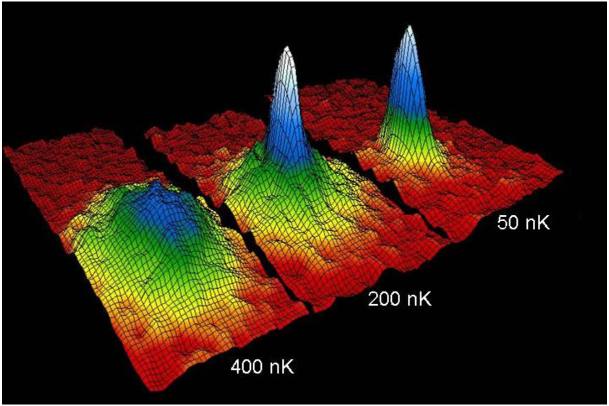
Bose-Einstein condensation and mean-field limits

Kay Kirkpatrick, UIUC

2015

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



Kay Kirkpatrick, Urbana-Champaign

IMA, May 2015

The big challenge: making physics rigorous

microscopic first principles $\rightsquigarrow$ zoom out $\rightsquigarrow$ $\textsc{Macroscopic states}$

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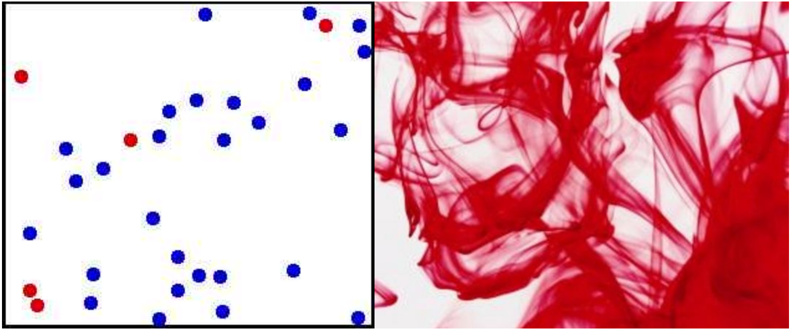

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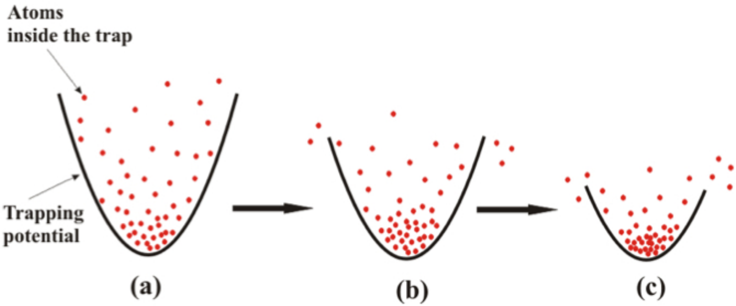
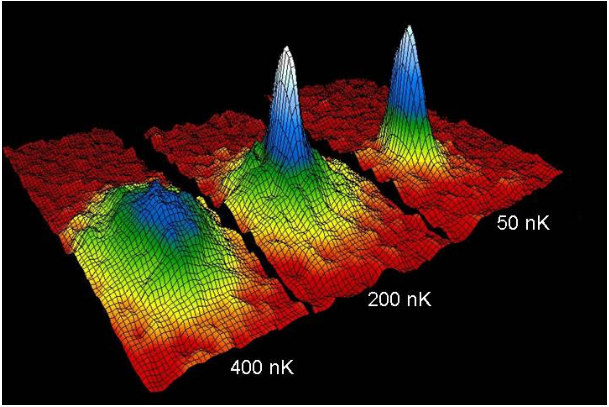


Cornell-Wieman and Ketterle 1995: trapped and condensed rubidium around 170 nK. (Courtesy U Michigan)

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

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

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Yes, via statistical mechanics...

