#### Bose-Einstein condensation and limit theorems

Kay Kirkpatrick, UIUC

2015

Bose-Einstein condensation: from many quantum particles to a quantum "superparticle"



#### Kay Kirkpatrick, UIUC/MSRI

TexAMP 2015



The big challenge: making physics rigorous

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microscopic first principles  $\rightsquigarrow$  zoom out  $\rightsquigarrow$  MACROSCOPIC  ${\rm STATES}$ 



Courtesy Greg L and Digital Vision/Getty Images

1925: predicting Bose-Einstein condensation (BEC)

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1995: Cornell-Wieman and Ketterle experiment



Courtesy U Michigan



#### 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)

#### The mathematics of BEC

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

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Can we rigorously connect the physics and the math?

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Can we rigorously connect the physics and the math?

Yes!

The outline (w/ G. Staffilani, B. Schlein, G. Ben Arous)

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

- N bosons → mean-field limit → Hartree equation
   N bosons → localizing limit → 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

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$$-\Delta = -\sum_{i=1}^{d} \partial_{x^i x^i} \ge 0$$

external trapping potential V<sub>ext</sub>

• solution 
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• 
$$\int |\psi_0|^2 = 1 \implies |\psi(x, t)|^2$$
 is a probability density for all t.  
Exercise: why?

Particle in a box



 $V_{ext} = ``\infty \cdot \mathbf{1}_{[0,1]}c"$  has ground state  $\psi(x) = \sqrt{2}\sin(\pi x)$ 

#### The microscopic *N*-particle model

Wavefunction  $\psi_N(\mathbf{x}, t) = \psi_N(x_1, ..., x_N, t) \in L^2(\mathbb{R}^{dN}) \ \forall t$  solves the *N*-body Schrödinger equation:

$$i\partial_t\psi_N = \sum_{j=1}^N -\Delta_{x_j}\psi_N + \sum_{i< j}^N U(x_i - x_j)\psi_N =: H_N\psi_N$$

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pair interaction potential U

• solution 
$$\psi_N(\mathbf{x}, t) = e^{-iH_N t} \psi_N^0(\mathbf{x})$$

• joint density 
$$|\psi_N(x_1,\ldots,x_N,t)|^2$$

#### More assumptions

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

 $\psi_N(x_{\sigma(1)},...,x_{\sigma(N)},t) = \psi_N(x_1,...,x_N,t)$  for  $\sigma \in S_N$ .

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Initial data is factorized (particles i.i.d.):

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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.,  $\psi_N(\mathbf{x}, t) \simeq \prod_{j=1}^N \varphi(x_j, t)$ , then " $\psi_N \to \varphi$ " and  $\varphi$  solves the Hartree equation:

$$i\partial_t \varphi = -\Delta \varphi + (V * |\varphi|^2) \varphi.$$

Convergence " $\psi_N \rightarrow \varphi$ " means in the sense of marginals:

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

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where  $|arphi
angle\langle arphi|(x_1,x_1')=\overline{arphi}(x_1)arphi(x_1')$  and

one-particle marginal density  $\gamma_N^{(1)} := Tr_{N-1} |\psi_N\rangle \langle \psi_N|$  has kernel

$$\gamma_{N}^{(1)}(\mathbf{x}_{1};\mathbf{x}_{1}',t):=\int \overline{\psi}_{N}(\mathbf{x}_{1},\mathbf{x}_{N-1},t)\psi_{N}(\mathbf{x}_{1}',\mathbf{x}_{N-1},t)d\mathbf{x}_{N-1}.$$

#### Other mean-field limit theorems

Erdös and Yau, 2001: Convergence of marginals for Coulomb interaction,  $V(\mathbf{x}) = 1/|\mathbf{x}|$ , not assuming approximate factorization.

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Preview of localizing interactions:  $(V_N * |\varphi|^2)\varphi \rightarrow (\delta * |\varphi|^2)\varphi$ Erdös, 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:

$$\gamma_{N}^{(1)} = Tr_{N-1} |\psi_{N}\rangle \langle \psi_{N}| \xrightarrow{N \to \infty} |\varphi\rangle \langle \varphi|.$$

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Generalizes factorized:  $\psi_N(\mathbf{x}) = \prod_{j=1}^N \varphi(x_j)$  is BEC into  $\varphi$ .

# BEC limit theorems with parameter $\beta \in (0, 1]$

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

$$H_N = \sum_{j=1}^N -\Delta_{x_j} + \frac{1}{N} \sum_{i< j}^N N^{d\beta} V(N^\beta(x_i - x_j)).$$

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Theorems (Erdös-Schlein-Yau 2006-2008 d = 3K.-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

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  $\mathcal{H}$ .

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The expectation of an observable A in a pure state is

$$\mathbb{E}_{\varphi}[A] := \langle arphi | A arphi 
angle = \int arphi(x) \overline{A arphi}(x) dx.$$

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  $\epsilon > 0$ ,

$$\limsup_{N\to\infty}\mathbb{P}_{\psi_N}\left\{\left|\frac{1}{N}\sum_{j=1}^N A_j\right.\right.\right.$$

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$$\limsup_{N\to\infty} \mathbb{P}_{\psi_N}\left\{ \left| \frac{1}{N} \sum_{j=1}^N A_j - \langle \varphi | A \varphi \rangle \right| \geq \epsilon \right\} = 0.$$



BEC can explode as a bosenova

# 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)

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

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$$\mathcal{A}_t := rac{1}{\sqrt{N}} \sum_{j=1}^N (A_j - \mathbb{E}_{arphi_t} A) \xrightarrow{distrib. \ as \ N o \infty} \mathcal{N}(0, \sigma_t^2).$$

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The variance that we would guess is correct at t = 0 only:

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 $\sigma_t^2$  has  $\varphi_0 \rightsquigarrow \varphi_t \dots$  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

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

with free quasi-free state  $\varphi_{\Omega}$ ,

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

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MH: quantum to classical; B-K: classical to quantum

How do physics, the world, and the universe work?

 $\downarrow$ 

# Physics

 $\uparrow$ 

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?

$$i\partial_t\psi_N=\sum-\Delta_{x_j}\psi_N+rac{1}{N}\sum\sum V(x_i-x_j)\psi_N$$

Particle 1 sees

$$\begin{split} \frac{1}{N}\sum_{j=2}^{N}V(x_1-x_j) &\simeq \frac{1}{N}\sum_{j=2}^{N}\int V(x_1-y)|\varphi(y)|^2dy\\ &= \frac{N-1}{N}\int V(x_1-y)|\varphi(y)|^2dy\\ &\xrightarrow{N\to\infty} (V*|\varphi|^2)(x_1) \end{split}$$