Quantitative Derivation of the Gross-Pitaevskii Equation

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Gas of N Bosons

- Wave function

$$\psi_N \in L^2(\mathbb{R}^{3N}),$$

symmetric w. r. t. permutation of the N particles.

- Hamiltonian in Gross-Pitaevskii scaling, repulsive interaction $V \geq 0$:

$$H_N^{\text{trap}} = \sum_{j=1}^{N} \Big(-\Delta_{x_j} + V_{\text{trap}}(x_j) \Big) + \underbrace{\sum_{i<j}^{N} N^2 V(N(x_i - x_j))}_{\text{rare but strong collisions}}.$$

Physical phenomenon: Bose-Einstein condensation

At very low temperatures (i. e. when approximately in the ground state):

$$\psi_N \simeq \underbrace{\varphi \otimes \ldots \otimes \varphi}_{N \text{ factors}}, \quad \text{with } \varphi \in L^2(\mathbb{R}^3).$$

Ground State Properties

- Energy (Lieb-Seiringer-Yngvason 2000): Define ground state energy

$$E_N := \min_{\substack{\psi_N \in L^2_{\text{symm}}(\mathbb{R}^{3N}) \\ \|\psi_N\|=1}} \langle \psi_N, H_N^{\text{trap}} \psi_N \rangle.$$

Define the Gross-Pitaevskii energy functional on $L^2(\mathbb{R}^3)$

$$\mathcal{E}_{\text{GP}}(\varphi) = \int_{\mathbb{R}^3} \mathrm{d}x \left(|\nabla \varphi|^2 + V_{\text{trap}} |\varphi|^2 + 4\pi a_0 |\varphi|^4 \right),$$

a_0: scattering length, constant depending on interaction potential V.

Then

$$\lim_{N\to\infty} \frac{E_N}{N} = \min_{\substack{\varphi \in L^2(\mathbb{R}^3) \\ \|\varphi\|=1}} \mathcal{E}_{\text{GP}}(\varphi).$$

Ground State Properties

- Bose-Einstein condensation (Lieb-Seiringer 2002):

  Let γ_{ψ_N} be the one-particle reduced density of the ground state ψ_N:

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

  Let $\varphi_{\mathrm{GP}} \in L^2(\mathbb{R}^3)$ be the minimizer of the GP functional $\mathcal{E}_{\mathrm{GP}}$.

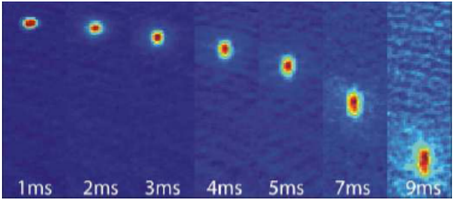
  Then (in trace norm)

  $$\gamma_{\psi_N} \longrightarrow |\varphi_{\mathrm{GP}}\rangle\langle\varphi_{\mathrm{GP}}| \qquad (N \to \infty).$$

  (We consider this the rigorous meaning of $\psi_N \simeq \varphi_{\mathrm{GP}} \otimes \ldots \otimes \varphi_{\mathrm{GP}}$.)

Dynamics of Bose-Einstein Condensate

- Experiment: Turn off the trap and watch evolution: e. g. cond-mat/0503044



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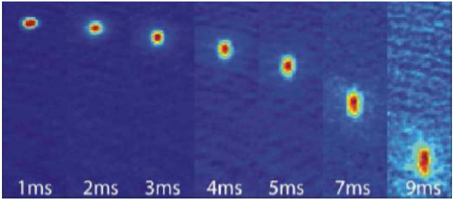

- Mathematics: Solve time-dependent Schrödinger equation

$$i\partial_t \psi_{N,t} = H_N \psi_{N,t}, \qquad \psi_{N,0} \simeq \varphi \otimes \ldots \otimes \varphi,$$

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

As $N \simeq 10^3 - \ldots$, it is difficult to make predictions.

