Semiclassical approximation and critical temperature shift for weakly interacting trapped bosons

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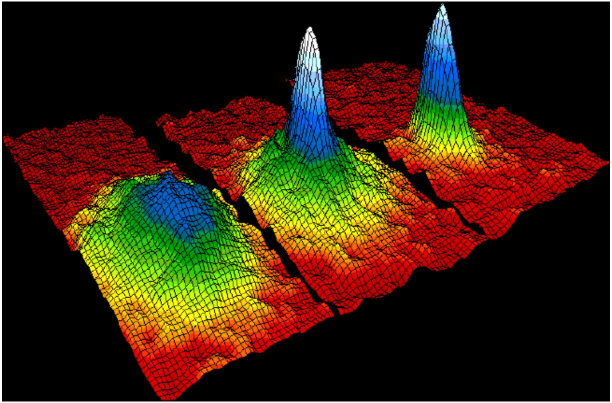
BEC – An experimental breakthrough



Nobel Prize in Physics 2001: Cornell, Ketterle and Wieman

Schrödinger equation

Fundamental description by **Schrödinger equation:**

$$H_N \Psi_N(x_1, ..., x_N) = E_N \Psi_N(x_1, ..., x_N),$$

with **Hamiltonian**

$$H_N = \sum_{i=1}^{N} \left(-\Delta_i + \frac{x_i^2}{4} \right) + \sum_{1 \leq i < j \leq N} v_N(x_i - x_j).$$

In experiments: $N = 10^2 - 10^6 \Rightarrow$ **Curse of dimensionality.**

Behavior of the system at zero temperature (MF case)

Mean-field limit: When $v_N(x) = N^{-1} v(x)$ we have

$$\Psi_N(x_1, ..., x_N) \approx \prod_{i=1}^{N} \Phi^{\mathrm{H}}(x_i) \quad \text{and} \quad E_N \approx N E^{\mathrm{H}},$$

where

$$\mathcal{E}^{\mathrm{H}}(\Phi) = \int_{\mathbb{R}^3} \overline{\Phi(x)} \left(-\Delta_i + \frac{x_i^2}{4} \right) \Phi(x) \, \mathrm{d}x + \frac{1}{2} \int_{\mathbb{R}^6} v(x-y) |\Phi(x)|^2 |\Phi(y)|^2 \, \mathrm{d}(x, y)$$

and Φ^{H} is the **unique minimizer** of $\mathcal{E}^{\mathrm{H}}$.

References:

- Lewin, Nam, Rougerie, Adv. Math. **254**, 570 (2014)
- Grech, Seiringer, Comm. Math. Phys. **322** (2), 559 (2013)

Behavior of the system at zero temperature (GP case)

Gross–Pitaevskii limit: When $v_N(x) = N^2 v(Nx)$ we have

$$\Psi_N(x_1, ..., x_N) \approx \prod_{i=1}^{N} \Phi^{\mathrm{GP}}(x_i) \quad \text{and} \quad E_N \approx N E^{\mathrm{GP}},$$

where

$$\mathcal{E}^{\mathrm{GP}}(\Phi) = \int_{\mathbb{R}^3} \overline{\Phi(x)} \left(-\Delta_i + \frac{x_i^2}{4} \right) \Phi(x) \, \mathrm{d}x + 4\pi a \int_{\mathbb{R}^3} |\Phi(x)|^4 \, \mathrm{d}(x)$$

and Φ^{GP} is the **unique minimizer** of $\mathcal{E}^{\mathrm{GP}}$.

References:

- Lieb, Seiringer, Yngvason, Phys. Rev. A **61**, 043602 (2000)
- Boccato, Brennecke, Cenatiempo, Schlein, Acta Math. **222**, 219 (2019)

Free energy and Gibbs variational principle

Let

$$\mathcal{S}_N = \left\{ \Gamma \in \mathcal{B}\left(L^2_{\mathrm{sym}}\left(\mathbb{R}^{3N}\right)\right) \,\middle|\, \Gamma \geq 0 \text{ and } \operatorname{Tr}\Gamma = 1 \right\},$$

denote the set of ***N*-particle states**.

