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

(Joint work with Zied Ammari and Boris Pawilowski)

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Outline

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).

Rate of convergence in Mathematics

- In mathematical physics, the rate of convergence towards mean-field limits is an active subject of investigation.
- A non-exhaustive list of recent results comprehends: Rodnianski and Schlein [2009]; Grillakis, Machedon and Margetis [2010]; Knowles and Pickl [2010]; L.Chen, Lee and Schlein [2011]; Anapolitanos [2011]; Pickl [2011]; X. Chen [2012]; F. [2013].
- 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 $\mathscr{H}$, that we denote $\mathscr{H}_N = \bigotimes_s^{(N)} \mathscr{H}$.
- We define an N-particle state (or density matrix) ρ_N as a positive, self-adjoint trace-class operator on $\mathscr{H}_N$ 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 $\mathscr{H}_p$ such that for any bounded operator $A \in \mathcal{L}(\mathscr{H})$:

$$\mathrm{Tr}[\rho_N A \otimes 1^{\otimes_{N-p}}] = \mathrm{Tr}[\rho_N^{(p)} A] \; .$$

- Remark: $\rho_N^{(p)}$ is indeed a positive, self-adjoint trace class operator on $\mathscr{H}_p$ 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 μ_0 on $\mathscr{H}$. The limit state has the form:

$$\rho_\infty^{(p)} = \int_{\mathscr{H}} |z^{\otimes_p}\rangle\langle z^{\otimes_p}| d\mu_0(z) \; .$$

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:

$$H_N = \sum_{j=1}^{N} \mathcal{D}_j + V_N \ .$$

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

- Example $[L^2_s(\mathbb{R}^{dN})]$: $\mathcal{D} = -\Delta_x$, $V_N = \frac{1}{N}\sum_{i<j}^{N} V(x_i - x_j)$, $V \in L^\infty(\mathbb{R}^d)$ 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 $\rho_\infty^{(p)}(t)$ such that:

$$\|\rho_N^{(p)}(t) - \rho_\infty^{(p)}(t)\|_1 \underset{N\to\infty}{\longrightarrow} 0 \; .$$

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]: $|\varphi^{\otimes N}\rangle\langle\varphi^{\otimes N}|$, $\varphi \in \mathscr{H}$.

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

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

or at least

$$\|\rho_N^{(p)} - \rho_\infty^{(p)}\|_1 \leq O\Bigl(\frac{1}{\alpha(N)}\Bigr) \;.$$

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* $N \geq \gamma p$*:*

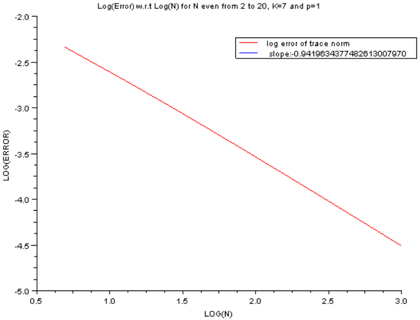
$$\|\rho_N^{(p)} - \rho_\infty^{(p)}\|_1 \leq C_0 \frac{C^p}{\alpha(N)} \ .$$

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.



- Time evolution cannot improve the rate of convergence. Suppose that $\|\rho_N^{(p)} - \rho_\infty^{(p)}\|_1 = O(\frac{1}{\ln N})$; and that at a certain time $t^* \in \mathbb{R}$, $\|\rho_N^{(p)}(t^*) - \rho_\infty^{(p)}(t^*)\|_1 = O(\frac{1}{N})$. Then applying the theorem backwards in time—with initial time t^* and final time zero—we would have $\|\rho_N^{(p)} - \rho_\infty^{(p)}\|_1 = O(\frac{1}{N})$, 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 $\Gamma_s(\mathscr{H})$.
- Let A^{Wick} be the Wick quantization of a p-particle operator. We write a mean field ("semiclassical") expansion of $\mathrm{Tr}[\rho_N(t)A^{\mathrm{Wick}}]$.
- Subtract the known classical limit $\int_{\mathscr{Z}}\langle z^{\otimes p}, A\, z^{\otimes p}\rangle\, d\mu_t$.
- For short times, bound $|\mathrm{Tr}[\rho_N(t)A^{\mathrm{Wick}}] - \int_{\mathscr{Z}}\langle z^{\otimes p}, A\, z^{\otimes p}\rangle\, d\mu_t|$ 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.

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