

BEC, Interactions and Disorder

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- The concept of BEC
- The concept of superfluidity
- Types of models
- What we would like to know
- What we know for sure
- A 1D example

The concept of BEC

Let $a(\varphi)^\dagger$, $a(\varphi)$ be creation and annihilation operators for a 1-particle state φ of bosons and let $\langle \cdot \rangle$ be some many-particle state (pure or mixed).

The **average occupation number** of φ in the state $\langle \cdot \rangle$ is

$$N_\varphi = \langle a(\varphi)^\dagger a(\varphi) \rangle.$$

Bose-Einstein Condensation (BEC) in the many particle state $\langle \cdot \rangle$ means that for some 1-particle state φ ,

$$\langle a(\varphi)^\dagger a(\varphi) \rangle = O(N).$$

for $N \rightarrow \infty$, more precisely,

$$N_\varphi/N \geq c > 0$$

for all (large enough) N . Here N is the (average) particle number in the state $\langle \cdot \rangle$.

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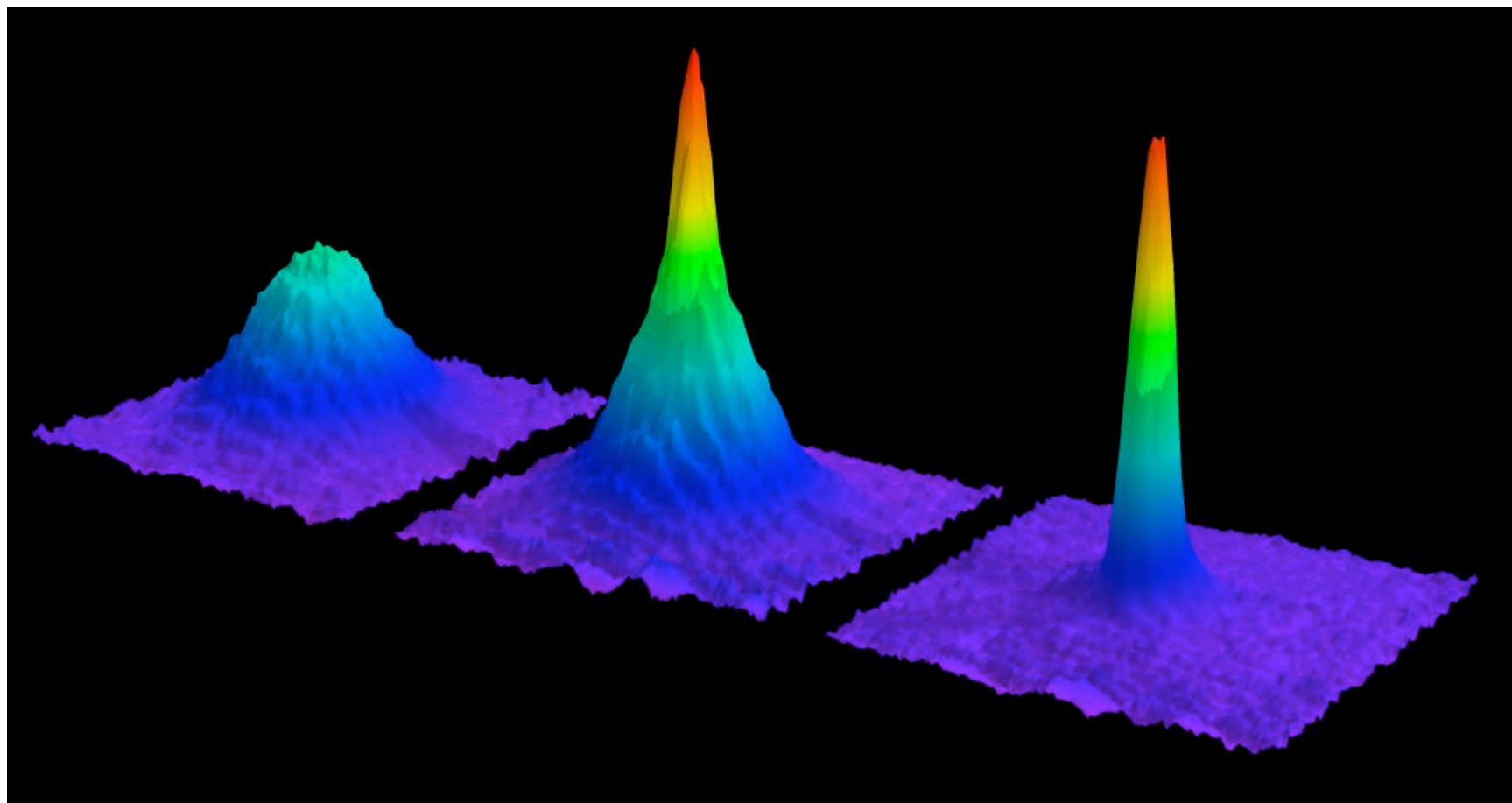
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Important remark:

