Bose-Einstein condensation and the nonlinear Schrödinger equation

Kay Kirkpatrick, MIT

Joint work with B. Schlein (Cambridge) and G. Staffilani (MIT).

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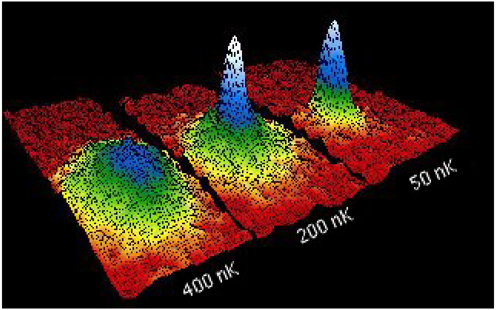

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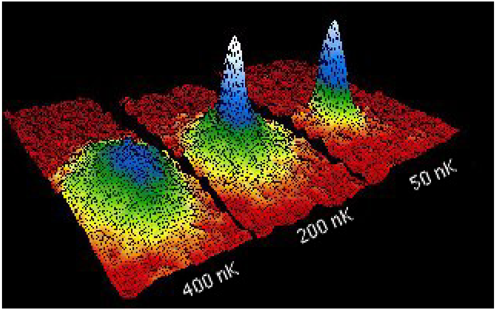

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The history of Bose-Einstein condensation

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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 evaporation and lasers.

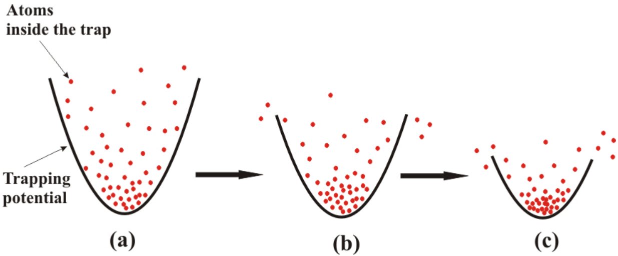

Figure: Particles condensing in the trap. (Courtesy of U Michigan)

The picture of Bose-Einstein condensation

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

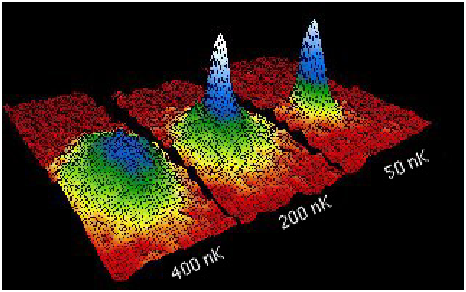

Figure: Snapshot of the particles' momenta after the trap is removed. (Courtesy of the Atomic Lab)

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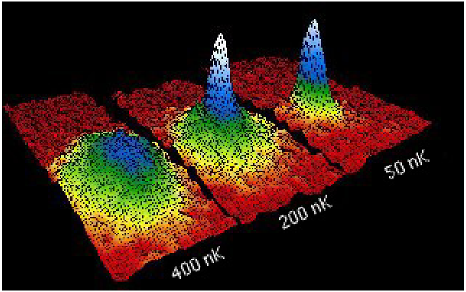

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Applications to interferometry and maybe quantum computing.

Outline

$$\begin{array}{ccc} \text{Microscopic first principles} & \rightsquigarrow & \text{Emergent phenomena} \\ N \text{ particles} & \xrightarrow{N\to\infty} & \text{continuum/cloud} \end{array}$$

Approximates $N \sim 10^3$ (dilute Bose gas) to $N \sim 10^{30}$ (boson star)

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One-particle microscopic models from quantum mechanics

A quantum particle in $\mathbb{R}^d$ is described by a wavefunction, $\psi(x,t) \in L^2(\mathbb{R}^d)$, satisfying the Schrödinger equation:

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

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- Solution operators form a semigroup: $\psi(x,t) = e^{-iHt}\psi_0(x)$.
- The probability amplitude, $|\psi(x,t)|^2$, gives the probability density of finding the particle at x at time t.

One-particle system with V_{ext} = infinite square well

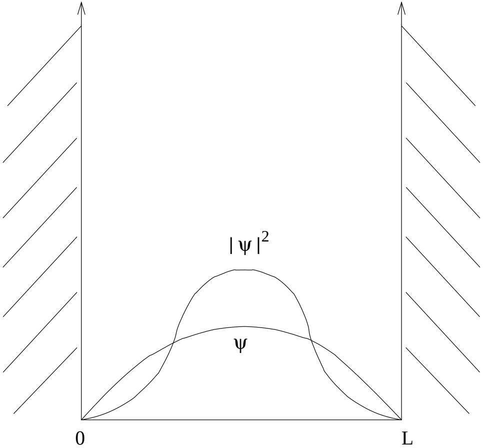

Figure: The "particle in a box" has ground state wavefunction $\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$ and probability amplitude $|\psi|^2$.