The outline

microscopic first principles $\rightsquigarrow \rightsquigarrow \rightsquigarrow$ MACROSCOPIC STATES

- N bosons $\rightsquigarrow$ mean-field limit $\rightsquigarrow$ HARTREE EQUATION
- N bosons $\rightsquigarrow$ localizing limit $\rightsquigarrow$ NLS
- Translate to quantum LLN
- Quantum CLT

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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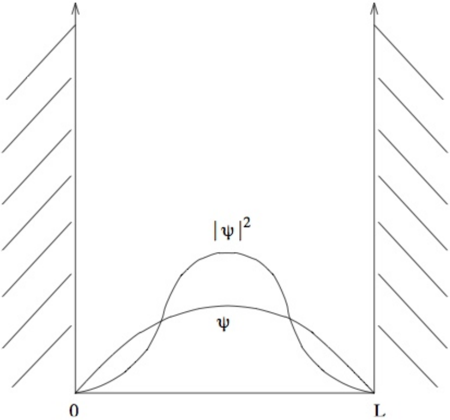
- solution $\psi(x,t) = e^{-iHt}\psi_0(x)$
- $\int |\psi_0|^2 = 1 \implies |\psi(x,t)|^2$ is a probability density for all t. Why?

Particle in a box



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

The microscopic N-particle model

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

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

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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 $|\psi_N(x_1, \dots, x_N, t)|^2$

Assumptions for N bosons

ψ_N is symmetric (particles exchangeable):

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

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But interactions kill independence for $t > 0$.

Mean-field pair interaction $U = \frac{1}{N} V$

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

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Spohn, 1980: If ψ_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 $\psi_N \to \varphi$ in the sense of marginals, and φ solves the Hartree equation:

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

Convergence $\psi_N \to \varphi$ in the sense of marginals means

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

where $|\varphi\rangle\langle\varphi|(x_1, x_1') = \overline{\varphi}(x_1)\varphi(x_1')$ and

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

$$\gamma_N^{(1)}(x_1; x_1', t) := \int \overline{\psi}_N(x_1, \mathbf{x}_{N-1}, t)\psi_N(x_1', \mathbf{x}_{N-1}, t) d\mathbf{x}_{N-1}.$$

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

$$\left\| \gamma_N^{(1)} - |\varphi\rangle\langle\varphi| \right\|_{Tr} \leq \frac{Ce^{Kt}}{N}.$$

Definition of BEC at zero temperature

Almost all particles are in same one-particle state.

Sequence $\{\psi_N \in L^2_s(\mathbb{R}^{3N})\}_{N\in\mathbb{N}}$ exhibits **Bose-Einstein condensation** with one-particle quantum state $\varphi \in L^2(\mathbb{R}^3)$ iff

one-particle marginals converge in trace norm:

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Like factorized, $\psi_N(\mathbf{x}) = \prod_{j=1}^N \varphi(x_j)$ is BEC with φ, but weaker.

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

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

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

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Theorems (Erdös-Schlein-Yau 2006-2008 $d = 3$
K.-Schlein-Staffilani 2009 $d = 2$ **plane and torus):**
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

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

$$\begin{array}{lccccl} & & \text{N-body Schrod.} & & \\ \textit{micro}: & \psi_N^0 & \longrightarrow & \psi_N & \\ \text{init. BEC} & \downarrow & & \downarrow & \textbf{marg.} \\ \textit{MACRO}: & \varphi_0 & \longrightarrow & \varphi & \\ & & \textbf{NLS evolution} & & \end{array}$$

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

Note: $|\varphi|^2$ is a probability density function for all time.

Translating to quantum probability space $(\mathcal{H}, \mathcal{P}, \varphi)$

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Quantum random variables or observables are operators on $\mathcal{H}$.

The expectation of an observable A in a pure state is

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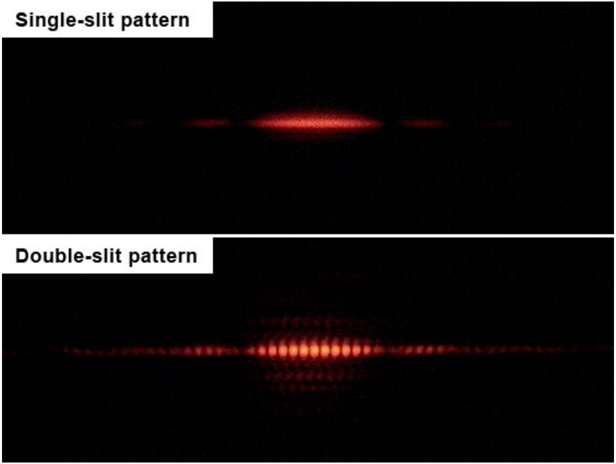
Position observable $X(\varphi)(x) := x\varphi(x)$ has density $|\varphi|^2$.

N position RVs $\{X_i = M_{x_i}\}_{i=1}^{N}$ have joint density $|\psi_N|^2$.