The definition is only precise if the **dependence of the many body state $\langle \cdot \rangle$ on N is specified**. There may be more than one physically relevant possibilities (**thermodynamic limit**, **Gross-Pitaevskii (GP) limit**, **mean-field limit**...)

Note also that the 1-particle state φ used to test for BEC may depend on N

The concept of BEC (cont.)

More concrete description for 1-particle Hilbert space $L^2(\mathbb{R}^d)$ (or $\ell^2(\mathbb{Z}^d)$): Consider the *1-particle density matrix*

$$\rho^{(1)}(\mathbf{x}, \mathbf{x}') = \langle a(\mathbf{x})^\dagger a(\mathbf{x}') \rangle$$

If $\langle \cdot \rangle$ is a pure state given by a wave function Ψ , then

$$\rho^{(1)}(\mathbf{x}, \mathbf{x}') = N \int \Psi(\mathbf{x}, \mathbf{x}_2, \dots, \mathbf{x}_N) \Psi(\mathbf{x}', \mathbf{x}_2, \dots, \mathbf{x}_N)^* d\mathbf{x}_2 \cdots d\mathbf{x}_N.$$

More generally, $\rho^{(1)}(\mathbf{x}, \mathbf{x}')$ is a superposition of such expressions.

Spectral decomposition:

$$\rho^{(1)}(\mathbf{x}, \mathbf{x}') = \sum_i N_i \varphi_i(\mathbf{x}) \varphi_i^*(\mathbf{x}')$$

with $N_0 \geq N_1 \geq \dots$ and orthonormal φ_i .

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The concept of BEC (cont.)

BEC in the state $\langle \cdot \rangle$ means that

$$N_0 = O(N)$$

while other N_i are of lower order. The **condensate fraction** is defined as $n_{\text{BEC}} = N_0/N$.

The eigenfunction $\varphi_0(\mathbf{x})$ of the integral kernel $\rho^{(1)}(\mathbf{x}, \mathbf{x}')$ is referred to as the **wave function of the condensate**.

Fragmented condensation means that there are $1 < k \ll N$ modes with a macroscopic occupation.

There is also the even more general concept of condensation where in the thermodynamic limit no single mode has macroscopic occupation but there is still **macroscopic occupation in an infinitesimal energy interval** near the bottom of the spectrum (generalized, or “type III” condensation.).

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Superfluidity, definition

Let E_0 denote the ground state energy of the system in the rest frame and $E_0(\mathbf{v})$ the ground state energy, measured in the moving frame, when a **velocity field** \mathbf{v} is imposed. Then for small \mathbf{v} and **uniformly in** N

$$\frac{E_0(\mathbf{v})}{N} = \frac{E_0}{N} + (\rho_s/\rho)\frac{1}{2}m\mathbf{v}^2 + O(|\mathbf{v}|^4) \quad (*)$$

where N is the particle number and m the particle mass. This defines the **superfluid fraction** $n_{\text{SF}} = \rho_s/\rho$. At positive temperatures the ground state energy should be replaced by the free energy.

Remark: It is important here that (*) holds uniformly for all large N ; i.e., that the error term $O(|\mathbf{v}|^4)$ can be bounded independently of N . For fixed N and a finite box, (*) with $n_{\text{SF}} = 1$ always holds for a Bose gas with an arbitrary interaction if \mathbf{v} is small enough, owing to the discreteness of the energy spectrum.

