Bose-Einstein condensation and limit theorems

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2015
Bose-Einstein condensation: from many quantum particles to a quantum “superparticle”

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TexAMP 2015
The big challenge: making physics rigorous
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microscopic first principles $\rightsquigarrow$ zoom out $\rightsquigarrow$ Macroscopic states

Courtesy Greg L and Digital Vision/Getty Images
1925: predicting Bose-Einstein condensation (BEC)
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1995: Cornell-Wieman and Ketterle experiment

![Diagram of Bose-Einstein condensation](image-url)
After the trap was turned off

BEC stayed coherent like a single macroscopic quantum particle.

Momentum is concentrated after release at 50 nK. (Atomic Lab)
Gross and Pitaevskii, 1961: a good model of BEC is the cubic nonlinear Schrödinger equation (NLS):

\[ i \partial_t \varphi = -\Delta \varphi + \mu |\varphi|^2 \varphi \]

Fruitful NLS research: competition between two RHS terms
The mathematics of BEC

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Can we rigorously connect the physics and the math?
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Fruitful NLS research: competition between two RHS terms

Can we rigorously connect the physics and the math? Yes!
The outline (w/ G. Staffilani, B. Schlein, G. Ben Arous)

microscopic first principles $\rightsquigarrow$ $\rightsquigarrow$ Macroscopic states

1. $N$ bosons $\rightsquigarrow$ mean-field limit $\rightsquigarrow$ Hartree equation
2. $N$ bosons $\rightsquigarrow$ localizing limit $\rightsquigarrow$ NLS
3. Quantum probability and CLTs
A quantum “particle” is really a wavefunction

For each \( t \), \( \psi(x, t) \in L^2(\mathbb{R}^d) \) solves a Schrödinger equation

\[
i \partial_t \psi = -\Delta \psi + V_{ext}(x) \psi
\]
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For each $t$, $\psi(x, t) \in L^2(\mathbb{R}^d)$ solves a Schrödinger equation

$$i \partial_t \psi = -\Delta \psi + V_{\text{ext}}(x)\psi =: H \psi$$

- $-\Delta = -\sum_{i=1}^d \partial_{x_i}^2 \geq 0$
- external trapping potential $V_{\text{ext}}$
- solution $\psi(x, t) = e^{-iHt}\psi_0(x)$
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- \(-\Delta = -\sum_{i=1}^{d} \partial_{x_i x_i} \geq 0\)
- external trapping potential \( V_{\text{ext}} \)
- solution \( \psi(x, t) = e^{-iHt} \psi_0(x) \)
- \( \int |\psi_0|^2 = 1 \implies |\psi(x, t)|^2 \) is a probability density for all \( t \).

Exercise: why?
Particle in a box

\[ V_{\text{ext}} = \infty \cdot 1_{[0,1]} \] has ground state \( \psi(x) = \sqrt{2} \sin(\pi x) \)
The microscopic $N$-particle model

Wavefunction $\psi_N(\mathbf{x}, t) = \psi_N(x_1, ..., x_N, t) \in L^2(\mathbb{R}^{dN}) \quad \forall t$

solves the $N$-body Schrödinger equation:

$$i \partial_t \psi_N = \sum_{j=1}^{N} -\Delta_{x_j} \psi_N + \sum_{i<j} U(x_i - x_j) \psi_N =: H_N \psi_N$$
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- pair interaction potential $U$
- solution $\psi_N(x, t) = e^{-iH_N t} \psi^0_N(x)$
- joint density $|\psi_N(x_1, \ldots, x_N, t)|^2$
More assumptions

For $N$ bosons, $\psi_N$ is symmetric (particles are exchangeable):

$$\psi_N(x_{\sigma(1)}, \ldots, x_{\sigma(N)}, t) = \psi_N(x_1, \ldots, x_N, t) \text{ for } \sigma \in S_N.$$
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Initial data is factorized (particles i.i.d.):

$$\psi_0^N(x) = \prod_{j=1}^{N} \varphi_0(x_j) \in L^2_s(\mathbb{R}^{3N}).$$
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But interactions create correlations for $t > 0$. 
Mean-field pair interaction $U = \frac{1}{N} V$

Weak: order $1/N$. Long distance: $V \in L^\infty(\mathbb{R}^3)$.