The **free energy** can be characterized by the **Gibbs variational principle**

$$F(T,N) = \inf_{\Gamma \in \mathcal{S}_N} \underbrace{\{\operatorname{Tr}[H_N \Gamma] - TS(\Gamma)\}}_{=\mathcal{F}(\Gamma)} \quad \text{with} \quad \underbrace{S(\Gamma) = -\operatorname{Tr}[\Gamma \ln(\Gamma)]}_{\text{Von Neumann entropy}}.$$

The unique minimizer of $\mathcal{F}$ is the **Gibbs state**

$$G_N = \frac{e^{-H_N/T}}{\mathrm{Tr}\left[e^{-H_N/T}\right]}.$$

1-pdm and BEC

The **one-particle reduced density matrix (1-pdm)** of an N-particle state $\Gamma_N \in \mathcal{S}_N$ can be defined via its integral kernel

$$\gamma^{(1)}_{\Gamma_N}(x, y) = N \int \Gamma_N(x, q_1, ..., q_{N-1}; y, q_1, ..., q_{N-1}) \, \mathrm{d}(q_1, ..., q_{N-1}).$$

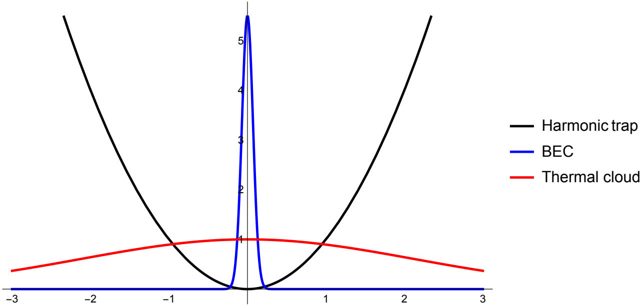
It is the quantum version of the **one-particle marginal** of an N-particle probability distribution.

A sequence of states Γ_N (indexed by the particle number) displays **Bose–Einstein condensation (BEC)** if

$$\liminf_{N\to\infty} \sup_{\|\phi\|_{L^2(\mathbb{R}^3)}} \frac{\langle \phi, \gamma^{(1)}_{\Gamma_N} \phi \rangle}{N} > 0.$$

Scales for ideal Bose gas as $N \to \infty$

Critical temperature of ideal gas: $T_\mathrm{c}(0) = \left(\frac{N}{\zeta(3)}\right)^{1/3}$.



- Free energy $F(T, N) \sim TN \sim N^{4/3}$
- Length scale density condensate: 1
- Length scale density thermal cloud: $N^{1/6}$

Scales for the interacting model as $N \to \infty$

Hamiltonian:

$$H_N = \sum_{i=1}^{N} \left(-\Delta_i + \frac{x_i^2}{4} \right) + \frac{1}{N^{2/3}} \sum_{1 \leq i < j \leq N} v\left(N^{-1/6}(x_i - x_j) \right)$$

Temperature:

$$T \lesssim T_{\mathrm{c}}(N) = \left(\frac{N}{\zeta(3)} \right)^{1/3}.$$

Scales for the interacting model as $N \to \infty$

Hamiltonian:

$$H_N = N^{1/3} \left\{ \sum_{i=1}^{N} \left(-\hbar^2 \Delta_i + \frac{x_i^2}{4} \right) + \frac{1}{N} \sum_{1 \leq i < j \leq N} v\left(x_i - x_j\right) \right\}$$

with $\hbar = N^{-1/3}$.

Temperature:

$$T \lesssim T_{\mathrm{c}}(N) = \left(\frac{N}{\zeta(3)} \right)^{1/3} .$$

The semiclassical mean-field limit

Hamiltonian:

$$H_N = \sum_{i=1}^{N} \left(-\hbar^2 \Delta_i + \frac{x_i^2}{4} \right) + \frac{1}{N} \sum_{1 \leq i < j \leq N} v\left(x_i - x_j\right)$$

with $\hbar = N^{-1/3}$.