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Superfluidity, definition (cont.)

Equivalent definition in terms of **twisted boundary conditions**:

Consider the system on a torus, i.e., on a cube of side length L with boundary conditions

$$\Psi_0((L, \mathbf{0}), \mathbf{x}_2, \dots, \mathbf{x}_N) = e^{i\theta} \Psi_0((0, \mathbf{0}), \mathbf{x}_2, \dots, \mathbf{x}_N)$$

Then the energy in dependence of θ is

$$\frac{E_N(\theta)}{N} = \frac{E_N(0)}{N} + (\rho_s/\rho) \frac{\hbar^2}{2m} \frac{\theta^2}{L^2} + O(\theta^4)$$

Remark: $n_{\text{SF}} \leq 1$ follows by taking $e^{i\theta x_1/L} \Psi_0$ as a trial function.

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Relation between BEC and SF

There is no simple relation between BEC and SF, although (experimentally) in homogeneous systems the two usually come together with $n_{\text{BEC}} \leq n_{\text{SF}}$.

In liquid He⁴ near absolute zero experiments and numerical computations indicate $n_{\text{SF}} \approx 1$ but $n_{\text{BEC}} \approx 0.1$.

In 2D (thin He⁴ films) one has $n_{\text{BEC}} = 0$ but $n_{\text{SF}} > 0$ is possible.

In random external potentials one expects the possibility that $n_{\text{BEC}} > 0$ while $n_{\text{SF}} = 0$ (Bose Glass phase, to be discussed.)

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BEC and SF have been studied in a variety of models and with a variety of methods:

- **Ideal gases**
- Particles in a box with short range interactions in the thermodynamic limit
- Various approximations of such models, sometimes exactly soluble: Bogoliubov approximation, mean field models, infinite-range hopping Hubbard model
- Trapped gases in the Gross-Pitaevskii and related limits
- The models can be continuous or discrete, and the dimension can be 3, 2 or 1
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Mathematical status of BEC and Superfluidity (non-random potentials)

BEC has so far been **rigorously proved** in the following cases

- Ideal gases (Einstein, ..., Lewis, Pulé, Verbeure, Zagrebnov,...)
- Some variants of the Bogoliubov Hamiltonian (Lewis, Pulé, Verbeure, Zagrebnov,...)
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- Hard core lattice gases at half filling, also with a weak periodic potential (Dyson, Lieb, Simon 1978; Kennedy, Lieb and Shastry 1988; Aizenman, Lieb, Seiringer, Solovej, JY 2004).
- In the GP limit (Lieb, Seiringer 2002).

In the first four cases BEC is proved in the thermodynamic limit and for positive temperatures (below a critical value).

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What we would like to know

The principal questions concern

- The effects of interactions on BEC and SF
- The effects of disorder on BEC and SF

Among physicists there is reasonable consensus that

- Interactions may enhance BEC in the sense that in a homogeneous system, the transition temperature for BEC is higher with interaction than for an ideal gas. On the other hand, in the ground state, interactions may lower the condensate fraction
- Disorder may enhance BEC (in a generalized sense) for ideal gases, but destroy both BEC and SF in interacting systems. BEC is, however, more robust than SF
- Disorder may induce Anderson localization in BE condensates

Can these points be confirmed or rejected by rigorous analysis?