$$i \partial_t \psi_N = \sum_{j=1}^{N} -\Delta_{x_j} \psi_N + \frac{1}{N} \sum_{i<j}^{N} V(x_i - x_j) \psi_N.$$
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Spohn, 1980: If $\psi_N$ is initially factorized and approximately factorized for all $t$, i.e., $\psi_N(x, t) \approx \prod_{j=1}^{N} \varphi(x_j, t)$, then "$\psi_N \to \varphi$" and $\varphi$ solves the Hartree equation:

$$i\partial_t \varphi = -\Delta \varphi + (V * |\varphi|^2)\varphi.$$
Convergence \( \psi_N \to \varphi \) means in the sense of marginals:

\[
\left\| \gamma_N^{(1)} - |\varphi\rangle\langle\varphi| \right\|_{Tr} \xrightarrow{N \to \infty} 0,
\]
Convergence "$\psi_N \to \varphi$" means in the sense of marginals:

$$\left\| \gamma^{(1)}_N - |\varphi\rangle\langle\varphi| \right\|_{Tr} \xrightarrow{N \to \infty} 0,$$

where $|\varphi\rangle\langle\varphi|(x_1, x'_1) = \overline{\varphi}(x_1)\varphi(x'_1)$ and one-particle marginal density $\gamma^{(1)}_N := Tr_{N-1}|\psi_N\rangle\langle\psi_N|$ has kernel

$$\gamma^{(1)}_N(x_1; x'_1, t) := \int \overline{\psi}_N(x_1, x_{N-1}, t)\psi_N(x'_1, x_{N-1}, t)dx_{N-1}.$$
Erdös and Yau, 2001: Convergence of marginals for Coulomb interaction, $V(x) = 1/|x|$, not assuming approximate factorization.
Other mean-field limit theorems

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Rodnianski-Schlein '08, Chen-Lee-Schlein, '11: convergence rate

$$\left\| \gamma_N^{(1)} - |\varphi\rangle\langle\varphi| \right\|_{Tr} \leq \frac{Ce^{Kt}}{N}.$$
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Preview of localizing interactions: $(V_N * |\varphi|^2)\varphi \rightarrow (\delta * |\varphi|^2)\varphi$

Erdős, Schlein, Yau, K., Staffilani, Chen, Pavlovic, Tzirakis...
Definition of BEC at zero temperature

Almost all particles are in the same one-particle state:

\[ \{ \psi_N \in L^2_s(\mathbb{R}^{3N}) \}_{N \in \mathbb{N}} \] exhibits Bose-Einstein condensation into one-particle quantum state \( \varphi \in L^2(\mathbb{R}^3) \) iff one-particle marginals converge in trace norm:

\[
\gamma^{(1)}_N = Tr_{N-1} |\psi_N\rangle\langle\psi_N| \xrightarrow{N \to \infty} |\varphi\rangle\langle\varphi|.
\]
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Almost all particles are in the same one-particle state:

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$$\gamma_N^{(1)} = \text{Tr}_{N-1} |\psi_N \rangle \langle \psi_N| \xrightarrow{N \to \infty} |\varphi \rangle \langle \varphi|.$$ 

Generalizes factorized: $$\psi_N(x) = \prod_{j=1}^N \varphi(x_j)$$ is BEC into $$\varphi.$$
BEC limit theorems with parameter $\beta \in (0, 1]$

Now localized strong interactions: $N^{d\beta} V(N^\beta(\cdot)) \to b_0 \delta$. 

$$H_N = \sum_{j=1}^{N} -\Delta x_j + \frac{1}{N} \sum_{i<j} N^{d\beta} V(N^\beta(x_i - x_j)).$$
BEC limit theorems with parameter $\beta \in (0, 1]$

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Theorems (Erdös-Schlein-Yau 2006-2008 $d = 3$
K.-Schlein-Staffilani 2009 $d = 2$ plane and rational tori): Systems that are initially BEC remain condensed for all time, and the macroscopic evolution is the NLS:

$$i \partial_t \varphi = -\Delta \varphi + b_0 |\varphi|^2 \varphi.$$
Our limit theorems make the physics of BEC rigorous

\[
H_N = \sum_{j=1}^{N} -\Delta x_j + \frac{1}{N} \sum_{i<j}^{N} N^{d\beta} V(N^\beta (x_i - x_j))
\]

\(N\)-body Schrod.

\textit{micro} : \(\psi^0_N \rightarrow \psi_N\)

init. BEC \(\downarrow\) \(\downarrow\) marg.

\textit{MACRO} : \(\varphi_0 \rightarrow \varphi\)

\textbf{NLS evolution}

\[i \partial_t \varphi = -\Delta \varphi + b_0 |\varphi|^2 \varphi.\]
A taste of quantum probability \((\mathcal{H}, \mathcal{P}, \varphi)\)

Hilbert space \(\mathcal{H}\), set of projections \(\mathcal{P}\), and state \(\varphi\).

Quantum random variables (RVs) or observables: operators on \(\mathcal{H}\).
A taste of quantum probability \((\mathcal{H}, \mathcal{P}, \varphi)\)

Hilbert space \(\mathcal{H}\), set of projections \(\mathcal{P}\), and state \(\varphi\).
Quantum random variables (RVs) or observables: operators on \(\mathcal{H}\).

