Quantitative derivation of the Gross-Pitaevskii equation

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This talk is about

- Mathematics of many-body quantum mechanics.
- Dynamics of Bose-Einstein condensates.
- Effective description.
- How the Gross-Pitaevskii PDE emerges.

Plan

1. Introduction
2. Theorem
3. Outline of the proof

Wave function for N Bosonic particles

- N-particle wave function:

$$\psi_{N,t}(x_1, \dots, x_N) \in \mathbb{C}, \qquad x_1, \dots, x_N \in \mathbb{R}^3, \qquad t \in \mathbb{R}.$$

- Square-integrable and normalized:

$$\psi_{N,t} \in L^2(\mathbb{R}^{3N}) \simeq L^2(\mathbb{R}^3) \otimes \cdots \otimes L^2(\mathbb{R}^3),$$

$$\int_{\mathbb{R}^{3N}} |\psi_{N,t}|^2 = 1.$$

- $|\psi_{N,t}|^2$ probability density.
- $\psi_{N,t}$ is symmetric in each pair of variables $x_1, \dots, x_N$.

Density operator

N-particle

$$\gamma_{\psi_{N,t}} = |\psi_{N,t}\rangle\langle\psi_{N,t}| \quad \text{on} \quad L^2(\mathbb{R}^{3N}).$$

$$\operatorname{Tr}\gamma_{\psi_{N,t}} = 1, \qquad \|\gamma_{\psi_{N,t}}\| := \operatorname{Tr}|\gamma_{\psi_{N,t}}|.$$

1-particle

$$\gamma^{(1)}_{\psi_{N,t}} = \operatorname{Tr}_{2\to N}\gamma_{\psi_{N,t}} \quad \text{on} \quad L^2(\mathbb{R}^3).$$

$\operatorname{Tr}_{2\to N}$ Integrate out $N-1$ variables of the integral kernel of $\gamma_{\psi_{N,t}}$.

$\gamma^{(1)}_{\psi_{N,t}}$ 1-particle marginal: Plays the role of 1-particle wave-function.

Bose-Einstein condensation

In experiments, since 1995 (Nobel Prize 2001)

Trapped cold ($T \sim 10^{-9} K$) dilute gas of $N \sim 10^3$ Bosons.

Heuristically

$$\psi_{N,t}(x_1, \ldots, x_N) \simeq \prod_{j=1}^{N} \varphi_t(x_j) \quad \text{where} \quad \varphi_t \in L^2(\mathbb{R}^3).$$

$$\gamma_{\psi_{N,t}} \simeq |\varphi_t\rangle\langle\varphi_t| \otimes \cdots \otimes |\varphi_t\rangle\langle\varphi_t|.$$

Mathematically

$$\mathrm{Tr}\, \left| \gamma^{(1)}_{\psi_{N,t}} - |\varphi_t\rangle\langle\varphi_t| \right| = 0.$$

Model (which is realistic)

Quantum Hamiltonian in the Gross-Pitaevskii regime

$$H_N^{\rm trap} = \sum_{j=1}^{N} \big(-\Delta_{x_j} + V_{\rm trap}(x_j)\big) + \frac{1}{N}\sum_{i<j}^{N} N^3 V(N(x_i - x_j)),$$

$$V_{\rm trap}(y) = |y|^2 \quad \text{and} \quad V \geq 0,\ V(x) = V(|x|),\ \text{compact supp.}$$

Very heuristically

$$\frac{1}{N} N^3 V(N\,\cdot\,) \sim \frac{1}{N}\delta(\cdot) \qquad \text{for large } N$$

models rare but strong collisions.

Mean-field character

Expect:

- Approximate factorization of condensate $\psi_{N,t}$ for large N

  $\Longrightarrow$

- Approximate independence of particles

  $\Longrightarrow$ (by the Law of Large Numbers)

Potential experienced by the jth particle

$$= \frac{1}{N}\sum_{i<j}^{N} W(x_i - x_j) \simeq \int dy\, W(x_j - y)|\varphi_t(y)|^2$$

$$= (W * |\varphi_t|^2)(x_j).$$

$\Longrightarrow$

- Should have

$$i\partial_t\varphi_t = (-\Delta + V^{\mathrm{trap}})\varphi_t + W * |\varphi_t|^2\varphi_t.$$

Correlations between particles

Non-interacting gas

Condensate state: product state, no correlations.

Weakly interacting gas

Leading order 2-particle correlation can be modeled by the solution f to the zero-energy scattering equation:

$$\Big(-\Delta + \frac{1}{2}V\Big)f = 0 \quad \text{with} \quad f(x) \to 1 \text{ as } |x| \to \infty.$$

- $f(x) \simeq 1 - a|x|^{-1}$ as $|x| \to \infty$ where $a := (8\pi)^{-1} \int fV$.
- $f(N\cdot)$ solves zero-energy scatt. eqn. with $V \rightsquigarrow N^2 V(N\cdot)$.