Temperature:

$$T \lesssim T_{\mathrm{c}}(1) = \left(\frac{1}{\zeta(3)} \right)^{1/3}.$$

The semiclassical mean-field limit

Hamiltonian:

$$H_N = \sum_{i=1}^{N} \left(-\hbar^2 \Delta_i + \frac{x_i^2}{4} \right) + \frac{1}{N} \sum_{1 \leq i < j \leq N} v\left(x_i - x_j\right)$$

with $\hbar = N^{-1/3}$.

Temperature:

$$T \lesssim T_{\mathrm{c}}(1) = \left(\frac{1}{\zeta(3)} \right)^{1/3}.$$

Goal: Prove BEC and quantify how the critical temperature depends on the interaction potential v.

Heuristics

MF interaction $v_N(x) = N^{-1}v(x)$ implies

$$\mathrm{Tr}\left[\sum_{1\leq i<j\leq N} v(x_i - x_j)\Gamma_N\right] \approx \frac{1}{2}\int_{\mathbb{R}^6} v(x-y)\varrho_{\Gamma_N}(x)\varrho_{\Gamma_N}(y)\,\mathrm{d}(x,y)$$

where $\varrho_{\Gamma_N}(x) = \gamma^{(1)}_{\Gamma_N}(x,x)$. $\Rightarrow$ Expect that energy can be expressed as a nonlinear function of **1-pdm**.

Semiclassical parameter $-\hbar^2\Delta$ implies that for "nice" functions f:

$$\mathrm{tr}\left[f\left(-\hbar^2\Delta + V(x)\right)\right] = \int_{\mathbb{R}^6} f\left(p^2 + V(q)\right)\frac{\mathrm{d}(p,q)}{(2\pi\hbar)^3} + O\left(\hbar^{-2}\right).$$

Effective model: The semiclassical free energy functional

Let $g \in [0,1]$ and $\gamma(p,q) \geq 0$ be such that

$$\int_{\mathbb{R}^6} \gamma(p,q) \frac{\mathrm{d}(p,q)}{(2\pi)^3} + g = 1.$$

The **semiclassical free energy functional** is defined by

$$\mathcal{F}^{\mathrm{sc}}(\gamma, g) = \int_{\mathbb{R}^6} \left(p^2 + \frac{q^2}{4} \right) \gamma(p,q) \frac{\mathrm{d}(p,q)}{(2\pi)^3} - T S^{\mathrm{sc}}(\gamma) + \frac{1}{2} \int_{\mathbb{R}^6} v(q-q') \varrho(q) \varrho(q') \, \mathrm{d}(q,q'),$$

with the **density** $\varrho(q) = \int_{\mathbb{R}^3} \gamma(p,q) \frac{\mathrm{d}p}{(2\pi)^3} + g\delta(q)$ and the **entropy**

$$S^{\mathrm{sc}}(\gamma) = -\int_{\mathbb{R}^6} \left(\gamma \ln(\gamma) - (1+\gamma) \ln(1+\gamma) \right)(p,q) \frac{\mathrm{d}(p,q)}{(2\pi)^3}.$$

Selected literature

Semiclassical MF limit for fermions

- Fournais, Lewin, Solovej, Calc. Var. Partial Differ. Equ. pp. 57 (2018)
- Lewin, Madsen, Triay, J. Math. Phys. **60**, 091901 (2019)

Dynamics of fermions in semiclassical MF limit

- Benedikter, Porta, Schlein, Commun. Math. Phys. 331, 1087 (2014)
- Benedikter, Jaksic, Porta, Saffirio, Schlein, Commun. Pure Appl. Math. 69, 2250 (2014)

Semiclassical MF limit and Gross–Pitaevskii limit for bosons

- Baumgartner, Narnhofer, Thirring, Annals of Physics **150**, 373 (1983)
- Deuchert, Seiringer, Yngvason, Commun. Math. Phys. **368**, 723 (2019)

