# Bose-Einstein condensation and quantum many-body systems

Kay Kirkpatrick, UIUC

Joint work with B. Schlein (Cambridge), G. Staffilani (MIT), S. Chatterjee and G. Ben Arous (Courant), J. Blanchet (Columbia).

February 14, 2010

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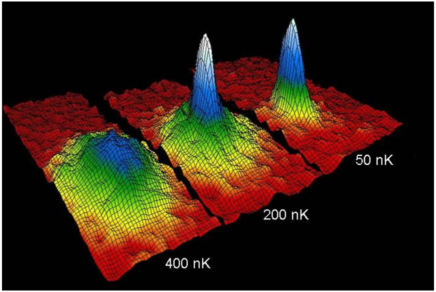

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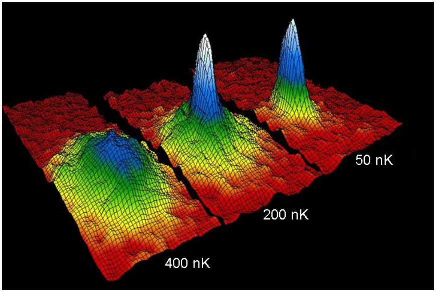

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# The physics of Bose-Einstein condensation

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Cornell-Wieman and Ketterle 1995: First observed Bose-Einstein condensation. They trapped a rubidium gas magnetically and cooled it to about 170 nK by evaporational cooling and lasers.

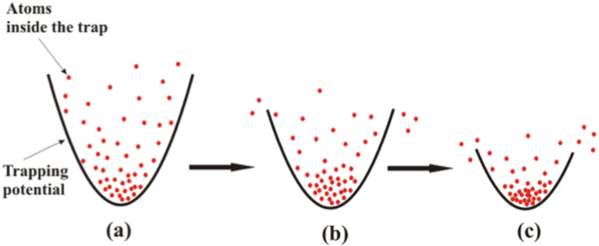

Figure: Particles condensing in the trap. (Courtesy of U Michigan)

# The physics of BEC, cont.

When they turned off the trap, the gas remained coherent and moved as if it were a single macroscopic quantum particle, an "atom laser."

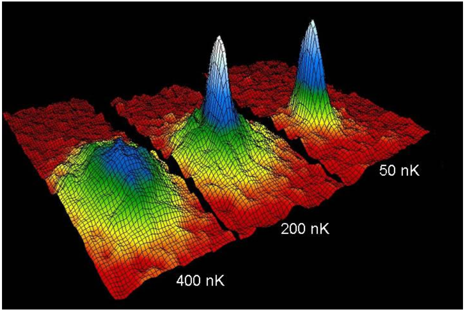

Figure: Snapshot of bosons' momenta after the trap is removed. (Atomic Lab)

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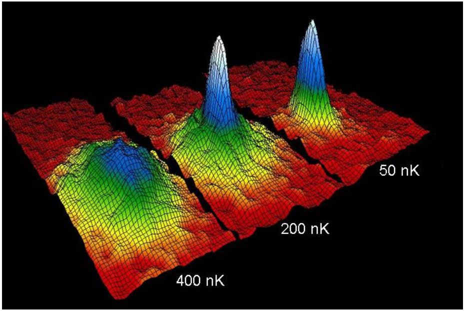

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Applications to interferometry, quantum computing, and more.

# The mathematics of BEC

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Fruitful NLS research in hopes of understanding BEC: big idea being dispersion vs. nonlinearity.

- Dispersion wins: solutions exist and can be nice. (e.g., $\mu = 1$)
- Nonlinearity wins: blow-up. (e.g., $\mu = -1$ in 3D)
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Yes, via statistical mechanics...

# The outline

Hilbert 6: Microscopic first principles for $N$ particles
$\rightsquigarrow N \to \infty \rightsquigarrow$ Macroscopic description of phenomena

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$\rightsquigarrow N \to \infty \rightsquigarrow$ Macroscopic description of phenomena

- First approximation of BEC: Systems of $N$ bosons with mean-field interactions $\rightsquigarrow$ Hartree equation
- Holy grail: Collapse of BEC and quantum control

  Attacks via CLT, discretization, and computation.

