Dynamics of a BEC in the Thomas-Fermi regime

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Physical Setting

Goal: study the dynamics of N identical bosons in a box Λ with periodic BC

- Thermodynamic limit: with fixed density $\rho := N/|\Lambda|$, study of the limit of infinite volume of the energy per particle

$$\mathfrak{e}(\rho) := \lim_{N\to+\infty} \frac{\inf \sigma(H_N)}{N}$$

$$= 4\pi\rho a\left(1+\frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3}+o\left(\sqrt{\rho a^3}\right)\right) \qquad \text{(LHY)}$$

- Dilute limit: if ρa^3 is small (a scattering length, effective length of the interaction) we obtain the Lee-Huang-Yang formula (LHY)

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Physical Setting

For the variational problem, in a dilute limit (at $T = 0$) one expects that the macroscopic ground state of the system Ψ^{GS} is well approximated by a one-particle state, i.e., there is Bose-Einstein Condensation (BEC)

$$H_N \Psi^{\mathrm{GS}} = E_0(N)\, \Psi^{\mathrm{GS}}$$
$$\Psi^{\mathrm{GS}} \approx \left(\varphi^{\mathrm{GS}}\right)^{\otimes N}$$

φ^{GS} ground state of a nonlinear effective one-particle functional

$$\mathcal{E}^{\mathrm{eff}}[\varphi] := \langle \varphi, h\varphi \rangle + \langle \varphi, \mathcal{V}_{\mathrm{eff}}(\varphi) \rangle$$

with h one-particle Hamiltonian and $\mathcal{V}_{\mathrm{eff}}$ an effective nonlinear potential

Dilute Limits

Let v_N be the (N-dependent) pair interaction

- Mean-Field (Hartree)

$$v_N(\mathrm{x}) := \frac{1}{N} v(\mathrm{x}), \qquad \mathcal{V}_{\text{eff}}(\psi) = \frac{1}{2}\left(v * |\psi|^2\right)|\psi|^2$$

- Gross-Pitaevskii (GP)

$$v_N(\mathrm{x}) := N^2 v(N\mathrm{x}), \qquad \mathcal{V}_{\text{eff}}(\psi) = \frac{1}{2} g\, |\psi|^4$$

- Intermediate regimes ($\beta \in (0,1)$)

$$v_N(\mathrm{x}) := N^{3\beta-1} v\left(N^{\beta}\mathrm{x}\right), \quad \mathcal{V}_{\text{eff}}(\psi) = \frac{1}{2}\left(\int v\right)|\psi|^4$$

In all these cases a_N the scattering length of v_N satisfies $8\pi N a_N \to g$, with g constant ($\rho a_N^3 \approx N^{-2} \ll 1$)

Dilute Limits

Let v_N be the (N-dependent) pair interaction

- Mean-Field (Hartree) ($\beta = 0$)

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- Gross-Pitaevskii (GP) ($\beta = 1$)

$$v_N(\mathsf{x}) := N^2 v(N\mathsf{x}), \qquad \mathcal{V}_{\text{eff}}(\psi) = \frac{1}{2} g\,|\psi|^4$$

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Thomas-Fermi Regime

In experimental settings, in particular in considering rotating systems, $Na_N \gg 1$; this is called Thomas-Fermi regime, in analogy with the density theory for large atoms

We consider a pair interaction such that $8\pi a_N \to +\infty$, compatibly with the dilute condition $\rho a_N^3 \ll 1$

Thomas-Fermi Regime

Fix the size of Λ and consider the following many-body Hamiltonian

$$H_N := \sum_{j=1}^{N} (-\Delta_j) + g_N N^{3\beta-1} \sum_{1\leq j<k\leq N} v\left(N^{\beta}\left(\mathsf{x}_j - \mathsf{x}_k\right)\right)$$

defined on $\mathcal{H}_N := \mathfrak{h}^{\otimes_s N}$, with $\mathfrak{h} = L^2(\Lambda)$

- Without loss of generality $\int v = 1$; then the scattering length of $g_N N^{3\beta-1} v\left(N^{\beta}\cdot\right)$ is given for $\beta \in [0,1)$ by

$$Na_N = \frac{1}{8\pi} g_N \left(1 + o\left(1\right)\right)$$

  therefore we require $g_N \gg 1$ (TF regime)
- If $g_N \leq N^{2/3}$ this is still a *dilute limit*

Mathematical Setting

To evaluate one-particle observables on many-body states $\Psi \in \mathcal{H}_N$ it is convenient to introduce the 1-particle reduced density matrix $\gamma_\Psi^{(1)}$ defined so that

$$\left\langle \Psi, \sum_{j=1}^{N} A_j \Psi \right\rangle = N \operatorname{tr}\left[\gamma_\Psi^{(1)} A\right]$$

for any A a one-particle observable

Complete BEC

Given a many-body state $\Psi \in \mathcal{H}_N$ and a one-particle state $\varphi \in \mathfrak{h}$

$$\gamma_\Psi^{(1)} \to P_\varphi := |\varphi\rangle \langle\varphi| , \qquad \text{in } \mathfrak{S}_1(\mathfrak{h})$$

i.e., a macroscopic fraction of the particles occupies the same one-particle state