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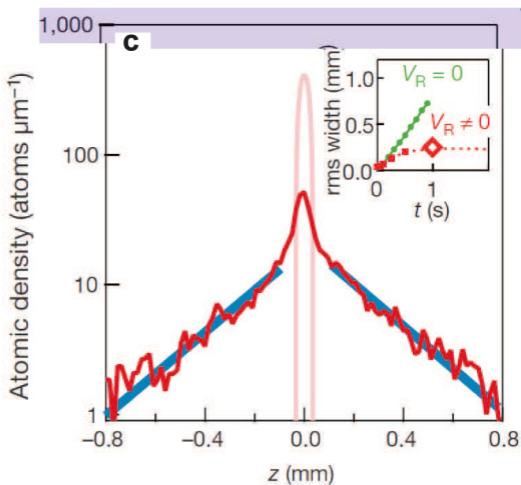
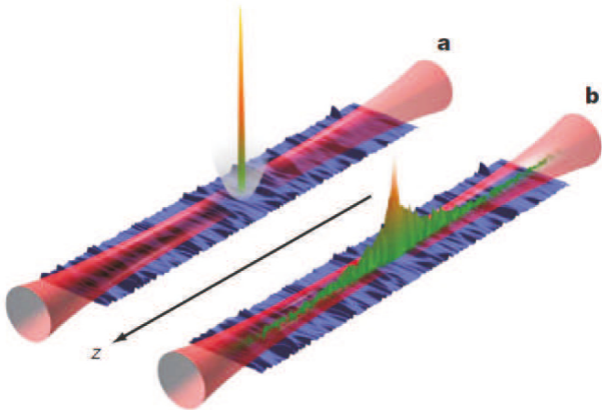


FIG. 2: Geometry of the localization experiment in random disorder: a) an interacting Bose-Einstein condensate is initially prepared in a harmonic trap; b) the condensate is then let free to expand into a 1D guide, where it is exposed to the speckle potential. c) Experimental observation of localization: for sufficiently large disorder strengths the condensate expansion stops, and the tails of its density distribution acquire an exponential decay behaviour. Figure reprinted with permission from [49]. Copyright 2010 by Macmillan Publisher Ltd.

