Effective equations for two-component Bose-Einstein Condensates

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Introduction: An example from classical physics

Kinetic theory of a gas of N particles

- **Microscopic theory.** Newtons's equations for the trajectories $(x_1, x_2, \dots, x_N)$ of N particles:

$$\begin{aligned} \dot{x}_j &= v_j \\ \dot{v}_j &= -\sum_{i \neq j}^{N} \nabla V(x_j - x_i). \end{aligned}$$

Here $x_j = x_j(t)$ and V is a short range potential.

Introduction: An example from classical physics

Kinetic theory of gas of N particles

- **Macroscopic theory.** Boltzmann's equation for the density of particles $f = f(x, v, t)$ at time t:

$$\partial_t f + v \cdot \nabla_x f = \int_{\mathbb{R}^3} dv' \int_{S^2} d\omega \, B(v - v', \omega) \times [f(x, v_{out}, t) f(x, v'_{out}, t) - f(x, v, t) f(x, v', t)].$$

Incoming particles with v and v' collide. Outcoming with

$$v_{out} = v + \omega \cdot (v' - v)\omega,$$
$$v'_{out} = v' - \omega \cdot (v' - v)\omega.$$

Here $B(v - v', \omega)$ is proportional do the cross section.

Introduction: An example from classical physics

Kinetic theory of gas of N particles

- **Scaling limit.** Boltzmann's equation becomes correct in the Boltzmann-Grad limit:

$$\text{density } \rho \to 0, \qquad N \to \infty, \qquad N\rho^2 = \text{const.}$$

- **Mathematical derivation.** Lanford ('75) proved: In the Boltzmann-Grad limit, Boltzmann's equation follows from Newton's equation (at least for short times).
- **Extensions.** Later, to a larger class of potentials V.

As the above example illustrates

Typical steps in a derivation program

- **Microscopic theory.** Physical law; Many degrees of freedom; Arbitrary initial data; Detailed solutions: impractical or not very useful.
- **Scaling limit.** Appropriate regime of parameters.
- **Macroscopic theory.** Statistical description; Effective theory (or equation); Restricted initial data (possibly).
- **Mathematical results.** Detailed analysis of the problem.
- **Extensions.** Less regular interactions; More general initial data.

An example from quantum theory

- **Thomas-Fermi theory for large atoms and molecules.** Neutral quantum system of N electrons and M nuclei. Ground state energy:

$$E(N) = \inf \langle \psi, H_N \psi \rangle.$$

For large N:

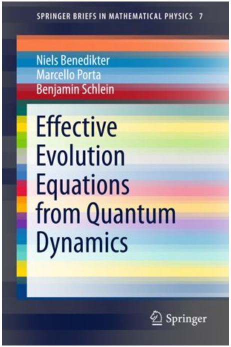
$$E(N) \approx E_{TF}(N) = \inf \{\mathcal{E}_{TF}(\rho) \,|\, \int dx \,|\rho(x)| = N\},$$

where $\mathcal{E}_{TF}(\rho)$ is the Thomas-Fermi functional.

Theorem (Lieb-Simon '77). Approximation becomes exact as $N \to \infty$.

Main background reference for this talk

N. Benedikter, M. Porta and B. Schlein (2016).



The references for the work that we mention can be found there.

Plan

1. Introduction (completed)
2. One-component Bose gases (easier to explain)
3. Two-component Bose gases (similar)

Wave function for N Bosonic particles

- N-particle wave function:

$$\psi_t(x_1, \ldots, x_N) \in \mathbb{C}, \qquad x_1, \ldots, x_N \in \mathbb{R}^3, \qquad t \in \mathbb{R}.$$

- Square-integrable and normalized:

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

$$\int_{\mathbb{R}^{3N}} |\psi_t|^2 = 1.$$

- $|\psi_t|^2$ probability density.
- ψ_t is symmetric in each pair of variables $x_1, \ldots, x_N$.

Density operator

N-particle

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

$$\operatorname{Tr}\gamma_{\psi_t} = 1, \qquad \|\gamma_{\psi_t}\| := \operatorname{Tr}|\gamma_{\psi_t}|.$$

1-particle

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

$\operatorname{Tr}_{2\to N}$ Integrate out $N-1$ variables of the integral kernel of γ_{ψ_t}.