Main caveat is interference (Courtesy of Jordgette)



Only some probability facts have quantum probability analogues.

The limit theorems are really Q LLNs

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then under the previous assumptions, for each $\epsilon > 0$,

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

Note $\mathbb{P}_{\psi_N}\{S\} = \int_S |\psi_N|^2$. Proof: Chebyshev and convergence rate.

Control theory for quantum computing

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- Central limit theorem for BEC (Ben Arous-K.-Schlein, 2011).

  Our quantum CLT has correlations coming from interactions.
- Large deviations principle for quantum many-body systems.

Our CLT for interacting quantum many-body systems

Theorem (Ben Arous, K., Schlein, 2013): If the initial state is factorized $\psi_N^0 = \varphi_0^{\otimes N}$ with normalized $\varphi_0 \in H^1(\mathbb{R}^3)$, and A is compact self-adjoint on $L^2(\mathbb{R}^3)$, and $V \leq 1/|\cdot|$, then for $t \in \mathbb{R}$

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Distribution of $\mathcal{A}_t$ from $\psi_N = \psi_{N,t}$.

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The obvious variance is correct at $t = 0$ only (i.i.d.):

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The variance σ_t^2 is more subtle than replacing φ_0 by φ_t.

Our novel use of the bosonic Bogoliubov transform

$$\Theta_{t,s} : (\varphi(\cdot, t), \overline{\varphi}(\cdot, t)) \mapsto (\varphi(\cdot, s), \overline{\varphi}(\cdot, s))$$

written

$$\Theta_{t,0} = \begin{pmatrix} U_t & JV_tJ \\ V_t & JU_tJ \end{pmatrix},$$

Here $Jf = \overline{f}$ and U_t, V_t are bounded linear maps on $L^2(\mathbb{R}^3)$ s.t.

$$U_t^* U_t - V_t^* V_t = 1, \qquad U_t^* J V_t J = V_t^* J U_t J.$$

Then the correct variance is twisted by $\Theta_{t,0}$:

$$\sigma_t^2 = ||U_t A \varphi_t + J V_t A \varphi_t||^2 - |\langle \varphi_t | U_t A \varphi_t + J V_t A \varphi_t \rangle|^2.$$

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$$|\mathbb{E}_{\psi_N} \mathcal{A}_t| = \left| \frac{1}{\sqrt{N}} \sum_{j=1}^{N} Tr\, A(\gamma_N^{(1)} - |\varphi\rangle\langle\varphi|) \right|$$

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

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(Also regularize interaction potential to handle Coulomb.)

Convergence of the second moment

$$\mathbb{E}_{\psi_N}\left(\frac{1}{\sqrt{N}}\sum_{j=1}^{N}(A_j - \mathbb{E}_{\varphi_t}A)\right)^2 = Tr\,\gamma_N^{(1)}\widetilde{A}^2 + NTr\,\gamma_N^{(2)}(\widetilde{A}\otimes\widetilde{A})$$

First term: $\|\widetilde{A}\varphi_t\|^2$, same as for i.i.d. case $\varphi_t^{\otimes N}$.

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Higher moments: Bounds on moments of observables w.r.t. fluctuation dynamics $\mathcal{U}_N(t,s) = W^*(\sqrt{N}\varphi_t)e^{-i\mathcal{H}_N(t-s)}W(\sqrt{N}\varphi_s)$ around the mean-field approximation $W(\sqrt{N}\varphi_t)\Omega$, and the limiting dynamics $\mathcal{U}_\infty(t,s)$ given by the Bogoliubov transform.

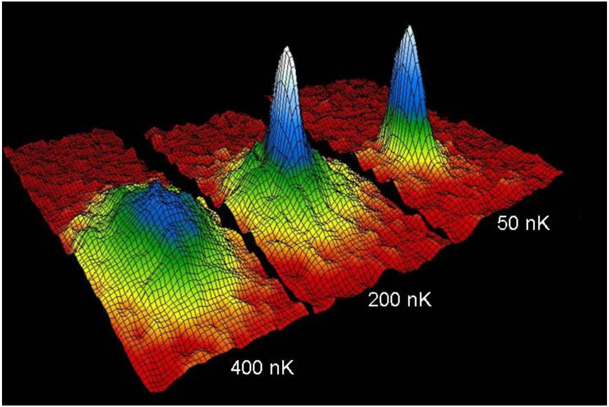
Plus combinatorics. Plus Fock space and coherent states.