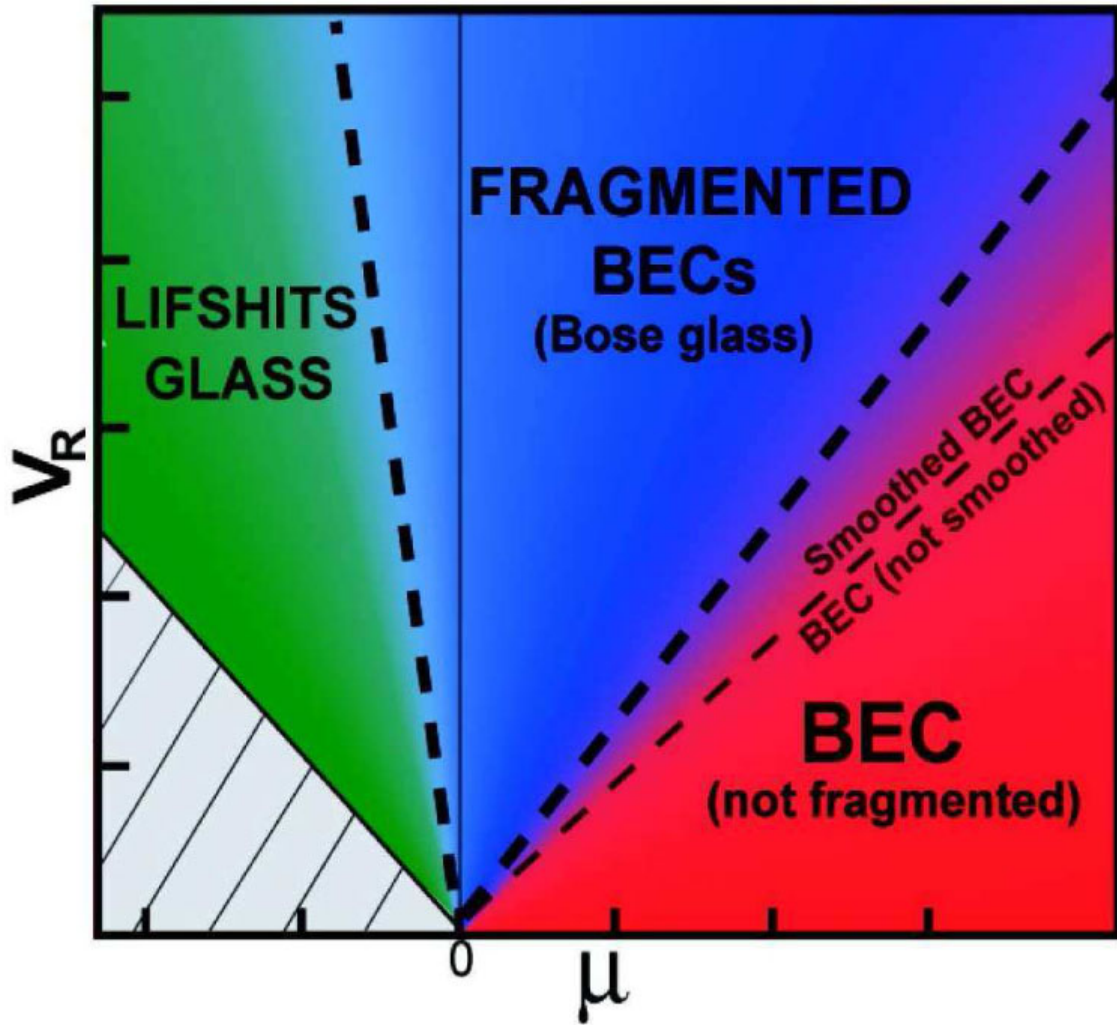


Figure 1: (color online) Schematic quantum-state diagram of an interacting ultracold Bose gas in 1D disorder. The dashed lines represent the boundaries (corresponding to *crossovers*) which are controlled by the parameter $\alpha_R = \hbar^2/2m\sigma_R^2V_R$ (fixed in the figure, see text), where V_R and σ_R are the amplitude and correlation length of the random potential. The hatched part corresponds to a forbidden zone ($\mu < V_{\min}$).

Table 1. Summary of the most common phases for dirty bosons in a lattice and the associated properties.

	Superfluid	Compressible	Gapless	Fragmented
BEC	Y	Y	Y	N
Glass Lifshits	N	Y	Y	Y
Bose	N	Y	Y	N
Mott insulator	N	N	N	N

