Entropy Chaos and Bose-Einstein Condensation

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Introduction

In this talk we give some convergence results about Bose-Einstein condensation in the Gross-Pitaevskii scaling limit.
The novelty of this approach consist in using Nelson's stochastic formulation of Quantum Mechanics. It permits us to prove some new consequence of the classical results on this subjects. In particular, using the probabilistic perspective and exploiting some new concepts from the theory of interacting particles systems, we prove that the stochastic system associated with the quantum one is entropy chaotic.

Nelson's Stochastic Mechanics

Nelson's Stochastic Mechanics is an alternative formulation of Quantum Mechanics which allows to study quantum phenomena using a well determined class of diffusion processes. Consider a solution to the Schrodinger equation

$$i\partial_t(\psi(x,t)) = H(t)(\psi)(x,t),$$

where $x \in \mathbb{R}^{3N}$ and $H(t)$ is the N particles Hamiltonian operator

$$H(t) = \sum_{k=1}^{N} \frac{-\hbar}{2m}\Delta_k + V(x,t),$$

and density

$$\rho_t(x) = |\psi(x,t)|^2.$$

We define two vector fields on $\mathbb{R}^N$

$$
\begin{aligned}
u(x,t) &= \mathrm{Re}\left(\frac{\nabla\psi(x,t)}{\psi(x,t)}\right) = \frac{1}{2}\frac{\nabla\rho_t}{\rho_t} \\
v(x,t) &= \mathrm{Im}\left(\frac{\nabla\psi(x,t)}{\psi(x,t)}\right)
\end{aligned}
$$

Putting

$$b(x,t) = v(x,t) + u(x,t),$$

we consider the solution $x_t \in \mathbb{R}^{3N}$ of the SDE

$$dx_t = b(x_t,t)dt + \sqrt{\frac{\hbar}{m}}dW_t$$

with initial probability density $p_0(x) = \rho_0(x) = |\psi(x,0)|^2$.

It is possible to prove that if

$$\int_{\mathbb{R}^{3N}} \left((\|v(x,t)\|^2 + \|u(x,t)\|^2 \right) \rho_t(x) dx = \int_{\mathbb{R}^{3N}} \|\nabla \psi\|^2 < +\infty,$$

there exists an unique process x_t and, so, an unique probability measure $\mathbb{P}$ on the path space $C^0((0,+\infty],\mathbb{R}^{3N})$, solution to the previous SDE.

We can recover many concepts and ideas of quantum mechanics from the process x_t. Indeed for example x_t admits $\rho_t(x,t) = |\psi(x,t)|^2$ as probability density, it solves a variational stochastic problem, it is possible to define an energy function whose mean is conserved etc.

The most important feature of Stochastic Mechanics is that it provides an alternative formulation of Quantum Mechanics where it is possible to speak both of trajectories of a particle and of the probability of its position.

Bose-Einstein condensation and Gross-Pitaevskii limit

We consider the ground state Ψ_N of N identical particles Hamiltonian

$$H = \sum_{k=1}^{N} \left(\frac{-\hbar}{2m} \Delta_k + V(x_k) + \sum_{j<k} v_N(\|x_k - x_j\|) \right),$$

where

$$v_N(r) = \frac{v_1\left(\frac{r}{a}\right)}{a^2},$$

and where

$$a = \frac{g}{4\pi N},$$

and $v_1(r)$ is a function with scattering length equal to 1.

We consider the solution Φ_{GP} of the Gross-Pitaevskii equation

$$\frac{-\hbar^2}{2m}\Delta(\Phi_{GP}) + \hbar V(x)\Phi_{GP} + 2g|\Phi_{GP}|^2\Phi_{GP} = \lambda_{GP}\Phi_{GP},$$

where λ_{GP} is the ground state eigenvalues, and denote by $\rho_{GP} = \Phi_{GP}\overline{\Phi}_{GP}$.

Theorem (Lieb, Yngvason, Seiringer 2000)

The following limit holds

$$\lim_{N\to+\infty}\int_{\mathbb{R}^{3(N-1)}} |\Psi_N(x, x^2, ..., x^N)|^2 dx^2 ... dx^N = \rho_{GP}(x),$$

in the sense of weak L^1 convergence.

The second classical result that we use in our proof is the following.

Theorem (Lieb, Yngvason, Seiringer, 2000)

Put

$$E_N = \int_{\mathbb{R}^{3N}} \left(\sum_i \frac{\hbar}{2m} \|\nabla_i \Psi_N\|^2 + \left(V(x^i) + \sum_{i<j} (v_N(x^i - x^j)) \right) |\Psi|^2 \right) dx,$$

and

$$E_{GP} = \int_{\mathbb{R}^3} \left(\frac{\hbar}{2m} \|\nabla \Phi_{GP}\|^2 + V|\Phi_{GP}|^2 + g|\Phi_{GP}|^4 \right) dx.$$

Then

$$\lim_{N \to +\infty} \frac{1}{N} E_N = E_{GP}.$$

Bose-Einstein condensation and Stochastic Mechanics

We want to know what happens in Stochastic Mechanics of Bose-Einstein condensation. If Ψ_N is the N particles ground state we define

$$\begin{aligned} b_N(x) &= \frac{\nabla \Psi_N(x)}{\Psi_N} \\ dx_{N,t} &= b_N(x_{N,t})dt + \sqrt{\frac{\hbar}{2m}}dW_t. \end{aligned}$$

with initial condition $p_0(x) = \rho_N(x)$.