Effective Evolution Equation

- Approximate dynamics (Erdös-Schlein-Yau 2006–2008, Pickl 2010):

  Assume bounded energy per particle

$$\frac{\langle \psi_{N,0}, H_N \psi_{N,0} \rangle}{N} \leq C$$

  and condensation into an orbital $\varphi \in H^1(\mathbb{R}^3)$:

$$\gamma_{\psi_{N,0}} \longrightarrow |\varphi\rangle\langle\varphi| \quad (N \to \infty).$$

  Let $\gamma_{\psi_{N,t}}$ be the reduced density associated with the solution of the Schrödinger equation

$$\psi_{N,t} = e^{-iH_N t} \psi_{N,0}.$$

  Let $\varphi_t \in L^2(\mathbb{R}^3)$ be the solution of the Gross-Pitaevskii equation

$$i\partial_t \varphi_t = -\Delta \varphi_t + 8\pi a_0 |\varphi_t|^2 \varphi_t \quad \text{with initial data } \varphi_0 = \varphi.$$

  Then

$$\gamma_{\psi_{N,t}} \longrightarrow |\varphi_t\rangle\langle\varphi_t| \quad (N \to \infty).$$

Rate of Convergence using Coherent States?

What is the rate of convergence, $\operatorname{tr}\left|\gamma_{\psi_{N,t}} - |\varphi_t\rangle\langle\varphi_t|\right| \leq \frac{C(t)}{N^\alpha}$?

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In analogy with mean-field systems (Rodnianski-Schlein 2009), one can try coherent states approach:

- Embed in bosonic Fock space:

$$\mathcal{F} = \bigoplus_{n=0}^{\infty} L^2(\mathbb{R}^{3n}) = \mathbb{C} \oplus L^2(\mathbb{R}^3) \oplus \ldots \oplus L^2(\mathbb{R}^{3N}) \oplus \ldots$$

$$\mathcal{H}_N = \int \mathrm{d}x \nabla_x a_x^* \nabla_x a_x + \frac{1}{2}\int \mathrm{d}x\mathrm{d}y\, N^2 V(N(x-y)) a_x^* a_y^* a_y a_x.$$

- Study evolution of coherent states

$$\psi_{N,0} = W(\sqrt{N}\varphi)\Omega \in \mathcal{F},$$

where $\|\varphi\| = 1$ guarantees $\langle \psi_{N,0}, \mathcal{N}\psi_{N,0}\rangle = N$.

Rate of Convergence using Coherent States?

- If coherence approximately preserved by time evolution:

$$e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)\Omega \simeq W(\sqrt{N}\varphi_t)\Omega \;\Leftrightarrow\; \underbrace{W^*(\sqrt{N}\varphi_t)e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)}_{=:\,U_N(t)\text{ fluctuation dynamics}}\Omega \simeq \Omega,$$

  where φ_t would solve the Gross-Pitaevskii equation.
- By an elementary calculation

$$\operatorname{tr}\left|\gamma_{\psi_{N,t}} - |\varphi_t\rangle\langle\varphi_t|\right| \leq \frac{C}{N^{1/2}}\langle\Omega, U_N^*(t)\mathcal{N}U_N(t)\Omega\rangle.$$

- So it is sufficient to prove

$$\langle\Omega, U_N^*(t)\mathcal{N}U_N(t)\Omega\rangle \leq C(t) \qquad \text{(r.h.s. independent of } N\text{).} \qquad (*)$$

- Problem: We find that $(*)$ does not hold.

Heuristically, $e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)\Omega$ develops singular correlations, which are not captured by approximate evolution $W(\sqrt{N}\varphi_t)\Omega$.

Bogoliubov Transformation Approach

Solution: Implement correlations by a Bogoliubov transformation.