Dirty bosons phase diagram

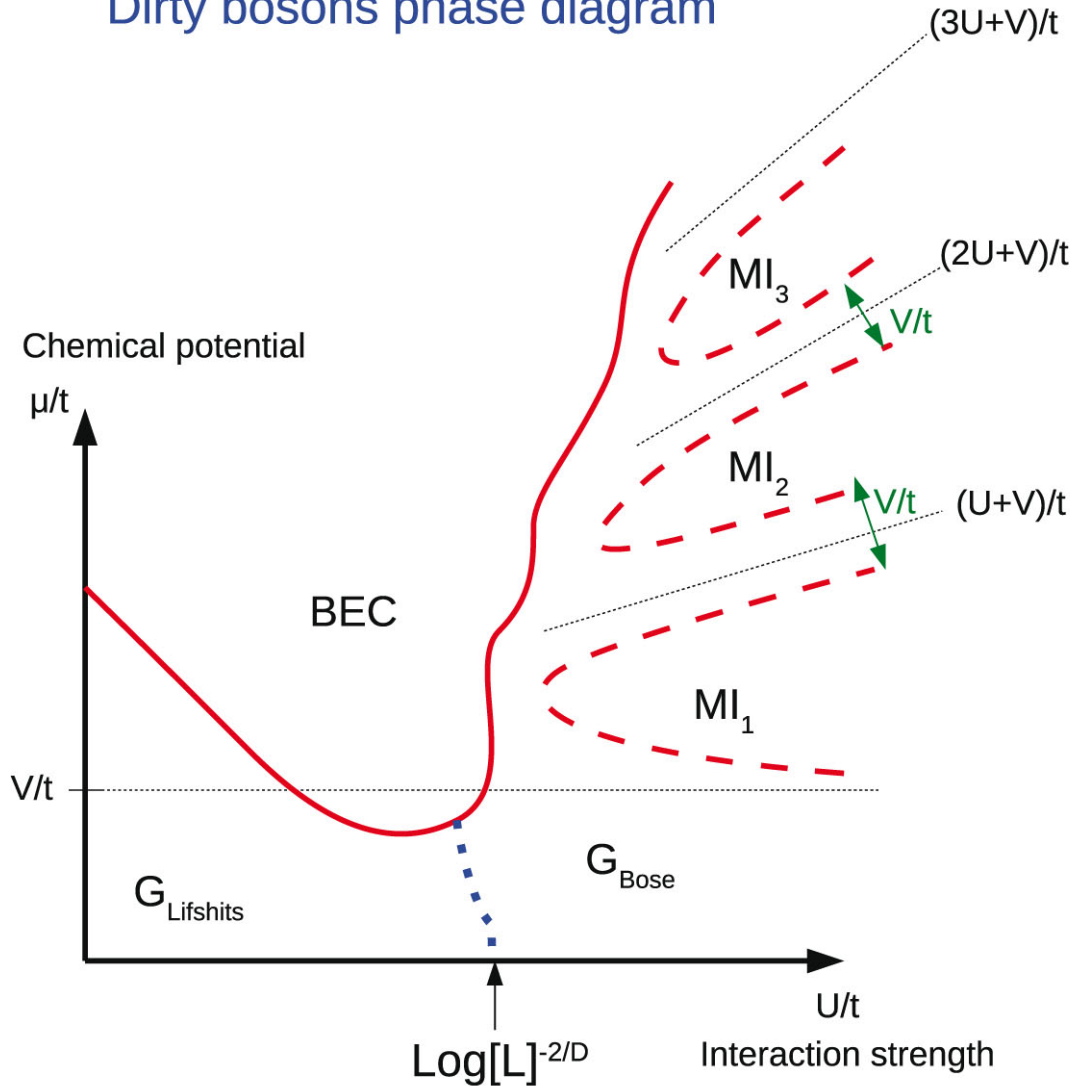


Figure 1. Schematic phase diagram for dirty bosons at zero temperature as a function of interactions (U) and chemical potential (μ) containing the glassy (G), superfluid (BEC) and Mott insulating (MI) phases. The continuous and dashed lines mark, respectively, the superfluid–insulator and glass–Mott transition, while the dotted line indicates a crossover from the Lifshits glass (heavily fragmented) to the Bose glass (extended) region. Outside of the BEC region, the one-body density matrix $\rho(\mathbf{r}, \mathbf{r}')$ decays as $|\mathbf{r} - \mathbf{r}'| \rightarrow \infty$. The Mott insulator lobes appear at sufficiently strong interactions, as the inclusion theorem guarantees that there may be no MI for $U < V$.

Bose-Hubbard model

One model that has received particular attention of physicists is the Bose-Hubbard model of a lattice gas with Hamiltonian

$$H_{\text{BH}} = -\frac{1}{2} \sum_{\langle \mathbf{x}\mathbf{y} \rangle} (a_{\mathbf{x}}^\dagger a_{\mathbf{y}} + a_{\mathbf{x}} a_{\mathbf{y}}^\dagger) + U \sum_{\mathbf{x}} a_{\mathbf{x}}^\dagger a_{\mathbf{x}} (a_{\mathbf{x}}^\dagger a_{\mathbf{x}} - 1).$$

The seminal paper of M.Fisher et al (1989) predicted a phase diagram with a BEC/SF phase and a Mott insulator phase and, in the presence of randomness, a glassy phase with BEC but no SF.

Systems of this kind (mostly without a random potential) have for more than 10 years been realized experimentally in optical lattices with tunable parameters, and the Mott/SF transition has been observed, but the glassy phase is still elusive.

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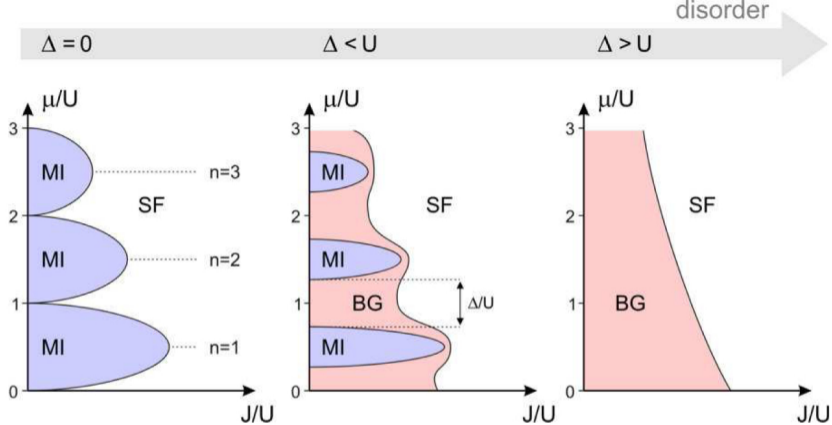