# One quantum particle in a potential

A quantum "particle" is really a wavefunction $\phi(x,t)$ in $L^2(\mathbb{R}^d)$ for each $t$, that satisfies a linear Schrödinger equation:

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

- $\Delta = \sum_{i=1}^{d} \partial_{x^i x^i}$ so $-\Delta \geq 0$; and $V_{ext}$ is external potential.

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- Solution is given by semigroup of operators applied to the initial condition: $\phi(x,t) = e^{-iHt}\phi_0(x)$.
- The probability amplitude, $|\phi(x,t)|^2$, is the probability density for some "quantum random variable."

# The “particle in a box/infinite square well”

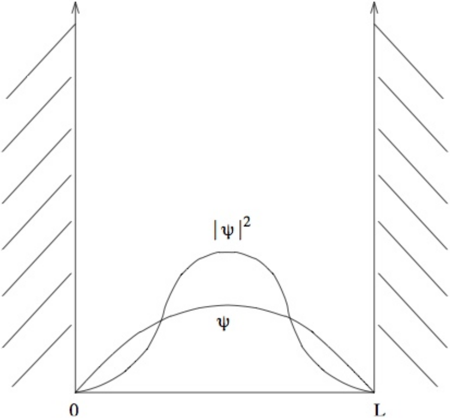

Figure: If $V_{ext} =$ “$\infty \cdot \mathbf{1}_{[0,L]^c}$” then the ground state is $\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$ with probability amplitude $|\psi|^2$.

# Quantum probability for one particle

$(\Omega, \mathcal{F}, P)$ is replaced by $(\mathcal{H} = L^2(\mathbb{R}^d), \mathcal{P}, \phi)$, with $\mathcal{P}$ being the set of orthogonal projections $P_M$, and $\phi$ a **state** or wavefunction.

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Random variables: **observables** A on $\mathcal{H}$, form a $*$-algebra $\mathcal{A}$.

The expectation of $A$ in a state $\phi$ is $\mathbb{E}_\phi[A] := \phi(A)$, and if $\phi$ is **pure** then:

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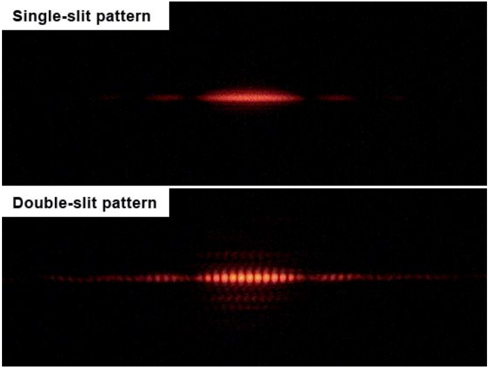
Why? Moments of $X_t$ are $\langle \phi | X_t^n \phi \rangle = \int x^n |\phi(x,t)|^2 dx$.

# Caveats about quantum probability

Main obstacle: interference effects. (Courtesy of Jordgette)



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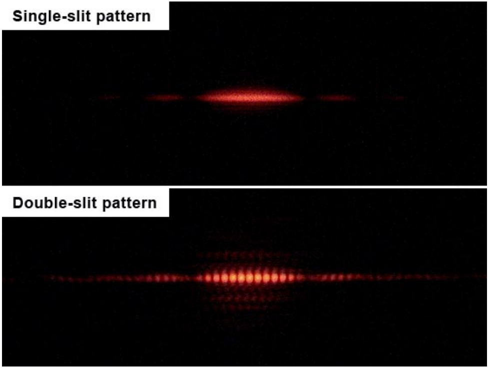

Some limit theorems have quantum analogues, but not others.

# The general $N$-particle microscopic model

The wavefunction $\psi_N(\mathbf{x}, t) = \psi_N(x_1, ..., x_N, t) \in L^2(\mathbb{R}^{dN})$, for a system of $N$ particles, satisfies 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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- Solution written as semigroup of operators applied to the initial condition: $\psi_N(\mathbf{x}, t) = e^{-iH_N t}\psi_N^0(\mathbf{x})$
- Now $|\psi_N(x_1, \ldots, x_N, t)|^2$ is a joint probability density.