Time-independent theory

Ground state energy per particle

Lieb, Seiringer and Yngvason (2000):

$$\lim_{N\to\infty} \frac{1}{N} \inf \operatorname{spec} H_N^{\mathrm{trap}} = \min\{\mathcal{E}_{GP}(\varphi) \,|\, \varphi \in L^2(\mathbb{R}^3),\ \|\varphi\| = 1\}$$

where

$$\mathcal{E}_{GP}(\varphi) = \int \Big(|\nabla\varphi|^2 + V_{\mathrm{trap}}|\varphi|^2 + 4\pi a |\varphi|^4 \Big).$$

The minimizer φ_{GP} of $\mathcal{E}_{GP}$ obeys

$$\operatorname{Tr}\Big|\, \gamma_{\psi_N^{\mathrm{gs}}} - |\varphi_{GP}\rangle\langle\varphi_{GP}| \,\Big| \to 0 \quad \text{as} \quad N \to \infty.$$

Gross-Pitaevskii character

Recall

$$i\partial_t \varphi_t = (-\Delta + V^{\mathrm{trap}})\varphi_t + W * |\varphi_t|^2 \varphi_t .$$

Observe that (formally)

$$N^3 V(N\,\cdot) \to b\,\delta(\cdot) \qquad \text{where} \qquad b = \int V .$$

Taking into account correlations

$$N^3 V(N\,\cdot) f(N\,\cdot) \to 8\pi a\,\delta(\cdot) \quad \text{where} \quad a = (8\pi)^{-1} \int f\, V .$$

Time evolution of condensates

Initial data

$\psi_{N,0} = \theta_N =$ condensate state with correlations (not a product)

We construct initial data θ in Fock space:

$$\theta = \theta_0 \oplus \theta_1 \oplus \cdots \oplus \theta_N \oplus \cdots \in \bigoplus_{n \geq 0} L^2_{sym}(\mathbb{R}^{3n})$$

with N particles in average:

$$\langle \theta, \mathcal{N} \theta \rangle \simeq N.$$

$\mathcal{N}$ number of particles operator on Fock space:

$$(\mathcal{N}\theta)_n = n\, \theta_n.$$

Initial data

Modified coherent state

$$\theta = W(\sqrt{N}\varphi)T(k)\Omega.$$

$$\begin{aligned} \Omega &= \text{finite particle state (e.g. Vac} = 1 \oplus 0 \oplus 0 \oplus \cdots) \\ T(k) &= \text{Bogoliubov transformation (models correlations)} \\ k(x,y) &= -N(1 - f(N(x-y)))\varphi(x)\varphi(y) \end{aligned}$$

$$\langle \theta, \mathcal{N}\theta \rangle \simeq N.$$

Coherent state

$$\xi = W(\sqrt{N}\varphi)\,\text{Vac} = e^{-N\|\varphi\|^2/2}\left[1 \oplus \varphi \oplus \frac{\varphi^{\otimes 2}}{\sqrt{2!}} \oplus \frac{\varphi^{\otimes 3}}{\sqrt{3!}} \oplus \cdots\right]$$

$$\langle \xi, \mathcal{N}\xi \rangle = N.$$

Schrödinger equation on Fock space

Condensate state reached; traps are turned off

$$H_N = H_N^{\mathrm{trap}} \text{ with } V_{\mathrm{trap}} \equiv 0.$$

Hamiltonian on Fock space

$$\mathcal{H} = H_0 \oplus H_1 \oplus \cdots \oplus H_N \oplus \cdots$$

Time evolution is observed

$$\begin{cases} i\partial_t \Psi_t = \mathcal{H}\Psi_t \\ \Psi_0 = W(\sqrt{N}\varphi)T(k)\Omega \end{cases} \qquad \text{as} \quad N \to \infty.$$

Theorem [Benedikter, Oliveira, Schlein, CPAM 2014]

$V \in L^1 \cap L^3(\mathbb{R}^3, (1+|x|^6)dx)$, $V \geq 0$, $\varphi \in H^4(\mathbb{R}^3)$,
$\langle \Omega, (\mathcal{N} + 1 + \mathcal{N}^2/N + \mathcal{H})\Omega \rangle \leq C$.
Consider the solution

$$\Psi_t = e^{-i\mathcal{H}t} W(\sqrt{N}\varphi) T(k)\Omega.$$

Let

$$\Gamma^{(1)}_{N,t} = \text{one-particle reduced density operator of } \Psi.$$

Then

$$\text{Tr} \left| \Gamma^{(1)}_{N,t} - |\varphi_t\rangle\langle\varphi_t| \right| \leq C \exp(C \exp(C|t|)) \frac{1}{\sqrt{N}}$$

for all t and N, where φ_t solves (time-dep. Gross-Pitaevskii eqn.)

$$i\partial_t \varphi_t = -\Delta\varphi_t + 8\pi a |\varphi_t|^2 \varphi_t \qquad \text{with} \qquad \varphi_0 = \varphi,$$

$a > 0$ (scattering length of V).