Fig. 14. Qualitative phase diagram for a disordered system of lattice interacting bosons. Three phases can be identified: a superfluid (SF), a Mott insulator (MI) and a Bose glass (BG).

Bose-Hubbard model (cont.)

There are some rigorous results on the BH model (without randomness), in particular by Fröhlich and Ueltschi (2006), confirming the existence of a Mott phase, but so far not BEC.

The BH model with infinite-range hopping has been studied by Bru and Dorlas (2001-2003) without randomness, and by Zagrebnov with randomness (lecture of VZ!)

The 1D model can be regarded as a discrete version of the Lieb-Liniger model. This model has been studied by Bishop and Wehr (2013) for weak interactions and with Bernoulli disorder. (The continuum LL model with Poisson disorder will be discussed below).

Hard core lattice gas

Another model that has *some* features in common with the BH model is a lattice gas of hard bosons in a tunable periodic potential. The Hamiltonian is

$$H = -\frac{1}{2} \sum_{\langle xy \rangle} (a_x^\dagger a_y + a_x a_y^\dagger) + \lambda \sum_{\mathbf{x}} (-1)^{\mathbf{x}} a_{\mathbf{x}}^\dagger a_{\mathbf{x}}.$$

The operators $a_{\mathbf{x}}^\#$ in this model commute at different sites as appropriate for Bosons but satisfy anti-commutation relations on the same site, reflecting the hard-core condition.

At half filling (which is in particular a **strongly interacting** case) this has been studied rigorously by Aizenman, Lieb, Solovej, Seiringer, JY (2003), proving BEC for small λ and a Mott phase for large λ .

It is natural to study this model also with the fixed λ replaced by random potential strengths λ_x^ω . Some results on this have been obtained by a student of Simone Warzel.

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λ

Mott insulator
(at low T)

exp. decay of correlations
no BEC

BEC

T



The diagram shows a phase space defined by interaction strength λ (vertical axis) and temperature T (horizontal axis). A shaded gray region at the top represents the Mott insulator phase at low temperatures. A blue hatched region at the bottom left represents the Bose-Einstein Condensate (BEC) phase. A white region in the middle and right represents the state with exponential decay of correlations and no BEC. The boundaries between these phases are marked by curved lines.

Gross-Pitaevskii theory

The time independent Gross-Pitaevskii equation in \mathbb{R}^d

$$-\frac{1}{2}\Delta\psi + V\psi + g|\psi|^2\psi = \lambda\psi$$

with an external confining potential V (possibly including a random part), is the variational equation for the energy functional

$$\mathcal{E}[\psi] = \int_{\mathbb{R}^d} \left\{ \frac{1}{2}|\nabla\psi|^2 + V|\psi|^2 + \frac{g}{2}|\psi|^4 \right\}$$

with an L^2 -normalization condition, $\int_{\mathbb{R}^d} |\psi|^2 = N$.

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Gross-Pitaevskii theory (cont.)

Basic fact behind the nonlinear term: For a *dilute* homogeneous gas of Bosons in 3D, interacting with a *repulsive short range 2-body potential* with *scattering length* a the *ground state energy density* is $\approx 4\pi a \rho^2$ where ρ is the particle density (Lieb, JY 1998). *Dilute* means here that

$$a^3 \rho \ll 1$$

i.e. a is much smaller than the mean particle distance $\rho^{-1/3}$.

Interpreting $\rho(x) = |\psi(x)|^2$ as a local particle density makes the energy functional and hence the GP equation plausible with $g = 8\pi a$.

