Bounds on the convergence towards mean field dynamics for systems of many bosons

(Joint work with Zied Ammari and Boris Pawilowski)
Outline

1 Introduction: Mean field between Physics and Mathematics

2 Mathematical framework

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Mean field in physics

- In many physical situations the number of degrees of freedom of the system under consideration is extremely high (even if finite).

- This is due to the presence of a high number of “fundamental constituents” (particles) in interaction.

- It is not uncommon, e.g. in condensed matter physics, to consider systems with $N = 10^4 - 10^7$ particles.

- To describe these systems, the so-called mean field approximation is often used: any particle is subjected to an effective (nonlinear) self-interaction, that represents the averaged effect of all other particles.

- An $N$-dimensional problem is reduced to a one-dimensional problem.
How good is the approximation?

- Mean field dynamics becomes exact only in the limit $N \to \infty$.

- Do we have to take into account the error? At which (small) value of $N$ does it becomes significant?

- Example (Grossmann and Holthaus [1996]; Dalfovo et al. [1999]). In Bose-Einstein condensation ($10^2 - 10^7$ atoms) the leading error term is of order $N^{-1/3}$, and becomes insignificant when $N \gtrsim 10^4$; higher order corrections are experimentally indistinguishable for $N \gtrsim 10^3$.

- It is thus physically relevant to provide an upper bound on the first order corrections (of mean field approximations).
In mathematical physics, the rate of convergence towards mean-field limits is an active subject of investigation.


The “optimal” rate of convergence after time evolution is considered to be $N^{-1}$, but it is obtained only for initial states with special structure (factorized, coherent). Also, the rate seems to depend on the singularity of the interaction.
Our contribution aims to clarify the following aspects:

- rate of convergence for general states;
- “optimality” of $N^{-1}$;
- influence of time evolution on the rate of convergence.
A quantum bosonic system

- A quantum system with a fixed number $N$ of identical $d$-dimensional particles is usually set in a suitable subspace of $\bigotimes^{(N)} L^2(\mathbb{R}^d)$.

- If the particles are bosons, we take the symmetric subspace; we will assume our Hilbert space to be the $N$-fold symmetric tensor copy of a separable Hilbert space $\mathcal{H}$, that we denote $\mathcal{H}_N = \bigotimes_s^{(N)} \mathcal{H}$.

- We define an $N$-particle state (or density matrix) $\rho_N$ as a positive, self-adjoint trace-class operator on $\mathcal{H}_N$ with trace one.

- Suppose that we have an operator that acts only on $p \leq N$ particles at a time; then in some sense the other degrees of freedom of the $N$-particle state are “useless”. It is then convenient to introduce the reduced density matrix $\rho_N^{(p)}$, an “inherited $p$-particle state” where the additional $N - p$ degrees of freedom have been taken out.
The \( p \)-particle reduced density matrix is therefore the state \( \rho_{N}^{(p)} \) on \( \mathcal{H}_{p} \) such that for any bounded operator \( A \in \mathcal{L}(\mathcal{H}) \):

\[
\text{Tr}[\rho_{N}A \otimes 1 \otimes N - p] = \text{Tr}[\rho_{N}^{(p)} A] .
\]

**Remark:** \( \rho_{N}^{(p)} \) is indeed a positive, self-adjoint trace class operator on \( \mathcal{H}_{p} \) with trace one.

Under suitable regularity conditions, the reduced density matrices converge in the limit \( N \to \infty \). In the limit, \( p \) remains fixed.

We will always assume that the reduced density matrices \( \rho_{N}^{(p)} \) converge for any \( p \in \mathbb{N}^{*} \), to a limit \( \rho_{\infty}^{(p)} \) characterized by a unique Wigner measure \( \mu_{0} \) on \( \mathcal{H} \). The limit state has the form:

\[
\rho_{\infty}^{(p)} = \int_{\mathcal{H}} |z \otimes p \rangle \langle z \otimes p | d\mu_{0}(z) .
\]

Convergence has to be intended in the topology induced by the trace norm (that we will denote by \( \| \cdot \|_{1} \)).
Time evolution

- We consider a simple dynamics on our system, namely one described by a Hamiltonian operator of the form:

\[ H_N = \sum_{j=1}^{N} D_j + V_N. \]

- \( D \) is a self-adjoint operator on the one-particle space \( \mathcal{H} \); \( V_N \) is a bounded operator on \( \mathcal{H}_N \) with \( N \)-dependent bound.

- Example \( [L^2_s(\mathbb{R}^{dN})] \): \( D = -\Delta_x, \ V_N = \frac{1}{N} \sum_{i<j} V(x_i - x_j), \ V \in L^\infty(\mathbb{R}^d) \) and symmetric.
The time-evolution of the state is $\rho_N(t) = e^{-itH_N} \rho_N e^{itH_N}$.