- Let $f : \mathbb{R}^3 \to \mathbb{C}$ solve the zero-energy two-particle scattering equ.

$$\left(-\Delta + \frac{1}{2}V\right) f = 0, \quad \text{where} \;\; f(x) \to 1 \text{ as } |x| \to \infty.$$

- Define a Bogoliubov transformation

$$T(k_t) = \exp\left(\frac{1}{2}\int \mathrm{d}x\mathrm{d}y\, k_t(x;y) a_x^* a_y^* - \text{h.c.}\right),$$

$$k_t(x;y) = N\Big(f(N(x-y)) - 1\Big)\varphi_t(x)\varphi_t(y).$$

- Add short-scale correlations: New initial data

$$\psi_{N,0} = W(\sqrt{N}\varphi)\,T(k_0)\Omega.$$

Bogoliubov Transformation Approach

- By elementary calculation

$$\operatorname{tr}\left|\gamma_{\psi_{N,t}} - |\varphi_t\rangle\langle\varphi_t|\right| \leq \frac{C}{N^{1/2}} \langle \Omega, \tilde{U}_N^*(t) \mathcal{N} \tilde{U}_N(t) \Omega \rangle$$

with the modified fluctuation dynamics

$$\tilde{U}_N(t) := T^*(k_t) W^*(\sqrt{N}\varphi_t) e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi) T(k_0).$$

- If we can show

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle \Omega, \tilde{U}_N^*(t) \mathcal{N} \tilde{U}_N(t) \Omega \rangle \leq C \langle \Omega, \tilde{U}_N^*(t) \mathcal{N} \tilde{U}_N(t) \Omega \rangle \qquad (*)$$

then by Gronwall's lemma

$$\langle \Omega, \tilde{U}_N^*(t) \mathcal{N} \tilde{U}_N(t) \Omega \rangle \leq C e^{Kt}.$$

- To prove $(*)$ (or something similar) we calculate the time derivative and identify cancellations between Schrödinger evolution and Gross-Pitaevskii evolution.

Theorem (B-Oliveira-Schlein 2012, arXiv:1208.0373)

Let $\|\varphi\|_{L^2(\mathbb{R}^3)} = 1$. *Let* $V \geq 0$, *i. e. repulsive interaction.*
Let $\gamma_{\psi_{N,t}}$ *be the reduced density of* $\psi_{N,t} = e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi) T(k_0)\Omega$.
Let φ_t *solve the Gross-Pitaevskii equation*

$$i\partial_t \varphi_t = -\Delta\varphi_t + 8\pi a_0 |\varphi_t|^2 \varphi_t, \quad \textit{with initial data } \varphi_0 = \varphi.$$

Then

$$\operatorname{tr}\left|\gamma_{\psi_{N,t}} - |\varphi_t\rangle\langle\varphi_t|\right| \leq \frac{const.}{\sqrt{N}} e^{c_1 e^{c_2 |t|}}.$$

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$$\operatorname{tr}\left|\gamma_{\psi_{N,t}} - |\varphi_t\rangle\langle\varphi_t|\right| \leq \frac{const.}{\sqrt{N}} e^{c_1 e^{c_2|t|}}.$$

1. Instead of the vacuum Ω, we can use $\omega_N \in \mathcal{F}$ with $\langle \omega_N, (\mathcal{N} + \frac{1}{N}\mathcal{N}^2 + \mathcal{H}_N)\omega_N\rangle \leq C$ (where C is independent of N).
2. If $\|\varphi_t\|_{H^4} \leq C$, then $e^{c_1|t|}$ instead of $e^{c_1 e^{c_2|t|}}$.
3. The initial data $W(\sqrt{N}\varphi)T(k_0)\omega$ has 'correct energy': $\langle W(\sqrt{N}\varphi)T(k_0)\omega, \mathcal{H}_N W(\sqrt{N}\varphi)T(k_0)\omega\rangle = N\mathcal{E}_{\mathrm{GP}}(\varphi) + \mathcal{O}(\sqrt{N})$.
4. We can project on some states with fixed number of particles. Work in progress: Does this cover e. g. the ground state in a trap?