The N-particle microscopic model–general set-up

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:

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

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- V_{ext}: the external potential, which we will take to be zero
- U: potential energy from pair interactions
- Initial condition: $\psi_N(\mathbf{x}, t = 0) = \psi_N^0(\mathbf{x})$
- Solution written as: $\psi_N(\mathbf{x}, t) = e^{-iH_N t}\psi_N^0(\mathbf{x})$
- The probability density of finding particle 1 at x_1, particle 2 at x_2, etc., at time t, is given by: $|\psi_N(x_1, \ldots, x_N, t)|^2$.

Additional assumptions for N-boson models

The wavefunction for a system of N **bosons** is symmetric with respect to permutations (i.e., Pauli exclusion principle doesn't apply): $\psi_N(x_{\sigma(1)}, ..., x_{\sigma(N)}, t) = \psi_N(x_1, ..., x_N, t)$ for any $\sigma \in S_N$.

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We will consider two types of pair interactions for U:

- Weak and diffuse (mean-field systems)
- Later: Strong, short-scale, and repulsive (BEC)

The microscopic model for mean-field systems, 3D

For mean-field systems we consider the pair interaction potential $U = \frac{1}{N} V$ and the model:

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Diffuse: interactions occur at any distance, i.e., $V \in L^\infty(\mathbb{R}^3)$.

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We also assume that the initial data is factorized:

$$\psi_N^0(\mathbf{x}) = \prod_{j=1}^{N} \phi_0(x_j) \in L^2(\mathbb{R}^{3N}).$$

This is because states close to the ground state are the most interesting and are approximately described this way.

The scaling limit for mean-field systems

Theorem (Spohn, 1980): Suppose additionally that the solution of the N-boson system has factorization approximately preserved, i.e., $\psi_N(\mathbf{x}, t) \simeq \prod_{j=1}^{N} \phi(x_j, t)$. Then in the mean-field limit, we have convergence in the sense of marginals:

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$$\psi_N \xrightarrow{N \to \infty} \phi.$$

And ϕ satisfies the Hartree equation:

$$\begin{aligned} i\partial_t \phi &= -\Delta\phi + (V * |\phi|^2)\phi, \\ \phi(x, 0) &= \phi_0(x). \end{aligned}$$

This is a kind of “de-localized” Schrödinger equation.

Convergence in the sense of marginals

We define an operator $\gamma_N^{(k)}$ on $L^2(\mathbb{R}^{3k+1})$, for $k = 1, \ldots, N$, called the k-**particle marginal density matrix**, with kernel given by:

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

where $\mathbf{x}_k = (x_1, \ldots, x_k) \in \mathbb{R}^{3k}$, $\mathbf{x}_{N-k} = (x_{k+1}, \ldots, x_N) \in \mathbb{R}^{3(N-k)}$.

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In other words, $\gamma_N^{(k)}$ is the partial trace of the orthogonal projection $\gamma_N = |\psi_N\rangle\langle\psi_N|$ over the last $N-k$ particles. Key: $\gamma_N^{(k)}$ is finite.

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The meaning of $\psi_N \to \phi$ in the theorem:

$$\forall k, \quad \gamma_N^{(k)} \to |\phi\rangle\langle\phi|^{\otimes k} \text{ in trace as } N \to \infty.$$

Another result along these lines

Erdös and Yau, 2001: If $V(\mathbf{x}) = \frac{1}{|\mathbf{x}|}$, then in the mean-field limit, $\psi_N \xrightarrow{N\to\infty} \phi$ in the sense of marginals as before.