$\gamma^{(1)}_{\psi_t}$ 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

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

$$\gamma_{\psi_t} \simeq |\varphi_t\rangle\langle\varphi_t| \otimes \cdots \otimes |\varphi_t\rangle\langle\varphi_t|.$$

Mathematically

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

Models

Quantum Hamiltonian in the mean-field regime

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

Quantum Hamiltonian in the Gross-Pitaevskii regime

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

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

Basic problems

Ground state energy

$$E(N) = \inf \langle \psi, H_N^{\mathrm{trap}} \psi \rangle = \inf \operatorname{spec} H_N^{\mathrm{trap}}.$$

Initial value problem

$$H_N = (H_N^{\mathrm{trap}} \text{ with } V_{\mathrm{trap}} = 0)$$

$$\begin{aligned} i\partial_t \psi_t &= H_N \psi_t \\ \psi_{t=0} &= \psi. \end{aligned}$$

In the mean-field regime

Expect:

- Approximate factorization of condensate ψ_t for large N

  $\implies$

- Approximate independence of particles

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

$$\text{Potential experienced by the } j\text{th particle}$$

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

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

$\implies$ (separation of variables)

- The Schrödinger equation should factor into products

$$i\partial_t \varphi_t = -\Delta \varphi_t + V * |\varphi_t|^2 \varphi_t.$$

In the Gross-Pitaevskii regime

Very heuristically

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

models rare but strong collisions.

In this talk, we focus on mean-field.

We may skip the slides about Gross-Pitaevskii.

Time-independent theory

Mean-field regime

Ground state energy per particle:

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

where

$$\mathcal{E}_{MF}(\varphi) = \int \Big(|\nabla\varphi|^2 + V_{\mathrm{trap}}|\varphi|^2 + \frac{1}{2}(V * |\varphi|^2)|\varphi|^2 \Big).$$

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

$$\operatorname{Tr}\Big|\, \gamma^{(1)}_{\psi^{\mathrm{gs}}} - |\varphi_{MF}\rangle\langle\varphi_{MF}|\, \Big| \to 0 \quad \text{as} \quad N \to \infty.$$

(Modern proof: Lewin-Nam-Rougerie ('14))

Time-independent theory

Gross-Pitaevski regime

Ground state energy per particle:

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

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

$$\operatorname{Tr} \Big| \, \gamma^{(1)}_{\psi^{\mathrm{gs}}} - |\varphi_{GP}\rangle\langle\varphi_{GP}| \, \Big| \to 0 \quad \text{as} \quad N \to \infty.$$

(Lieb-Seiringer-Yngvason ('00))

Fock space

$$\mathcal{F} = \mathbb{C} \oplus \bigoplus_{n \geq 1} L^2_{sym}(\mathbb{R}^{3n}).$$

State $\psi \in \mathcal{F}$:

$$\psi = \psi_0 \oplus \psi_1 \oplus \psi_2 \oplus \cdots \oplus \psi_N \oplus \cdots$$

Vacuum state $\Omega \in \mathcal{F}$:

$$\Omega = 1 \oplus 0 \oplus 0 \oplus \cdots$$

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

$$(\mathcal{N}\psi)_n = n\,\psi_n.$$

For example $\langle \Omega, \mathcal{N}\Omega \rangle = 0$.

Time evolution of condensates — Initial data

Product state in $L^2_{\text{sym}}(\mathbb{R}^{3N})$

$$\psi_{t=0} = \varphi^{\otimes N}.$$

Coherent state in $\mathcal{F}$

$$\begin{aligned}\Psi_{t=0} &= W(\sqrt{N}\varphi)\,\Omega \\ &= e^{-N\|\varphi\|^2/2}\left[1 \oplus \varphi \oplus \frac{\varphi^{\otimes 2}}{\sqrt{2!}} \oplus \frac{\varphi^{\otimes 3}}{\sqrt{3!}} \oplus \cdots \oplus \frac{\varphi^{\otimes N}}{\sqrt{N!}} \oplus \cdots\right]\end{aligned}$$

We have

$$\langle \Psi_{t=0}, \mathcal{N}\Psi_{t=0}\rangle = N.$$

Schrödinger equation on Fock space

Condensate state reached – Traps are turned off

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

Hamiltonian on Fock space

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

Time evolution is observed

$$\begin{cases} i\partial_t \Psi_t = \mathcal{H}\Psi_t \\ \Psi_{t=0} = \Psi \end{cases} \quad \text{as} \quad N \to \infty.$$

Mean-field regime

Theorem (Rodnianski-Schlein, CMP '09)
Consider the solution

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

Let

$$\Gamma_t^{(1)} = \text{one-particle reduced density operator of } \Psi_t.$$

Then

$$\operatorname{Tr} \left| \, \Gamma_t^{(1)} - |\varphi_t\rangle\langle\varphi_t| \, \right| \leq C \exp(C|t|) \frac{1}{N}$$

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

$$i\partial_t \varphi_t = -\Delta\varphi_t + (V * |\varphi_t|^2)\varphi_t \qquad \text{with} \qquad \varphi_0 = \varphi.$$

Gross-Pitaevskii regime

Theorem (Benedikter–de Oliveira–Schlein, CPAM '14)]
Consider the solution

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

Let

$$\Gamma_t^{(1)} = \text{one-particle reduced density operator of } \Psi_t.$$

Then

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

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).

