{O}\Big(\frac{\mathfrak{a}}{\ell}\ln(\ell/\mathfrak{a})\Big)\Big)$$

Pointwise estimates

- $|1 - \ell^3 f(x,y)| \leq C\kappa \left(\frac{1}{|x-y|+1}\right)$
- $|\nabla_{x+y} f(x,y)| \leq C\kappa\ell^{-3}\big(d\big(\frac{x+y}{2}\big)^{5/3} + 1\big)^{-1}$,

  where $d(x)$ is the distance of x to the boundary of the box Λ_ℓ.
  (The last estimate is crucial for the control of linear terms.)