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$$i\partial_t \phi = -\Delta\phi + \left(\frac{1}{|\cdot|} * |\phi|^2\right)\phi.$$

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Preview of next section: if V were the delta function in a sense, then the Hartree equation becomes a cubic nonlinear Schrödinger (or, Gross-Pitaevskii) equation:

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

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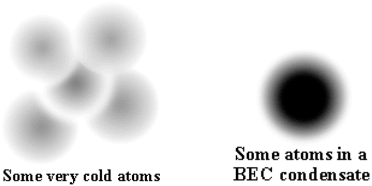

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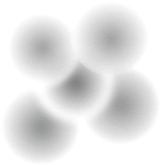

Some very cold atoms

Some atoms in a BEC condensate

  - 3D Bose-Einstein condensate (Erdös-Schlein-Yau, 2006-2008)
  - Planar and toroidal BEC (K.-Schlein-Staffilani, 2008)
- The holy grail: Phase transitions to and from BEC

The definition of Bose-Einstein condensation

BEC happens when a non-vanishing fraction of the N particles are described by the same one-particle state, as $N \to \infty$.

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More precisely, 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

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Example: $\psi_N(\mathbf{x}) = \prod_{j=1}^N \phi(x_j)$ exhibits BEC into ϕ. But more than just factorized solutions can exhibit BEC.

The microscopic model for BEC

To model BEC, we consider a family of N-boson systems with localized interactions, indexed by β. The Hamiltonian is:

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

Here $V \geq 0$ is radial and decays, and $\beta \in (0, 1]$.

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Mean-field corresponds to $\beta = 0$; the physics of BEC is very different, but the same overall strategy works for the proofs.

The scaling limit for the 3D BEC

Erdös, Schlein, and Yau, 2006-08: Suppose that the initial state ψ_N^0 is BEC with $\phi_0 \in L^2(\mathbb{R}^3)$, and appropriate assumptions are made: bounded energy per particle, etc.

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

Here $b_0(\beta = 1) = \int_{\mathbb{R}^3} V(x)dx$.

The 2D BEC model

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

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If the initial state is BEC with $\phi_0 \in L^2(\Lambda)$, and energy per particle is bounded, 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 GP (cubic NLS) equation on Λ:

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

A diagram of what's going on

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

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

The main points of the theorem are the convergence in the sense of marginals and the Gross-Pitaevskii evolution of the limit.

The strategy of the proof

The marginals evolve according to the **BBGKY hierarchy**:

$$i\partial_t \gamma_N^{(k)} = \sum_{j=1}^{k} (-\Delta_{x_j} + \Delta_{x_j'}) \gamma_N^{(k)} + \frac{1}{N} \sum_{j=1}^{k} (V_N(x_i - x_j) - V_N(x_i' - x_j')) \gamma_N^{(k)}$$

$$+ \left(\frac{N-k}{N} \right) \sum_{j=1}^{k} Tr_{k+1} (V_N(x_i - x_{k+1}) - V_N(x_i' - x_{k+1})) \gamma_N^{(k+1)}.$$

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Then as $N \to \infty$, it converges formally to the **GP hierarchy**:

$$i\partial_t \gamma_\infty^{(k)} = \sum_{j=1}^{k} (-\Delta_{x_j} + \Delta_{x_j'}) \gamma_\infty^{(k)}$$

$$+ b_0 \sum_{j=1}^{k} Tr_{k+1} (\delta(x_i - x_{k+1}) - \delta(x_i' - x_{k+1})) \gamma_\infty^{(k+1)}.$$

The strategy of the proof, cont.

This suggests proving the following:

- $\{\gamma_N^{(k)}\}_{k=1}^N$ is compact in an appropriate weak topology (uniformly in time).
- Limit points, $\gamma_\infty^{(k)}$, are solutions of the infinite hierarchy.
- Explicitly identify solution of the infinite hierarchy: the factorized solution.

The strategy of the proof, cont.

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- $\{\gamma_N^{(k)}\}_{k=1}^N$ is compact in an appropriate weak topology (uniformly in time).
- Limit points, $\gamma_\infty^{(k)}$, are solutions of the infinite hierarchy.
- Explicitly identify solution of the infinite hierarchy: the factorized solution.
- Show uniqueness of the solution of the infinite hierarchy.

The last step is the hardest, and this is where the number theory comes in for the case $\Lambda = [-1, 1]^2$.

The main novelty of the proof

For uniqueness in the $\mathbb{R}^d$ case, we need to bound integrals that come from Fourier transforms.

Erdös, Schlein, and Yau did this by a Feynman-graph approach.

Klainerman and Machedon (2008) achieved the same thing instead by space-time estimates for the free Schrödinger evolution.

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Remark: this method works for square tori only; otherwise, we'd need precise estimates for lattice points on ellipses–not available.