# Additional assumptions for $N$-boson models

The wavefunction $\psi_N$ for a system of $N$ **bosons** is symmetric with respect to permutations:

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

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For $t > 0$, interactions kill independence. Mean-field interactions...

# The mean-field case in 3D, and a limit theorem

Consider the mean-field pair interaction $U = \frac{1}{N} V$:

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

Weak: each interaction is of strength $1/N$.
Diffuse: interactions can occur at any distance, in $supp(V)$.

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Spohn, 1980: Let $V \in L^\infty(\mathbb{R}^3)$ and $\psi_N$ initially factorized and approx. factorized for all $t$: $\psi_N(\mathbf{x}, t) \simeq \prod_{j=1}^{N} \phi(x_j, t)$.

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

# Improved limit theorems and the marginals

Erdös and Yau, 2001: Same for Coulomb, $V(\mathbf{x}) = 1/|\mathbf{x}|$, and also no unsatisfactory approximate factorization assumption.

Macroscopic Hartree evolution: $i\partial_t \phi = -\Delta\phi + (\frac{1}{|\cdot|} * |\phi|^2)\phi$.

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Here $\gamma_N^{(1)}$ is one-particle marginal density matrix $\gamma_N^{(1)} := Tr_{N-1}|\psi_N\rangle\langle\psi_N|$, with kernel given by:

$$\gamma_N^{(1)}(x_1; x_1') := \int \overline{\psi}_N(x_1, \mathbf{x}_{N-1})\psi_N(x_1', \mathbf{x}_{N-1}) d\mathbf{x}_{N-1}.$$

# Translating to a (weak) law of large numbers

1-particle observable $\sum_{j=1}^{N} A^{(j)}$, with $A$ in the $j^{th}$ slot:

$$A^{(j)} = 1 \otimes 1 \otimes \cdots \otimes A \otimes 1 \cdots \otimes 1$$

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Preview of next section: Central limit theorem? Large deviations?

Preview of last section: if the potential $V$ were the delta function, then the Hartree equation would become the cubic NLS:

$$i\partial_t \phi = -\Delta \phi + (\delta * |\phi|^2)\phi = -\Delta \phi + |\phi|^2 \phi.$$

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Quantum control, to build materials like quantum computers.

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- Central limit theorem for BEC (Ben Arous-K.-Schlein, 2011)
- Phase transition in the discrete NLS (Chatterjee-K., 2010)
- LDP and computational quantum many-body systems (with Ben Arous, Schlein, Blanchet, both in progress)

# A CLT for quantum many-body dynamics

**Theorem (Ben Arous, K., Schlein, 2011):** Factorized initial state $\psi_N^0 = \phi_0^{\otimes N}$ with normed $\phi_0 \in H^1$. If $A$ is a compact self-adjoint operator on $L^2(\mathbb{R}^3)$ and $t \in \mathbb{R}$, and $V \leq 1/|\cdot|$.

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$$\text{Then fluctuations } \mathcal{A}_t := \frac{1}{\sqrt{N}} \sum_{j=1}^{N} (A^{(j)} - \mathbb{E}_\phi A),$$

with $j^{th}$ particle observable $A^{(j)} = 1 \otimes 1 \otimes \cdots \otimes A \otimes 1 \cdots \otimes 1$, (and law of $\mathcal{A}_t$ is from $\psi_N$), converge to centered normal random variables with variance:

$$\sigma_t^2 = ||U_t A\phi + JV_t A\phi||^2 - |\langle \phi | U_t A\phi + JV_t A\phi \rangle|^2.$$

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IID particles at $t = 0$ only, and $\sigma_{t=0}^2 = ||A\phi_0||^2 - \langle \phi_0 | A\phi_0 \rangle^2$. Interactions change the variance, but don't destroy the CLT.