Main results (non-technical version)

Theorem (Characterization of BEC and MF shift of T_{c})

The **full quantum mechanical model** *displays BEC if and only if the semiclassical free energy functional displays BEC.*

Denote by $g(T)$ **the condensate fraction** *of the* **interacting Gibbs state***. Assume that* v *is replaced by* λv *with* $0 < \lambda \leq 1$*. Then there exists* $\lambda_0 > 0$ *such that for all* $\lambda \leq \lambda_0$ *we have the following statements*

- *There exits a* **unique** *critical temperature* $T_{\mathrm{c}}(\lambda)$ *such that* $g(T) = 0$ *for* $T \geq T_{\mathrm{c}}(\lambda)$ *and* $g(T) > 0$ *for* $T < T_{\mathrm{c}}(\lambda)$*.*
- *The* **critical temperature** *satisfies* $T_{\mathrm{c}}(\lambda) = T_{\mathrm{c}}(0) - \lambda\Theta + O(\lambda^2)$ *with*

$$\Theta = \frac{1}{24\pi^3} \int_{\mathbb{R}^6} \gamma_0^2(p,x) \exp\left(\frac{1}{T_{\mathrm{c}}(0)} \left(p^2 + \frac{x^2}{4} \right) \right) (v * \varrho_0(0) - v * \varrho_0(x)) \, \mathrm{d}(p,x).$$

1st stage of simplification: Hartree free energy functional

We define the set of **1-pdms**

$$\mathcal{D}_N^{\mathrm{H}} = \left\{ \gamma \in \mathcal{B}\left(L^2\left(\mathbb{R}^3\right)\right) \;\middle|\; \gamma \geq 0,\ \mathrm{tr}[\gamma] = N \right\}.$$

For an operator $\gamma \in \mathcal{D}_N^{\mathrm{H}}$ the **Hartree free energy functional** is defined by

$$\mathcal{F}^{\mathrm{H}}(\gamma) = \mathrm{tr}\left[\left(-\hbar^2 \Delta + \frac{x^2}{4} + \frac{1}{2N} v * \varrho_\gamma\right)\gamma\right] - Ts(\gamma),$$

where $\varrho_\gamma(x) = \gamma(x,x)$ and where the **bosonic entropy** is defined by

$$s(\gamma) = -\mathrm{tr}\left[\gamma \ln(\gamma) - (1+\gamma)\ln(1+\gamma)\right].$$

Finally, γ^{H} denotes the **unique minimizer** of $\mathcal{F}^{\mathrm{H}}$ and

$$F^{\mathrm{H}}(T,N) = \mathcal{F}^{\mathrm{H}}\left(\gamma^{\mathrm{H}}\right).$$

Main results: 1st stage of simplification (technical version)

Theorem (Validity of Hartree theory)

In the limit $N \to \infty$ with $T \lesssim T_{\mathrm{c}}(0)$ we have

$$\left|F(T,N) - F^{\mathrm{H}}(T,N)\right| \lesssim N^{1/3}.$$

Moreover, for any **sequence of states** $\Gamma_N \in \mathcal{S}_N$ *with 1-pdm* γ_N *and*

$$\left|\mathcal{F}(\Gamma_N) - F^{\mathrm{H}}(T,N)\right| \leq \delta$$

for some $\delta > 0$, we have

$$\left\|\gamma_{\Gamma_N} - \gamma^{\mathrm{H}}\right\|_1 \lesssim N^{5/6}(1+\delta)^{1/4}.$$

Main results: 2nd stage of simplification (technical version)

For a given 1-pdm γ we define the **Husimi function** by

$$m_\gamma(p,q) = \langle \ell^\hbar_{p,q}, \gamma \ell^\hbar_{p,q} \rangle \quad \text{with} \quad \ell^\hbar_{p,q} = \hbar^{-3/4} \ell((x-q)/(\hbar^{1/2})) e^{ipx/\hbar}.$$

Theorem (Validity of the semiclassical approximation)