The lemma of Gauss, illustrated

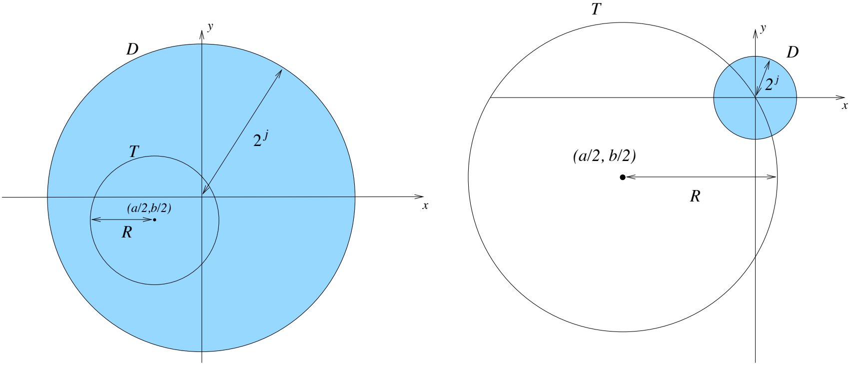

Figure: R small: #lattice pts $\leq R^{\epsilon}$. R large: #lattice pts ≤ 2.

Recent results on transitions to the BEC phase

Aizenmann-Lieb-Seiringer-Solovej-Yngvason, 2004: Quantum phase transition in an optical lattice:

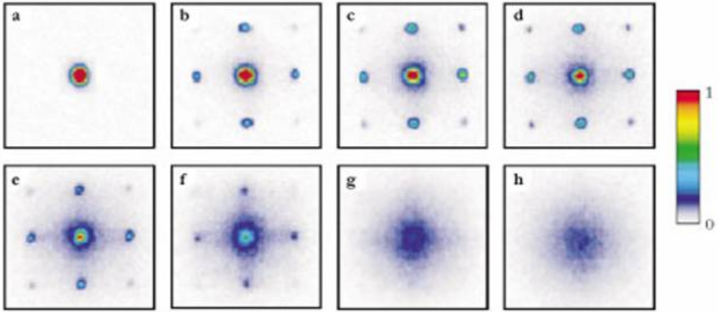

Figure: a - e: BEC; ∼f: transition; g - h: Mott insulator

Recent results on transitions to the BEC phase, cont.

Anapolitanos-Sigal, 2009: Phase transition between T$=0$ and T_{BEC}.

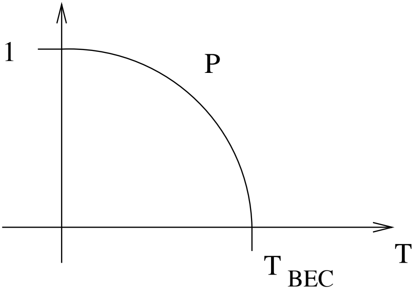

Figure: P(T) is the proportion of particles condensed at temperature T.

Other recent results and the way forward

Rezakhanlou-Hammond-Yaghouti, 2007: coagulation and the Smoluchowski equation (classical analogue of BEC).

Rodnianski-Schlein, 2008: Rate of convergence for mean-field.

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Future:

- 3D periodic Bose-Einstein condensation
- Rate of convergence for Bose-Einstein condensation
- Higher-order interactions

Inspiration from experimental physics

L. Hau, 1999-2007: Slowed light to 17 m/s and momentarily stopped it with BEC. Transformed light into matter and back.

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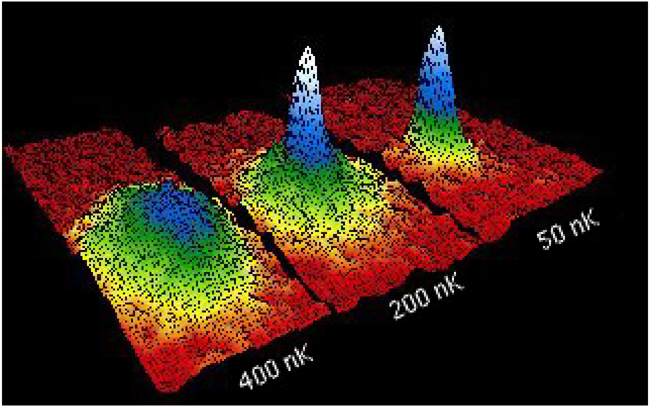
A BEC that is quickly warmed undergoes an irreversible phase transition: it implodes and then explodes, similar to a supernova.

(Loading Supernova.mp4)

To explain the **bosenova** would be fantastic.

The end



arXiv:0808.0505