The expectation of an observable \(A\) in a pure state is

\[
E_{\varphi}[A] := \langle \varphi | A\varphi \rangle = \int \varphi(x) \overline{A\varphi(x)} \, dx.
\]

Position observable is \(X(\varphi)(x) := x\varphi(x)\) with density \(|\varphi|^2\).
Only some probability facts have quantum analogues

Courtesy of Jordgette
The BEC limit theorems imply quantum LLNs

If $A$ is a one-particle observable and

$$A_j = 1 \otimes \cdots \otimes 1 \otimes A \otimes 1 \otimes \cdots \otimes 1,$$

then for each $\epsilon > 0,$

$$\limsup_{N \to \infty} \mathbb{P}_{\psi_N} \left\{ \left| \frac{1}{N} \sum_{j=1}^{N} A_j \right| \geq \epsilon \right\} = 0.$$
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BEC can explode as a bosenova
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We need a control theory of BEC

- Central limit theorem for BEC (Ben Arous-K.-Schlein, 2013)
  Our quantum CLT has correlations coming from interactions
- CLT for quantum groups (Brannan-K., 2015)
Our CLT for interacting quantum many-body systems

**Theorem (Ben Arous, K., Schlein, 2013):** Under suitable assumptions on the initial state $\psi_0^N$, $\varphi_0$, $A$, and $V$, then for $t \in \mathbb{R}$
Our CLT for interacting quantum many-body systems

Theorem (Ben Arous, K., Schlein, 2013): Under suitable assumptions on the initial state $\psi^0_N$, $\varphi_0$, $A$, and $V$, then for $t \in \mathbb{R}$

$$A_t := \frac{1}{\sqrt{N}} \sum_{j=1}^{N} (A_j - \mathbb{E}_{\varphi_t} A) \xrightarrow{\text{distrib. as } N \to \infty} \mathcal{N}(0, \sigma^2_t).$$
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The variance that we would guess is correct at $t = 0$ only:

$$\sigma_0^2 = \mathbb{E}_{\varphi_0} [A^2] - (\mathbb{E}_{\varphi_0} A)^2$$

$\sigma_t^2$ has $\varphi_0 \sim \varphi_t$. ....
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$\sigma_t^2$ has $\varphi_0 \rightsquigarrow \varphi_t$.... and twisted by the Bogoliubov transform.
We studied freely independent RVs via quantum groups (instead of random matrices) with Michael Brannan (Texas A&M)
Theorem (Brannan, K. 2015): Deformed quantum groups have an action

ASK MIKE FOR HIS ACTION FIGURE TEX CODE

on Free Araki-Woods factors
Theorem (Brannan, K. 2015): Deformed quantum groups have an action
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on Free Araki-Woods factors

\[ \Gamma = \Gamma(\mathbb{R}^n, U_t)'' := \{ \ell(\xi) + \ell(\xi)^* : \xi \in H_\mathbb{R} \}_{''} \]

with free quasi-free state \( \varphi_\Omega \),

\[ \alpha(c_i) = \sum u_{ij} \otimes c_j, \quad U_t = A^{it}, \quad \text{some } A > 0. \]

Usually a full type III_\lambda factor for \( \lambda \in [0, 1] \). Best case: \( \lambda = 1! \)
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Usually a full type \( \text{III}_{\lambda} \) factor for \( \lambda \in [0, 1] \). Best case: \( \lambda = 1! \) (exciting new development from MSRI...
Theorem (Brannan, K. 2015): For all almost-periodic representations $U_t$ on $H_{\mathbb{R}}$, there is a sequence of quantum groups

$$\left\{ O_{F(n)}^+ \right\}_{n \geq 1}$$

that has Haar distributional limit

$$(\Gamma, \varphi_{\Omega}).$$
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MH: quantum to classical; B-K: classical to quantum
How do physics, the world, and the universe work?

Physics

↓    ↑

Analysis
Thanks

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arXiv:0808.0505 (AJM), 1009.5737 (CPAM), 1111.6999 (CMP), 1505.05137(PJM)
Why do interactions become the cubic nonlinearity?

\[ i \partial_t \psi_N = \sum -\Delta x_j \psi_N + \frac{1}{N} \sum \sum V(x_i - x_j) \psi_N \]

Particle 1 sees

\[ \frac{1}{N} \sum_{j=2}^{N} V(x_1 - x_j) \simeq \frac{1}{N} \sum_{j=2}^{N} \int V(x_1 - y)|\varphi(y)|^2 \, dy \]

\[ = \frac{N - 1}{N} \int V(x_1 - y)|\varphi(y)|^2 \, dy \]

\[ \xrightarrow{N \to \infty} (V * |\varphi|^2)(x_1) \]