Setting

We consider a trapped system in $\Lambda = \left[-\frac{1}{2}, \frac{1}{2}\right]^3$ $\left(\mathfrak{h} = L^2(\Lambda)\right)$

$$H_N := \sum_{j=1}^{N} (-\Delta_j) + g_N N^{3\beta-1} \sum_{1 \le j < k \le N} v\left(N^\beta (\mathsf{x}_j - \mathsf{x}_k)\right)$$

The solution to the Schrödinger equation is

$$\begin{cases} i\partial_t \Psi_{N,t} = H_N \Psi_{N,t} \\ \Psi_{N,t}\big|_{t=0} = \Psi_{N,0} \end{cases}$$

Goal: understand whether complete BEC is preserved by time evolution, i.e.

$$\gamma^{(1)}_{\Psi_{N,0}} \to P_{\varphi_0} \text{ in } \mathfrak{S}_1(\mathfrak{h}) \Longrightarrow \gamma^{(1)}_{\Psi_{N,t}} \to P_{\varphi_t^{\mathrm{GP}}} \text{ in } \mathfrak{S}_1(\mathfrak{h})$$

Gross-Pitaevskii Equation

Expected limiting equation: the time-dependent GP equation

$$\begin{cases} i\partial_t \varphi_t^{\mathrm{GP}} = -\Delta \varphi_t^{\mathrm{GP}} + g_N |\varphi_t^{\mathrm{GP}}|^2 \varphi_t^{\mathrm{GP}} \\ \varphi_t^{\mathrm{GP}}\big|_{t=0} = \varphi_0 \end{cases}$$

Energy of the system:

$$\mathcal{E}^{\mathrm{GP}}[\varphi] = \int_\Lambda d\mathbf{x} \, \left(\frac{1}{2} |\nabla \varphi(\mathbf{x})|^2 + \frac{g_N}{2} |\varphi(\mathbf{x})|^4 \right)$$
$$E^{\mathrm{GP}} = \inf_{\|\varphi\|_2 = 1} \mathcal{E}^{\mathrm{GP}}[\varphi]$$

Idea: for low energies the kinetic term is negligible if N is large

Thomas-Fermi Energy

Dropping the kinetic term we obtain the TF energy functional

$$\mathcal{E}^{\mathrm{TF}}[\rho] = \frac{g_N}{2} \int_{\Lambda} d\mathbf{x} \; \rho^2(\mathbf{x}),$$
$$E^{\mathrm{TF}} = \inf_{\|\rho\|_1 = 1, \; \rho \geq 0} \mathcal{E}^{\mathrm{TF}}[\rho]$$

Fact: in a box $E^{\mathrm{GP}} = E^{\mathrm{TF}} = \frac{g_N}{2}$
(in $\mathbb{R}^3$, $E^{\mathrm{GP}} \approx E^{\mathrm{TF}}$ at first order in N)

Intermediate Equation

To prove the approximation $\gamma^{(1)}_{\Psi_{N,t}} \approx P_{\varphi_t^{\mathrm{GP}}}$ it is helpful to introduce an intermediate effective equation, the time-dependent Hartree (H) equation

$$\begin{cases} i\partial_t \varphi_t^{\mathrm{H}} = -\Delta \varphi_t^{\mathrm{H}} + g_N v_N * \left|\varphi_t^{\mathrm{H}}\right|^2 \varphi_t^{\mathrm{H}} \\ \varphi_t^{\mathrm{H}}\big|_{t=0} = \varphi_0 \end{cases}$$

We exploit $v_N * |\varphi|^2 \to |\varphi|^2$, but we need control on $\|\varphi\|_\infty$ **indipendent on** g_N

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Conjecture

Let φ_0 be the initial datum of the GP equation

$$\varphi_0 \in L^\infty(\Lambda) \Longrightarrow \sup_{t\in\mathbb{R}} \left\|\varphi_t^{\mathrm{H}}\right\|_\infty \leq C$$

Theorem

Assume that $v \in L^2\left(\mathbb{R}^3\right) \cap L^1\left(\mathbb{R}^3, x dx\right)$, the Conjecture holds true and

$$\left\|\gamma^{(1)}_{\Psi_{N,0}} - P_{\varphi_0^{\mathrm{GP}}}\right\|_{\mathfrak{S}^1} \ll N^{-\frac{1-3\beta}{2}}$$
$$\mathcal{E}^{\mathrm{GP}}[\varphi_0] - E^{\mathrm{GP}} \ll \xi_N \leq \sqrt{g_N}$$
$$g_N \ll \log N$$

then for each $t \in \mathbb{R}$ and for any $\beta \in [0, 1/6)$ there is *complete BEC on* φ_t^{GP}, i.e.