# The CLT and the main ingredients

$$\frac{\sum_{j=1}^{N} A^{(j)} - \mathbb{E}_{\phi} A}{\sqrt{N}} \to \mathcal{N}(0, ||U_t A\phi + J V_t A\phi||^2 - |\langle \phi | U_t A\phi + J V_t A\phi \rangle|^2)$$

New in this context: bosonic Bogoliubov transform

$$\Theta(t;s) = \begin{pmatrix} U(t;s) & JV(t;s)J \\ V(t;s) & JU(t;s)J \end{pmatrix}$$

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for $Jf = \overline{f}$ and bounded linear maps $U(t;s), V(t;s)$ on $L^2(\mathbb{R}^3)$ s.t.

$$U^*(t;s)U(t;s) - V^*(t;s)V(t;s) = 1,$$

$$U^*(t;s)JV(t;s)J = V^*(t;s)JU(t;s)J.$$

# More

Note

$$\Theta(t;s) : (\phi(\cdot,t),\overline{\phi}(\cdot,t)) \mapsto (\phi(\cdot,s),\overline{\phi}(\cdot,s)).$$

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$$\leq \frac{||A||}{\sqrt{N}} \sum_{j=1}^{N} Tr \left| \gamma_N^{(1)} - |\phi\rangle\langle\phi| \right| \lesssim \frac{||A|| e^{K|t|}}{\sqrt{N}} \to 0.$$

# Convergence of the higher moments

- Bounds on all moments of the number-of-particles observable, the first one or two moments of the kinetic energy observable, with respect to the limiting dynamics and to the full fluctuation dynamics.

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- Bounds comparing the kinetic energy to the Hamiltonian and generators of the dynamics.
- Combinatorics

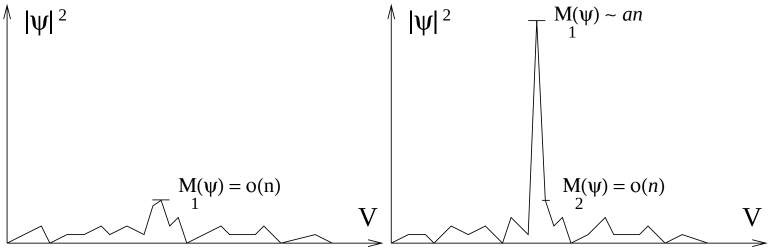
# Outline: Collapse of Bose-Einstein condensation

Quantum control, to build materials like quantum computers.

- Central limit theorem for BEC (Ben Arous-K.-Schlein, 2011)
- Phase transition in the discrete NLS (Chatterjee-K., 2010)
- LDP and computational quantum many-body systems (with Ben Arous, Schlein, Blanchet, both in progress)

# Impressionistic pictures of the two phases

Subcritical: Supercritical:



Non-condensed phase
$M_1(\psi)$ mass of heaviest site

Condensed phase
$M_2(\psi)$ second-largest site

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Problem: Gibbs measures probably can't be defined for 3D...

# Our way around this problem

Discrete NLS: $i\frac{d}{dt}f_x = -\widetilde{\Delta} f_x - |f_x|^2 f_x,$ on 3D torus,

$V = \{1/L, 2/L \ldots, 1\}^3$, spacing $h = 1/L$, and $n = L^3$ finite.

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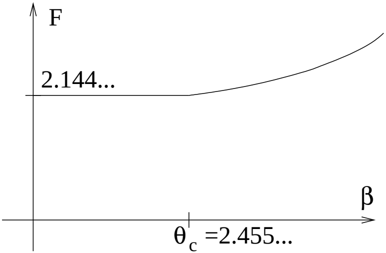
Natural invariant measures:

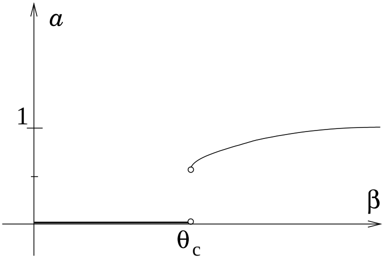
$$d\mu_{\beta,B} := Z^{-1}e^{-\beta H(f)}1_{\{N(f)\le B\}}\prod_{x\in V}df_x.$$

Partition function $Z$, inverse temperature $\beta$, and allowed mass $B$.

# The free energy and the mass at the heaviest site

Left: $Z(\beta, B) \sim e^{nF(\beta,B)}$, and mass is normalized, $B = 1$.