No stochastic process can canonically be associated with the solution to Gross-Pitaevskii equation. Indeed the Nelson's Stochastic Mechanics is defined only for solutions to linear Schrodinger equations. We can guess a process associated with Gross-Pitaevskii limit by defining

$$\begin{aligned} u^N_{GP}(x) &= \frac{\nabla \Phi^{\otimes N}_{GP}(x)}{\Phi^{\otimes N}_{GP}} \\ dx^N_{GP,t} &= u^N_{GP}(x_{GP,t})dt + \sqrt{\frac{\hbar}{2m}}dW_t. \end{aligned}$$

where $\Phi^{\otimes N}_{GP}$ is the functions obtained by making the product of N independent function of the form $\Phi_{GP}(x^k)$.

Entropy chaos

With the help of Stochastic Mechanics formulation of Quantum Mechanics we have transformed the problem of Bose-Einstein condensation in the Gross-Pitaevskii limit into a probabilistic problem which can be studied with appropriate convergence techniques.

The first result is on the process at fixed time t. We extend a result of Ugolini (2012) about the Kac chaoticity of the process $x_{N,t}$.

This means that if we define the measures

$$\rho^n_N(x^1, ..., x^n) = \int_{\mathbb{R}^{3(N-n)}} \rho_N(x^1, ..., x^n, y^{n+1}, ..., y^N) dy^{n+1} ... dy^N,$$

ρ^n_N converges weakly to $\rho_{GP}^{\otimes n}$.

We prove that the process $x_{N,t}$ (if the trapping potential $V(x)$ grow to infinity faster then $\|x\|^2$) is also entropy chaotic. This notion is introduced by Carlen, Carvalho, Le Roux, Loss and Villani (2010) and then recently investigated by Hauray and Mischler (2014).
A process is entropy chaotic if two conditions hold. The first condition is that the one-particle probability distribution

$$\rho_N^{(1)} \to \rho_{GP}$$

weakly in L^1. This is obviously a consequence of the classical theorem by Lieb, Yngvason, Seiringer (2000) about the convergence in Gross-Pitaevskii limit.

The second condition requests that the mean entropy of the n-particles probability distribution

$$H_N = \frac{1}{N}\int_{\mathbb{R}^{3N}} \log(\rho_N)\rho_N dx,$$

converges to the entropy of the weak limit

$$\int_{\mathbb{R}^3} \log(\rho_{GP})\rho_{GP} dx.$$

This fact can be proved using the relation between entropy and Fisher information and exploiting the convergence of kinetic energy in Gross-Pitaevskii limit.
The entropy chaos convergence implies the Kac chaos convergence. Furthermore the entropy chaos convergence guarantees that the one-particle probability density $\rho_N^{(1)}$ converges strongly in L^1 to ρ_{GP}.

Convergence of the measures on the path space

We investigate also the convergence of the one-particle probability measure $\mathbb{P}_N^{(1)}$ on the path space $C^0([0,T],\mathbb{R}^3)$, and not only the probability measure at fixed time ρ_N.
In this case Morato and Ugolini (2011) prove some interesting results. First of all, if we denote by τ_N the stopping time of the first interaction between two particles, $\tau_N \to +\infty$ as $N \to +\infty$.
Furthermore if we denote by $\mathbb{P}_N^{(1)}|_{\tau_N}$ the one-particle probability law projected on the σ algebra generated by τ_N we have that $\mathbb{P}_N^{(1)}|_{\tau_N} \to \mathbb{P}_{GP}$ in total variation.

What we have proved is a convergence result for the probability $\mathbb{P}^{(1)}_N$ and not only for the stopped $\mathbb{P}^{(1)}_N|_{\tau_N}$. First of all we use that the the relative entropy

$$\mathcal{H}_N = \int \log\left(\frac{d\mathbb{P}^{(1)}_N}{d\mathbb{P}_{GP}}\right) d\mathbb{P}_{GP},$$

is bounded for $N \to +\infty$. This guarantees the existence, passing to a subsequence, of a weak limit $\overline{\mathbb{P}}$ of the measures $\mathbb{P}^{(1)}_N$. Finally using the stopping time τ_N and the previously result, we are able to prove that the limit measure $\overline{\mathbb{P}}$ does not depend on the chosen subsequence and $\overline{\mathbb{P}} = \mathbb{P}_{GP}$. For our result the convergence is only weak an not in total variation.