Controlling Quantum Fluctuations in the Mean-Field Limit

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UA Tucson – 20 March 2010

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The quantum Bose gas

A quantum Bose gas of \( N \) particles is described by a normalized symmetric wave function

\[
\Psi_N \in L^2(\mathbb{R}^{dN}, dx_1 \cdots dx_N).
\]

The time evolution is given by the \( N \)-body Schrödinger equation

\[
i \partial_t \Psi_N(t) = H_N \Psi_N(t), \quad \Psi_N(0) = \Psi_{N,0}.
\]

The \( N \)-body Hamiltonian is

\[
H_N := \sum_{i=1}^{N} h_i + \lambda_N \sum_{1 \leq i < j \leq N} w(x_i - x_j).
\]
Goal: understand behaviour of $\Psi_N(t)$. This is hard!

Simplifications:

- Take the limit $N \to \infty$ (macroscopic gas).
- Consider factorized initial data (condensate): $\Psi_{N,0} = \varphi_0^\otimes N$ for $\varphi_0 \in L^2(\mathbb{R}^d)$.

A nontrivial limit necessitates that both terms of $H_N$ be of the same order in the limit $N \to \infty$. Set $\lambda_N = 1/N$: mean-field scaling.

$\Psi_N(t)$ is no longer factorized for $t > 0$. Heuristics: expect that

$$
\Psi_N(t) \approx \varphi(t)^\otimes N ,
$$

where

$$
i\partial_t \varphi(t) = h\varphi(t) + (w * |\varphi(t)|^2)\varphi(t) ,
$$

the Hartree equation.
Reduced density matrices

We need a means of quantifying the error in $\Psi_N \approx \varphi \otimes N$ (control the quantum fluctuations around $\varphi$). Define the reduced $k$-particle density matrix

$$
\gamma^{(k)}_N (x_1, \ldots, x_k; y_1, \ldots, y_k) := \int dx_{k+1} \cdots dx_N \Psi_N(x_1, \ldots, x_N)\overline{\Psi_N(y_1, \ldots, y_k, x_{k+1}, \ldots, x_N)}.
$$

Good indicator: trace norm distance

$$
R^{(k)}_N := \text{Tr} \left| \gamma^{(k)}_N - |\varphi\rangle \langle \varphi| \otimes^k \right|,
$$

where $\text{Tr}|A| = \sum_{\lambda \in \text{Sp}(A)} |\lambda|$. 
• (Rodnianski & Schlein, 2007) If $h = -\Delta$ and $w(x) = |x|^{-1}$ then

$$R_N^{(k)}(t) \leq \frac{C'(k)}{\sqrt{N}} e^{K(k)t}.$$ 

• (Erdős & Schlein, 2008) If $\hat{w} \in L^1$ then

$$R_N^{(k)}(t) \leq \frac{C'(k)}{N} e^{K(k)t}.$$
A different indicator of condensation

Define

\[ E^{(k)}_N := 1 - \langle \varphi \otimes k, \gamma^{(k)}_N \varphi \otimes k \rangle \]

Properties:

(i) \( E^{(k)}_N \leq k E^{(1)}_N \)

(ii) \( E^{(k)}_N \leq R^{(k)}_N \leq \sqrt{E^{(k)}_N} \)
Theorem

Assume that

(i) $h$ and $H_N$ are self-adjoint and bounded from below
(ii) $w \in L^{p_1} + L^{p_2}$ where $2 \leq p_1 \leq p_2 \leq \infty$

Then

$$E_N^{(1)}(t) \leq \left( E_N^{(1)}(0) + \frac{1}{N} \right) e^{\Phi(t)}$$

where

$$\Phi(t) := 32 \| w \|_{L^{p_1} + L^{p_2}} \int_0^t ds \left( \| \varphi(s) \|_{q_1} + \| \varphi(s) \|_{q_2} \right)$$

and

$$\frac{1}{2} = \frac{1}{p_i} + \frac{1}{q_i}$$
• For $d = 3$, allowed singularities in $w$ up to $|x|^{-3/2}$