We denote by $\rho_N^{(p)}(t)$ the corresponding $p$-particle reduced density matrices.

The regularity assumption on the state at time zero and on the Hamiltonian $H_N$ imply that for any $p \in \mathbb{N}^*$, $t \in \mathbb{R}$ there exists $\rho^{(p)}(t)$ such that:

$$\|\rho_N^{(p)}(t) - \rho^{(p)}(t)\|_1 \underset{N \to \infty}{\longrightarrow} 0.$$
Bounds at initial time

- If the quantum evolution has not yet taken place, it is relatively easy to obtain bounds on the rate of convergence.

- There are $N$-particle states whose $p$-particle marginals coincide with their limit.

  * Example [Hermite states]: $|\varphi^{\otimes N}\rangle \langle \varphi^{\otimes N}|$, $\varphi \in \mathcal{H}$.

- In general, given a state $\rho_N \in L^1(\mathcal{H}_N)$ we may expect to prove that there exist $\alpha(N) \xrightarrow{N \to \infty} \infty$ such that for any $p \in \mathbb{N}^*$

$$\|\rho_N^{(p)} - \rho_\infty^{(p)}\|_1 = O\left(\frac{1}{\alpha(N)}\right);$$

or at least

$$\|\rho_N^{(p)} - \rho_\infty^{(p)}\|_1 \leq O\left(\frac{1}{\alpha(N)}\right).$$
Bounds on the rate of convergence

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<th>Arbitrary time.</th>
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**Bounds after evolution**

- What happens if we “switch on” evolution?

- A priori the rate of convergence may be affected by time evolution, since the latter changes the structure of states.

**Theorem (Ammari, F., Pawilowski [2014])**

Assume there exist $C_0$, $C > 2$ and $\gamma \geq 1$ such that for all $N, p \in \mathbb{N}^*$ with $N \geq \gamma p$:

$$\|\rho_N^{(p)} - \rho_\infty^{(p)}\|_1 \leq C_0 \frac{C^p}{\alpha(N)}.$$

Then for any $T > 0$ there exists $C_T > 0$ such that for all $t \in [-T, T]$ and all $N, p \in \mathbb{N}^*$ with $N \geq \gamma p$,

$$\|\rho_N^{(p)}(t) - \rho_\infty^{(p)}(t)\|_1 \leq C_T \frac{C^p}{\min\{\alpha(N), N\}}.$$
Remarks

- Time evolution (in this regular situation) singles out the rate of convergence $O(N^{-1})$ as the best possible rate. Is it a true feature of the dynamics—$O(N^{-1})$ is therefore “optimal”—or is it just a technical limitation?

- Numerical calculations performed by B. Pawilowski strongly indicate $O(N^{-1})$ is optimal: the Hartree states—whose marginals coincide with their limit at time zero—show numerically a rate of convergence $O(N^{-1})$ after time evolution.

![Graph showing log-log plot with data points and trend line.](image-url)
Time evolution cannot improve the rate of convergence. Suppose that $\|\rho_N^{(p)} - \rho_\infty^{(p)}\|_1 = O\left(\frac{1}{\ln N}\right)$; and that at a certain time $t^* \in \mathbb{R}$, $\|\rho_N^{(p)}(t^*) - \rho_\infty^{(p)}(t^*)\|_1 = O\left(\frac{1}{N}\right)$. Then applying the theorem backwards in time—with initial time $t^*$ and final time zero—we would have $\|\rho_N^{(p)} - \rho_\infty^{(p)}\|_1 = O\left(\frac{1}{N}\right)$, that is in contradiction with the original hypothesis.
Open questions

- Does the evolution modify the rate of convergence more significantly in presence of singular interactions (e.g. Hartree with Coulomb potential, Gross-Pitaevskii...)?

- May the rate of convergence (after evolution) be better only for some particular $\bar{p}$-particle marginal?

- Is it possible to determine a bound if we have initial time informations only on some of the marginals?
Brief outline of the proof

- Translate the operator in the language of second quantization on the symmetric Fock space $\Gamma_s(\mathcal{H})$.

- Let $A^{\text{Wick}}$ be the Wick quantization of a $p$-particle operator. We write a mean field ("semiclassical") expansion of $\text{Tr}[\rho_N(t)A^{\text{Wick}}]$.

- Subtract the known classical limit $\int_Z \langle z^\otimes p, A z^\otimes p \rangle d\mu_t$.

- For short times, bound $|\text{Tr}[\rho_N(t)A^{\text{Wick}}] - \int_Z \langle z^\otimes p, A z^\otimes p \rangle d\mu_t|$ by bounding each term of the expansion.

- Iterate the procedure to extend the bound to arbitrary times.

- Observe that the error made bounding the difference above instead of $\|\rho_N^{(p)}(t) - \rho_\infty^{(p)}(t)\|_1$ is $\leq O(N^{-1})$. 
Thank you for the attention.
References