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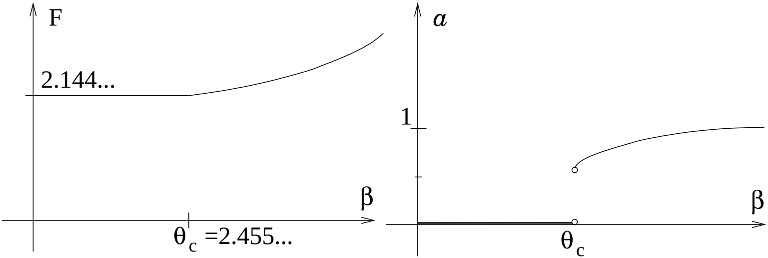

Right: $\psi$ picked from Gibbs measure $\mu$ is localized at $y$ for $\beta > \theta_c$:

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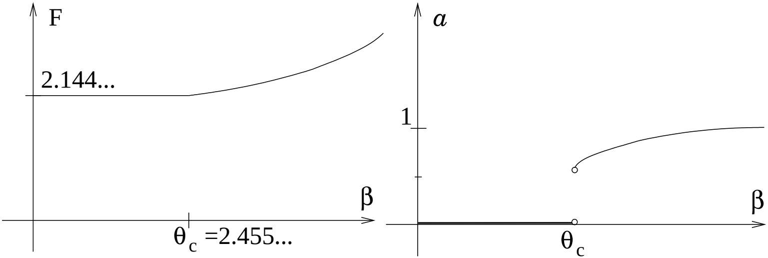

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This is a 1st order phase transition...

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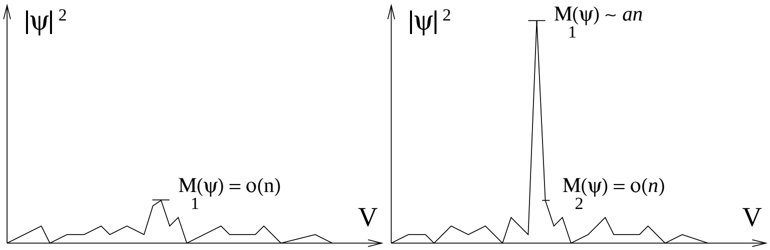

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Experiments: existence of a similar localized phase in 1D, a crossover from BEC to Anderson localization in physical space.

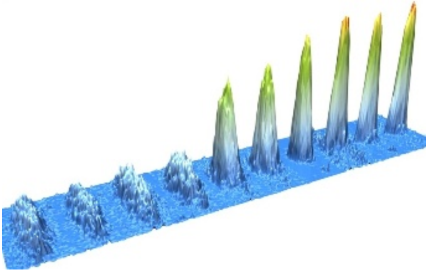

Figure: Weak (left) to strong (r) quasiperiodic potential. (LENS QDG)

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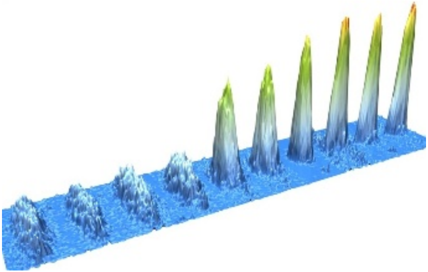

Figure: Weak (left) to strong (r) quasiperiodic potential. (LENS QDG)

Observing the condensed phase that we have discovered?

# Outline: better BEC model

- Microscopic model of BEC with localizing interactions
- 3D BEC scaling limit (Erdös-Schlein-Yau, 2006-2008)
- 2D BEC, both plane and torus (K.-Schlein-Staffilani, 2008)

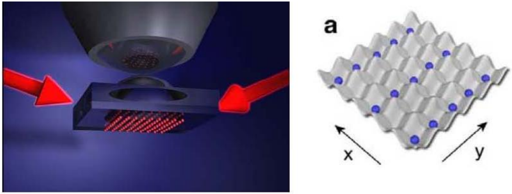

Figure: BEC loaded into 2D optical lattice (Courtesy of U Mass)

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Zero temperature: BEC happens when almost all of the particles are described by the same one-particle state.