$\frac{\mathrm{d}}{\mathrm{d}t}\langle\Omega, \tilde{U}_N^*(t)\mathcal{N}\tilde{U}_N(t)\Omega\rangle$: Coherent Part Cancellation

The generator $\mathcal{L}_N(t)\tilde{U}_N(t) = i\partial_t\tilde{U}_N(t)$ is found to be

$$\begin{aligned}\mathcal{L}_N(t) &= \cancel{i\frac{dT_t^*}{\mathrm{d}t}}T_t + T_t^*\left[i\frac{\mathrm{d}W_t^*}{\mathrm{d}t}W_t + W_t^*\mathcal{H}_N W_t\right]T_t \\ &\simeq T_t^*\Big[a^{\#}(\sqrt{N}i\dot{\varphi}_t) + \sqrt{N}a^{\#} + a^{\#}a^{\#} \\ &\qquad + \frac{1}{\sqrt{N}}a^{\#}a^{\#}a^{\#} + \frac{1}{N}a^{\#}a^{\#}a^{\#}a^{\#}\Big]T_t.\end{aligned}$$

Then we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\tilde{U}_N(t)\Omega, \mathcal{N}\tilde{U}_N(t)\Omega\rangle = \langle\tilde{U}_N(t)\Omega, [i\mathcal{L}_N(t), \mathcal{N}]\tilde{U}_N(t)\Omega\rangle.$$

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$$\simeq T_t^*\Big[a^\#(\sqrt{N}i\dot{\varphi}_t) + \sqrt{N}a^\# + a^\# a^\# + \frac{1}{\sqrt{N}}a^\# a^\# a^\# + \frac{1}{N}a^\# a^\# a^\# a^\#\Big]T_t.$$

Then we obtain

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Use the approximate Gross-Pitaevskii equation

$$i\partial_t\varphi_t = -\Delta\varphi_t + (N^3 f(N.)V(N.) * |\varphi_t|^2)\varphi_t$$

to get partial cancellation

$$a^\#(\sqrt{N}i\dot{\varphi}_t) + \sqrt{N}a^\# = \sqrt{N}a^\#\Big(N^3(1-f(N.))V(N.) * |\varphi_t|^2\varphi_t\Big).$$

$\frac{\mathrm{d}}{\mathrm{d}t}\langle\Omega, \tilde{U}_N^*(t)\mathcal{N}\tilde{U}_N(t)\Omega\rangle$: Bogoliubov Part Cancellation

After the coherent part cancellation, we know have

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\tilde{U}_N(t)\Omega, \mathcal{N}\tilde{U}_N(t)\Omega\rangle \simeq$$

$$\langle\tilde{U}_N(t)\Omega, T_t^* \underbrace{\left[\sqrt{N}a^\#(..) + a^\# a^\# + \frac{1}{\sqrt{N}}a^\# a^\# a^\# + \frac{1}{N}a^\# a^\# a^\# a^\#\right]}_{\text{normalordered}} T_t\tilde{U}_N(t)\Omega\rangle$$

Bogoliubov transf. $T_t^* a_x T_t \simeq a_x + a^*(k_t(\cdot, x))$ destroys normalorder.
Normalordering of cubic terms creates linear terms. $\rightsquigarrow$ Cancellations:

$$T_T^*\left(a^\# + a^\# a^\# a^\#\right) T_t = \text{linear} + \text{cubic,not normalordered}$$

$$= \cancel{\text{linear} - \text{linear}} + \text{cubic,normalordered.}$$

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Normalordering of quartic terms produces quadratic terms.
Scattering equation then implies cancellations among quadratics. □

Summary

- In Bose-Einstein condensates, short-scale correlations are important.
- Correlations can be implemented on length scale $1/N$ using a Bogoliubov transformation.
- We obtain the Gross-Pitaevskii equation with an error of order $N^{-1/2}$.