$$\left\|\gamma^{(1)}_{\Psi_{N,t}} - P_{\varphi_t^{\mathrm{GP}}}\right\|_{\mathfrak{S}^1} \ll 1$$

Remarks

- Similar result is achievable also in $d = 2$
- Open question is to go beyond $\beta = 1/6$; also related to stationary problem limitations
- (HP1) means that there is BEC in the initial datum $\Psi_{N,0}$ on the state φ_0
- (HP2) means that the GP initial datum φ_0 is close to a ground state in energy: important to prove that the Hartree solution is close to the GP solution
- (HP3) is necessary to prove condensation on a state φ_t^{H}; still allows for a dilute limit

$$\left\| \gamma^{(1)}_{\Psi_{N,0}} - P_{\varphi_0^{\mathrm{GP}}} \right\|_{\mathfrak{S}^1} \ll N^{-\frac{1-3\beta}{2}} \tag{HP1}$$

$$\mathcal{E}^{\mathrm{GP}}[\varphi_0] - E^{\mathrm{GP}} \ll \xi_N \leq \sqrt{g_N} \tag{HP2}$$

$$g_N \ll \log N \tag{HP3}$$

Sketch of the proof

Two parts:

- Approximate the $\gamma^{(1)}_{\Psi_{N,t}}$ with $P_{\varphi^{\mathrm{H}}_t}$
- Estimate the difference between φ^{H}_t and φ^{GP}_t

Main ingredients:

- Tools developed in **[P11]**
- Energy estimates for the one-particle problem

[P11] Pickl, "A Simple Derivation of Mean Field Limits for Quantum Systems"

Many-Body to Hartree

Similarly as in **[P11]**, the goal is obtaining a Grönwall-type estimate for

$$\alpha_t := 1 - \langle \Psi_{N,t}, \left(\left| \varphi_t^{\mathrm{H}} \right\rangle \left\langle \varphi_t^{\mathrm{H}} \right| \right)_1 \Psi_{N,t} \rangle$$

We need to estimate terms of the form

$$\left\| v_N * \left| \varphi_t^{\mathrm{H}} \right|^2 \right\|_\infty \leq \| v \|_1 \left\| \varphi_t^{\mathrm{H}} \right\|_\infty^2$$

Using the Conjecture we get the desired result; if we do not assume it, we can only use the kinetic energy: *we do not reach the time scale of vortices* (compare with **[JS15]**)

[JS15] Jerrard, Smets, "Vortex dynamics for the two-dimensional non-homogeneous Gross-Pitaevskii equation"

Hartree to Gross-Pitaevskii

$$\begin{aligned}\partial_t \left\|\varphi_t^{\mathrm{GP}} - \varphi_t^{\mathrm{H}}\right\|_2^2 &\leq g_N \left|\mathrm{Im}\langle \varphi_t^{\mathrm{H}}, \left(\left|\varphi_t^{\mathrm{GP}}\right|^2 - v_N * \left|\varphi_t^{\mathrm{H}}\right|^2\right) \varphi_t^{\mathrm{GP}}\rangle\right| \\ &\leq g_N \left|\langle \varphi_t^{\mathrm{H}}, \left(\left|\varphi_t^{\mathrm{GP}}\right|^2 - \left|\varphi_t^{\mathrm{H}}\right|^2\right) \varphi_t^{\mathrm{GP}}\rangle\right| \\ &\quad + g_N \left|\langle \varphi_t^{\mathrm{H}}, \left(\left|\varphi_t^{\mathrm{H}}\right|^2 - v_N * \left|\varphi_t^{\mathrm{H}}\right|^2\right) \varphi_t^{\mathrm{GP}}\rangle\right|\end{aligned}$$

To prove convergence of this last two terms use L^2 difference of the square of the solutions (energy bound) for the first term and $v_N \to \delta$ as a distribution for the second one:

$$\begin{aligned}&\left|\langle \varphi_t^{\mathrm{H}}, \left(\left|\varphi_t^{\mathrm{H}}\right|^2 - v_N * \left|\varphi_t^{\mathrm{H}}\right|^2\right) \varphi_t^{\mathrm{GP}}\rangle\right| \leq \\ &\qquad \leq \frac{C}{N^\beta} \left\|\nabla \varphi_t^{\mathrm{H}}\right\|_2 \left\|\varphi_t^{\mathrm{H}}\right\|_\infty \left\|\varphi_t^{\mathrm{H}}\right\|_4 \left\|\varphi_t^{\mathrm{GP}}\right\|_4\end{aligned}$$

Conclusion

- Condensation is preserved under suitable assumptions of regularity on the solution
  - **Q:** How to prove the Conjecture?
  - **Q:** Vortices are encoded in the vorticity measure, which depends on the gradient of the solution; can a similar result be proven in a stronger (e.g. H^1) norm?

- There is BEC in the Thomas Fermi limit, at least in a scaling with $\beta < 1/3$ (work in progress with M. Correggi and E. L. Giacomelli)
  - **Q:** Can we extend the result for $\beta > 1/6$?

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Thanks for the attention!