Two-component condensate

State space

$$L^2(\mathbb{R}^{3N_1}) \otimes L^2(\mathbb{R}^{3N_2}).$$

Hamiltonian (in the mean-field regime)

$$H_{N_1,N_2} = h_{N_1} \otimes I + I \otimes h_{N_2} + \mathcal{V}_{N_1,N_2}$$

where

$$h_{N_p} = \sum_{j=1}^{N_p} -\Delta_{x_j} + \frac{1}{N_p} \sum_{i<j}^{N_p} V_p(x_i - x_j)$$

and

$$\mathcal{V}_{N_1,N_2} = \frac{1}{N_1 + N_2} \sum_{j=1}^{N_1} \sum_{k=1}^{N_2} V_{12}(x_j - y_k).$$

Two-component condensate

(1,1)-particle density operator

$$\gamma^{(1,1)} = \mathrm{Tr}_{N_1-1,N_2-1}|\psi_t\rangle\langle\psi_t| \quad \text{on} \quad L^2(\mathbb{R}^3)\otimes L^2(\mathbb{R}^3).$$

We embed our model into

$$\mathcal{F}\otimes\mathcal{F}.$$

Hamiltonian

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{V}.$$

Initial data

$$\Psi_{t=0} = W(\sqrt{N_1}u)\Omega\otimes W(\sqrt{N_2}v)\Omega.$$

Two-component condensate

Theorem (de Oliveira-Michelangeli, RMP '19)
Consider the solution

$$\Psi_t = e^{-i\mathcal{H}t}[W(\sqrt{N_1}u)\Omega \otimes W(\sqrt{N_2}v)\Omega].$$

Let $\Gamma_t^{(1,1)}$ = (1,1)-particle reduced density operator of Ψ_t. Then

$$\mathrm{Tr}\left| \Gamma_t^{(1,1)} - |u_t \otimes v_t\rangle\langle u_t \otimes v_t| \right| \leq C \exp(C|t|) \left[\frac{1}{\sqrt{N_1}} + \frac{1}{\sqrt{N_2}} \right]$$

for all t, N_1 and N, where u_t and v_t solve (time-dep. Hartree sys.)

$$\begin{aligned} i\partial_t u_t &= -\Delta u_t + (V_1 * |u_t|^2)u_t + c_2(V_{12} * |v_t|^2)u_t, \\ i\partial_t v_t &= -\Delta v_t + (V_2 * |v_t|^2)v_t + c_1(V_{12} * |u_t|^2)v_t \end{aligned}$$

with $u_{t=0} = u$ and $v_{t=0} = v$ where $c_j = \lim_{N_1,N_2\to\infty} N_j/(N_1 + N_2)$.

Two-component condensate

Remarks

- Similar results for fixed number of particles (i.e. not in Fock space) can be found in Anapolitanos-Hott-Hundertmark, RMP '17 and Michelangeli-Olgiati, Anal. Math. Phys. '17.
- For fixed number of particles, the corresponding time-independent result (ground state energy per particle) can be found in Michelangeli-Nam-Olgiati RMP '18.
- Our proofs are based on the methods developed in Rodnianski-Schlein CMP '09.

Outline of the proof

In the one-component case.

The two-component case is similar.

Creation and annihilation operators on Fock space

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

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

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

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

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

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

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

Conjugation formulas

Weyl operator $W(f)$:

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

Fluctuation dynamics

Integral kernel of $\Gamma_t^{(1)} - |\varphi_t\rangle\langle\varphi_t|$:

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

We want to approximate

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

Define

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

We find the estimate

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

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)

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

To use Grönwall's Lemma, we compute

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

Cancellation

- 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 complete cancellation of linear terms in $W_t^* \mathcal{H} W_t$ with $(i\partial_t W_t^*)W_t$:

$$\text{linear in } W_t^* \mathcal{H} W_t$$
$$= \sqrt{N}\, a^*\big[-\Delta\varphi_t + (V * |\varphi_t|^2)\varphi_t\big] + \sqrt{N} a(\cdots).$$

Grönwall

- We are able to prove

$$\langle [i\mathcal{L}_N(t), \mathcal{N}] \rangle_t \leq C \langle \mathcal{N} + 1 \rangle_t .$$

- Hence

$$\frac{d}{dt} \langle \mathcal{N} \rangle_t \leq C \langle \mathcal{N} + 1 \rangle_t .$$

- Using Grönwall's Lemma, we obtain

$$\langle \mathcal{N} \rangle_t \leq C \exp(C|t|).$$

□

Thank you for your attention!