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A sequence $\{\psi_N \in L^2_s(\mathbb{R}^{3N})\}_{N\in\mathbb{N}}$ exhibits **Bose-Einstein condensation (BEC)** into the one-particle quantum state $\phi \in L^2(\mathbb{R}^3)$ iff the one-particle marginal $\gamma_N^{(1)} = Tr_{N-1}|\psi_N\rangle\langle\psi_N|$,

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Example: $\psi_N(\mathbf{x}) = \prod_{j=1}^N \phi(x_j)$ exhibits BEC into $\phi$. Others?

# The microscopic model for 3D BEC

Consider a family of $N$-boson systems parametrized by $\beta \in (0,1]$:

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j}\psi_N + \frac{1}{N}\sum_{i<j}^{N} N^{3\beta} V(N^{\beta}(x_i - x_j)).$$

The interactions are strong: $N^{3\beta-1}$; and short scale: $N^{\beta}$ factor.
They localize: $V \geq 0$ a bump function, so $N^{3\beta} V(N^{\beta}(\cdot)) \to b_0\delta$.

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Then for all $t \in \mathbb{R}$, $\psi_N$ is still BEC with $\phi$ solving the NLS:

$$i\partial_t\phi = -\Delta\phi + b_0|\phi|^2\phi.$$

# The 2D BEC models

**Theorem (K., Schlein, and Staffilani, 2008):** Consider a 2D domain $\Lambda = \mathbb{R}^2$, or $\Lambda = [-1, 1]^2$ with periodic boundary conditions, and the $N$-particle Schrödinger equation on $\Lambda$:

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If the initial state is BEC with $\phi_0 \in L^2(\Lambda)$, and other appropriate assumptions (bdd energy per particle, etc), then BEC persists for all $t$, and $\psi_N \to \phi$ in the sense of marginals. And the macroscopic evolution is governed by the NLS (a.k.a. Gross-Pitaevskii) equation on $\Lambda$:

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Here $\beta \in (0, 3/4)$ (technical restriction); and $b_0 = \int_\Lambda V(x)dx$.

# A diagram of what's going on

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j}\psi_N + \frac{1}{N}\sum_{i<j}^{N} N^{2\beta} V(N^{\beta}(x_i - x_j))$$

$$\begin{tikzcd}
micro : & \psi_N^0 \arrow[r, "N\text{-body Schrod.}"] \arrow[d, "\text{init. BEC}"'] & \psi_N \arrow[d, "\textbf{marg.}"] \\
MACRO : & \phi_0 \arrow[r, "\textbf{GP evolution}"'] & \phi
\end{tikzcd}$$

$$i\partial_t\phi = -\Delta\phi + b_0|\phi|^2\phi.$$

The conclusions of the theorem are in bold. So the physicist's heuristic of the GP/NLS effective evolution is now rigorous.

# The upshot and the outlook

- The physics of quantum many-body systems is rigorously connected to the mathematics of the nonlinear Schrödinger equation.
- Getting at this bosenova phase transition is tough: so far, CLT for quantum many-body systems, Gibbs for discrete NLS.

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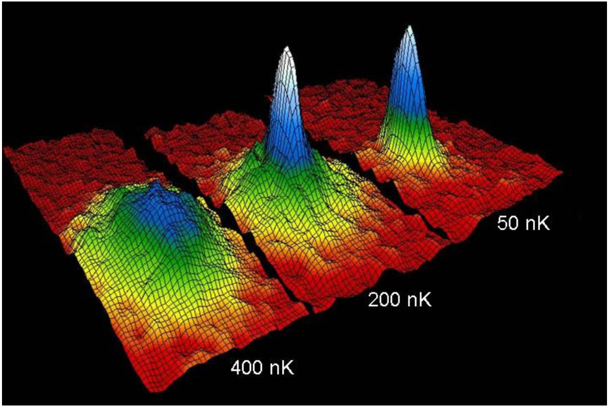
- Getting at this bosenova phase transition is tough: so far, CLT for quantum many-body systems, Gibbs for discrete NLS.

- LDP issues in noncommutative probability.
- Computational approach, in progress with J. Blanchet.

# Thank you



arXiv: 0808.0505 (AJM), 1009.5737 (CPAM), 1109.0274 (survey), 1111.6999