Remarks

Based on

- Hepp '74, Ginibre–Velo '79, Rodnianski–Schlein '09,. . .

Previous results

- Spohn '80, Erdös–Schlein–Yau '06, Pickl '10,. . .
  (no rate of convergence)

Other results

- Adami–Golse–Teta '07, Grillakis–Machedon–Margetis '10,. . .

Large bibliography. . .

Look at arXiv:1208.0373 (or Benedikter's review arXiv:1404.4568) and Schlein's notes arXiv:1210.1603.

Outline of the proof

Creation and annihilation operators on Fock space

$f \in L^2(\mathbb{R}^3)$ and ψ in Fock space:

$$(a^*(f)\psi)_n(x_1, \dots, x_n) = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} f(x_j)\psi_{n-1}(x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_n),$$

$$(a(f)\psi)_n(x_1, \dots, x_n) = \sqrt{n+1} \int dy\, f(y)\psi_{n+1}(y, x_1, \dots, x_n).$$

Commutation relations

$$[a(f), a^*(g)] = \langle f, g \rangle, \qquad [a(f), a(g)] = [a^*(f), a^*(g)] = 0.$$

Operator-valued distributions

$a_x, \ a_x^*, \ x \in \mathbb{R}^3$:

$$a^*(f) = \int dx\, f(x) a_x^* \qquad \text{and} \qquad a(f) = \int dx\, \overline{f(x)} a_x .$$

Commutation relations

$$[a_x, a_y^*] = \delta(x - y) \qquad \text{and} \qquad [a_x, a_y] = [a_x^*, a_y^*] = 0.$$

Operators on Fock space

$$\mathcal{N} = \int dx\, a_x^* a_x,$$

$$\mathcal{H} = \int dx\, \nabla_x a_x^* \nabla_x a_x + \frac{1}{2N} \int dxdy\, N^3 V(N(x-y)) a_x^* a_y^* a_y a_x,$$

$$W(f) = \exp(a^*(f) - a(f)),$$

$$T(k) = \exp\left[\frac{1}{2}\int dxdy\, k(x,y) a_x^* a_y^* - \frac{1}{2}\int dxdy\, \overline{k(x,y)} a_x a_y\right].$$

Conjugation formulas

Weyl operator $W(f)$:

$$W^*(f)a_x^*W(f) = a_x^* + \overline{f(x)}, \qquad W^*(f)a_xW(f) = a_x + f(x),$$

Bogoliubov transformation $T(k)$:

$$T^*(k)a_x^*T(k) = \int dy\,\big(\cosh(k)(y,x)a_y^* + \sinh(k)(y,x)a_y\big).$$

Fluctuation dynamics

Integral kernel of $\Gamma^{(1)}_{N,t} - |\varphi_t\rangle\langle\varphi_t|$:

$$\Gamma^{(1)}_{N,t}(x,y) - \overline{\varphi_t(y)}\varphi_t(x) = \frac{\langle \Psi_t, a_y^* a_x \Psi_t\rangle}{\langle \Psi_t, \mathcal{N}\Psi_t\rangle} - \overline{\varphi_t(y)}\varphi_t(x).$$

We want to approximate

$$\Psi_t = e^{-i\mathcal{H}t} W(\sqrt{N}\varphi) T(k)\Omega \simeq W(\sqrt{N}\varphi_t) T(k_t)\Omega.$$

Define

$$U_N(t) = T^*(k_t) W^*(\sqrt{N}\varphi_t) e^{-i\mathcal{H}t} W(\sqrt{N}\varphi) T(k).$$

We find the estimate

$$\operatorname{Tr}\left| \Gamma^{(1)}_{N,t} - |\varphi_t\rangle\langle\varphi_t| \right| \leq \frac{C}{\sqrt{N}} \langle U_N(t)\Omega, \mathcal{N} U_N(t)\Omega\rangle.$$