In the limit $N \to \infty$ with $T \lesssim T_c(0)$ we have

$$\left| F^{\mathrm{H}}(T,N) - N F^{\mathrm{sc}}(T) \right| \lesssim N^{2/3}.$$

Moreover, let P^{H} be the **projection** *onto the eigenspace of the* **largest eigenvalue** *of γ^{H} and define $Q^{\mathrm{H}} = 1 - P^{\mathrm{H}}$. We then have*

$$\left| N^{-1} \mathrm{tr}\left[P^{\mathrm{H}} \gamma^{\mathrm{H}} \right] - g^{\mathrm{sc}} \right| \lesssim N^{-1/9+\sigma} \quad \textit{as well as}$$

$$\int_{\mathbb{R}^6} \left| m_{Q^{\mathrm{H}} \gamma^{\mathrm{H}}}(p,x) - \gamma^{\mathrm{sc}}(p,x) \right| \mathrm{d}(p,x) \lesssim N^{-1/9+\sigma}$$

for any $\sigma > 0$.

Remarks

- **Optimal** error of bounds for free energies.
- **Zero temperature** limit included.
- All results remain true if $\mathcal{F}$ is minimized over general states on the Fock space with **fluctuating particle number**. In particular, we have **equivalence of ensembles** up to the given accuracy.
- **Power law traps** behaving as $|x|^s$ for $|x| \to \infty$ and some $s > 0$ can be treated with our approach.

Quantifying coercivity of semiclassical free energy

For $f(x) = x\ln(x) - (1+x)\ln(1+x)$ and two nonnegative functions $a, b \in L^1(\mathbb{R}^6)$ we define the **semiclassical relative entropy**

$$\mathcal{S}^{\mathrm{sc}}(a,b) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^6}\Big[f(a(p,x)) - f(b(p,x)) \\ - f'(b(p,x))\,(a(p,x)-b(p,x))\Big]\,\mathrm{d}(p,x).$$

Lemma (Quantitative coercivity)

There exists a constant $C > 0$ such that for any two nonnegative functions $a, b \in L^1(\mathbb{R}^6)$ we have

$$\mathcal{S}^{\mathrm{sc}}(a,b) \geq C\,\frac{\left(\int_{\mathbb{R}^6}|a(p,x)-b(p,x)|\,\mathrm{d}(p,x)\right)^2}{\int_{\mathbb{R}^6}(a(p,x)+b(p,x))\,(1+b(p,x))\,\mathrm{d}(p,x)}.$$

Quantifying coercivity of quantum free energy

For $f(x) = x\ln(x) - (1+x)\ln(1+x)$ and two nonnegative trace-class operators a, b we define the **bosonic relative entropy**

$$\mathcal{S}(a,b) = \mathrm{tr}\Big[f(a) - f(b) - f'(b)\,(a-b)\Big].$$

Lemma (Quantitative coercivity)

There exists a constant $C > 0$ such that for any two nonnegative trace-class operators a, b we have

$$\mathcal{S}\,(a,b) \geq C\,\frac{(\|a-b\|_1)^2}{\|1+b\|\mathrm{tr}[a+b]}.$$

Equivalence of ensembles for Hartree free energy

For $\Gamma \in \mathcal{S}_N$ we define the **canonical version** of the Hartree free energy by

$$\mathcal{F}^{\mathrm{H,c}}(\Gamma) = \mathrm{Tr}\left[\mathrm{d}\Upsilon\left(h + \frac{1}{2} v_N * \varrho_\Gamma\right)\Gamma\right] - TS(\Gamma)$$

and denote

$$F^{\mathrm{H,c}}(T,N) = \inf_{\Gamma \in \mathcal{S}_N} \mathcal{F}^{\mathrm{H,c}}(\Gamma).$$

Lemma (Equivalence of ensembles)

We have the bound

$$F^{\mathrm{H}}(T,N) \leq F^{\mathrm{H,c}}(T,N) \leq F^{\mathrm{H}}(T,N) + T\left(1 + \ln\left(1+N\right)\right).$$