We've made the physics of BEC rigorous

- Other mean-field models: my PhD students Leslie Ross (physics) and Tayyab Nawaz (math).
- Quantum groups models of freely independent RVs with Michael Brannnan.
- Gibbs measures and heat kernel estimates for dispersive PDEs with postdocs Janna Lierl and Samantha Xu.

Thanks

NSF DMS-1106770, OISE-0730136, CAREER DMS-1254791



arXiv:0808.0505 (AJM), 1009.5737 (CPAM), 1109.0274 (MMNP), 1111.6999 (CMP), forthcoming

Program

New Challenges in PDE: Deterministic Dynamics and Randomness in High and Infinite Dimensional Systems

August 17, 2015 to December 18, 2015

Organizers

Kay Kirkpatrick (University of Illinois at Urbana-Champaign), Yvan Martel (École Polytechnique), Jonathan Mattingly (Duke University), Andrea Nahmod (University of Massachusetts, Amherst), Pierre Raphael (Universite de Nice Sophia-Antipolis), Luc Rey-Bellet (University of Massachusetts, Amherst), LEAD Gigliola Staffilani (Massachusetts Institute of Technology), Daniel Tataru (University of California, Berkeley)

The bosonic Fock space

Fock space: $\mathcal{F} = \bigoplus_{n\geq 0} L_s^2(\mathbb{R}^{3n}, dx_1 \dots dx_n)$

Inner product:

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Number-of-particles operator: $\mathcal{N}\{\psi^{(n)}\}_{n \geq 0} = \{n\psi^{(n)}\}_{n \geq 0}$,
eigenvectors $\{0, \dots, 0, \psi^{(m)}, 0, \dots\}$.

Hamiltonian: $$\mathcal{H}_N^{(m)} = \sum_{j=1}^{m} -\Delta_{x_j} + \frac{1}{N} \sum_{i<j}^{m} V(x_i - x_j) \,.$$

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Hamiltonian: $$\mathcal{H}_N^{(m)} = \sum_{j=1}^{m} -\Delta_{x_j} + \frac{1}{N} \sum_{i<j}^{m} V(x_i - x_j) \, .$$

Then $e^{-i\mathcal{H}_N t}\{0, \dots, 0, \psi_N, 0, \dots\} = \{0, \dots, 0, e^{-iH_N t}\psi_N, 0, \dots\}$.

Advantage: Particle number not fixed.

Creation and annihilation operators

$$\left(a^*(f)\psi\right)^{(n)}(x_1,\ldots,x_n) = \frac{1}{\sqrt{n}}\sum_{j=1}^{n} f(x_j)\psi^{(n-1)}(x_1,\ldots,x_{j-1},x_{j+1},\ldots,x_n)$$

$$\left(a(f)\psi\right)^{(n)}(x_1,\ldots,x_n) = \sqrt{n+1}\int dx\, \overline{f(x)}\psi^{(n+1)}(x,x_1,\ldots,x_n)\,.$$

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Operator-valued distributions a_x, a_x^*:

$$a(f) = \int dx\overline{f(x)}a_x, \qquad \text{and} \qquad a^*(f) = \int dx\, f(x)\, a_x^*\,.$$

Hamiltonian (commutes w/ particle number op. $\mathcal{N} = \int dx\, a_x^* a_x$):

$$\mathcal{H}_N = \int dx\,\nabla_x a_x^*\,\nabla_x a_x + \frac{1}{2N}\int dxdy\; V(x-y)a_x^* a_y^* a_y a_x\,.$$

Replacement for product states

Product state with N particles all in state φ:

$$\{0,\ldots,0,\varphi^{\otimes N},0,\ldots\} = \frac{(a^*(\varphi))^N}{\sqrt{N!}}\Omega\,.$$

Here the vacuum vector is $\Omega = \{1,0,0,\ldots\}$.

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With respect to this coherent state, $\mathcal{N}$ is a Poisson($\|\varphi\|^2$) RV.

The fluctuation dynamics

Around the mean-field approximation $W(\sqrt{N}\varphi_t)\Omega$, fluctuations

$$\mathcal{U}_N(t;s) = W^*(\sqrt{N}\varphi_t)e^{-i\mathcal{H}_N(t-s)}W(\sqrt{N}\varphi_s),$$

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Limiting dynamics $\mathcal{U}_\infty(t,s)$ has generator $\mathcal{L}_\infty(t)$ and is described by the Bogoliubov transformation.