Controlling the number of fluctuations

We are left to prove that $\langle \mathcal{N} \rangle_t := \langle U_N(t)\Omega, \mathcal{N} U_N(t)\Omega \rangle \leq C$ where

$$i\partial_t U_N(t) = \mathcal{L}_N(t) U_N(t).$$

Explicitly (using shorthands)

$$\mathcal{L}_N(t) = (i\partial T_t^*) T_t + T_t^* [(i\partial_t W_t^*) W_t + W_t^* \mathcal{H} W_t] T_t.$$

To use Grönwall's Lemma, we compute

$$\frac{d}{dt} \langle \mathcal{N} \rangle_t = \langle [i\mathcal{L}_N(t), \mathcal{N}] \rangle_t \qquad \text{(notation } \langle \cdot \rangle_t \text{)}$$

The term $(i\partial T_t^*) T_t$ in $\mathcal{L}_N(t)$ is harmless. Let us focus on the second term.

Cancellations I

- We have

$$(i\partial_t W_t^*)W_t = -\sqrt{N}\big[a^*(i\partial_t\varphi_t) + a(\cdots)\big] + \text{irrelevant}$$

- For $W_t^*\mathcal{H}W_t$ we use the conjugation formulas and expand. We get terms:

linear in a, a^*	formally $O(N^{1/2})$.
quadratic	$O(1)$.
cubic	$O(N^{-1/2})$.
quartic	$O(N^{-1})$.

- There is no complete cancellation of linear terms in $W_t^*\mathcal{H}W_t$ with $(i\partial_t W_t^*)W_t$. We are left with

$$\sqrt{N}\, a^*\big[(N^3V(N\cdot)(1-f(N\cdot)) * |\varphi_t|^2)\varphi_t\big) + \sqrt{N}a(\cdots). \quad (*)$$

Conjugation by T_t gives cubic terms, not normal-ordered. Normal-ordering gives linear terms which cancel (*).

Cancellations II

- Conjugation by T_t gives quartic terms, not normal-ordered. Normal-ordering and using zero-energy scatt. eqn. cancels quadratic terms.
- We are able to prove

$$[i\mathcal{L}_N(t), \mathcal{N}] \leq \mathcal{H} + C_t(\mathcal{N}^2/N + \mathcal{N} + 1).$$

- Since $\mathcal{L}_N(t) = \mathcal{H} +$ other terms, we are able to prove

$$\mathcal{H} \leq C_t(\mathcal{L}_N(t) + \mathcal{N}^2/N + \mathcal{N} + 1). \qquad (**)$$

Thus

$$[i\mathcal{L}_N(t), \mathcal{N}] \leq C_t(\mathcal{L}_N(t) + \mathcal{N}^2/N + \mathcal{N} + 1).$$

Grönwall

- Control $\langle \mathcal{N}^2/N\rangle_t$ by $\langle(\mathcal{N}+1)^2/N\rangle_{t=0}$ and $\langle \mathcal{N}\rangle_t$. We get

$$\frac{d}{dt}\langle \mathcal{N}\rangle_t \leq C_t\langle \mathcal{N}+1+\mathcal{L}_N(t)\rangle_t + C_t\langle(\mathcal{N}+1)^2/N\rangle_{t=0}.$$

- To close the scheme, we need to bound $\langle \mathcal{L}_N(t)\rangle_t$. We find

$$\frac{d}{dt}\langle \mathcal{L}_N(t)\rangle_t \leq C_t\langle \mathcal{N}+1+\mathcal{L}_N(t)\rangle_t + C_t\langle(\mathcal{N}+1)^2/N\rangle_{t=0}.$$

Thus, for D_t to be fixed,

$$\frac{d}{dt}\langle D_t(\mathcal{N}+1)+\mathcal{L}_N(t)\rangle_t \leq C_t\langle D_t(\mathcal{N}+1)+\mathcal{L}_N(t)\rangle_t + C_t\langle(\mathcal{N}+1)^2/N\rangle_{t=0}.$$

Continuing Grönwall...

- Thus, by Grönwall's Lemma,

$$\langle D_t(\mathcal{N}+1)+\mathcal{L}_N(t)\rangle_t \le C\exp(C\exp(Ct))\langle \mathcal{L}_N(0)+\mathcal{N}+1+\mathcal{N}^2/N\rangle_{t=0}.$$

- But there exists $C_t > 0$ such that (using (**) and positivity)

$$\mathcal{L}_N(t)+C_t(\mathcal{N}^2/N+\mathcal{N}) \ge 0.$$

Choosing $D_t = C_t + 1$, we obtain

$$\langle \mathcal{N}\rangle_t \le \langle \mathcal{L}_N(t)+D_t(\mathcal{N}^2/N+N)\rangle_t \le C\exp(C\exp(Ct)).$$

□

Thank you for your attention!