• If $E_N^{(1)}(0) \leq C/N$ then

$$E_N^{(k)}(t) \leq C \frac{k}{N} e^{\Phi(t)} \quad \text{and} \quad R_N^{(k)}(t) \leq C \sqrt{\frac{k}{N} e^{\Phi(t)/2}}$$

$\implies$ control the condensation of $k = o(N)$ particles

### Examples

• The boson star: $h = \sqrt{1 - \Delta}$ and $w(x) = \lambda |x|^{-1}$ with $\lambda > -4/\pi$

• Scattering: If $\int dt \|\varphi(t)\|_{q_i} < \infty$ for $i = 1, 2$ then $\Phi(t) \leq C$

$\implies$ uniformity in time
“Venerable physical folklore”: \( h = -\Delta \) and \( w(x) = |x|^{-\zeta} \) for \( \zeta < 2 \) produces reasonable quantum dynamics for \( d = 3 \).

Mathematics:

- \( H_N \) is self-adjoint.
- Hartree equation is globally well-posed.

Does mean-field convergence hold?

Yes! Provided that \( w \in L^{6/5} + L^\infty \) (in \( d = 3 \))

\( \implies \) allowed singularities up to \( |x|^{-5/2} \).
Theorem

Assume that

(i) $h$ and $H_N$ are self-adjoint and bounded from below

(ii) $w \in L^p + L^\infty$ for $p_0 < p \leq 2$

(iii) $E_N^{(1)}(0) \to 0$ sufficiently fast in $N$

Then

$$E_N^{(1)}(t) \leq \frac{1}{N\eta} e^{\Phi(t)}$$

where

$$\eta := \frac{p/p_0 - 1}{2p/p_0 - p/2 - 1}$$

and

$$\Phi(t) = C \int_{0}^{t} ds \left( 1 + \|\varphi(s)\|_X^3 \right)$$

for $X \approx H^2 \cap L^\infty$. 

\[ 
\begin{array}{c|c|c|c|c|c|c|c|c}
\hline
p & 1.2 & 1.4 & 1.6 & 1.8 & 2 \\
\hline
\eta & 0.1 & 0.2 & 0.3 & 0.4 & 0.5 \\
\hline
\end{array} 
\]
Sketch of proofs

Control the quantity $\alpha := E_N^{(1)}(t)$. Set

$$p := |\varphi\rangle\langle\varphi|, \quad q := 1 - p,$$

and

$$W_\varphi := w * |\varphi|^2.$$

With the abbreviation $W_{ij} := w(x_i - x_j)$ we get

$$\dot{\alpha} = \frac{i}{2N} \langle \Psi, [(N - 1)W_{12} - NW_1^\varphi - NW_2^\varphi, q_1 + q_2] \Psi \rangle.$$

Main work: prove a bound of the form

$$\dot{\alpha}_N(t) \leq A_N(t) + B_N(t)\alpha_N(t)$$

with $\lim N A_N(t) = 0$. Then by Grönwall we are done.
To get (1), insert $1 = (p_1 + q_1)(p_2 + q_2)$ in front of both $\Psi$'s in

$$\frac{i}{2N} \langle \Psi, \left[ (N - 1)W_{12} - NW_1\varphi - NW_2\varphi, q_1 + q_2 \right] \Psi \rangle$$

and multiply everything out.

Only three types of terms survive:

$$p_1p_2(\cdot)q_1p_2, \quad q_1p_2(\cdot)q_1q_2, \quad p_1p_2(\cdot)q_1q_2.$$

Heuristics:

- $p$ controls singularities in $W_{12}$ (since $\varphi$ is smooth).
- $q$ is small: $\langle \Psi, q_1 \Psi \rangle = \alpha$.

Use energy estimates to control singularities.