Rigorous derivations of the GP equation from the many body Hamiltonian have been obtained in the time independent case by Lieb, Seiringer and JY (1998-2003), and in the time dependent case by Erdős, Yau and Schlein (2005–2008).

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Formally, the GP can be regarded as a mean-field Hartree approximation with the 2-body interaction potential replaced by a delta function, but in 3D this is a *wrong* picture since there are no genuine delta potentials in 3D! (And also not in 2D.)

In 1D on the other hand, the GP equation is obtained in a *high density* limit, and for δ -interactions it is, indeed, a mean field limit.

The 3D time independent GP equation has been derived rigorously from the full many body problem in the $N \rightarrow \infty$ limit, provided $a^3 \bar{\rho} \rightarrow 0$, in particular in the **GP limit** where the GP parameter

$$Na/L$$

with L the length scale of V is kept constant (Lieb, Seiringer, JY (2000)).

Remark: If a is fixed L must scale proportional to N and not $N^{1/3}$. Hence this is **not a thermodynamic limit** at positive density in 3D.

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In the GP limit there is **complete BEC** in the ground state (Lieb, Seiringer 2002).

If the trapping potential is **homogeneous** in the direction of the imposed velocity (periodic box, or rotational symmetry) there is also **complete superfluidity** in the same limit (Lieb, Seiringer, JY 2003).

Principal mathematical tools for the proofs are

- A lemma of Dyson (1957) transforming ‘hard’ potentials into ‘soft’ ones
- Generalized Poincaré inequalities

For the proof of SF also the diamagnetic inequality is used.

A 1D model (Seiringer, JY, Zagrebnoy 2012)

The model is the **Lieb-Liniger model** of bosons with contact interaction on the **unit interval** but with an additional **external random potential** V^ω . The Hamiltonian on the Hilbert space $L^2([0, 1], dz)^{\otimes_s N}$ is

$$H = \sum_{i=1}^N (-\partial_{z_i}^2 + V^\omega(z_i)) + \frac{\gamma}{N} \sum_{i < j} \delta(z_i - z_j)$$

with $\gamma \geq 0$ and periodic boundary conditions.

The random potential is taken to be

$$V^\omega(z) = \sigma \sum_j \delta(z - z_j^\omega)$$

with $\sigma \geq 0$ independent of the random sample ω while the **obstacles** $\{z_j^\omega\}$ are **Poisson distributed** with density $\nu \gg 1$.

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Our model is formulated in the fixed interval $[0, 1]$ so that the particle density ρ tends to infinity as $N \rightarrow \infty$. The parameters γ , ν and σ will also be allowed to tend to infinity as $N \rightarrow \infty$, but BEC requires that they can only grow rather slowly. In particular, the coupling constant γ/N will tend to zero as $N \rightarrow \infty$.

Instead of fixing the interval we could consider the model in an interval $[-L/2, L/2]$ and take N and $L \rightarrow \infty$ with $\rho = N/L$ fixed (thermodynamic Limit).

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BEC in the 1D model

For *fixed* γ , σ and ω there is **complete BEC in the ground state** in the sense that the 1-particle density matrix/ N converges to a one dimensional projector as $N \rightarrow \infty$. The corresponding **wave function of the condensate** is the normalized minimizer of the **Gross-Pitaevskii (GP) energy functional**

$$\mathcal{E}_\omega^{\text{GP}}[\psi] = \int_0^1 \{ |\psi'(z)|^2 + V^\omega(z)|\psi(z)|^2 + (\gamma/2)|\psi(z)|^4 \} dz$$

We want, however, to consider ν , σ and γ **large**. Hence it is important to estimate also the **rate of the convergence** of the 1-particle density matrix as $N \rightarrow \infty$, in dependence of the parameters and of ω .

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The Proof of BEC (sketch)

The proof of BEC is based on energy bounds:

- An **upper bound** to the many-body **ground state energy** E_0^{QM} by taking $\psi_0^{\otimes N}$ as a trial function for H where ψ_0 is the minimizer of the GP energy functional, normalized so that $\|\psi_0\|_2 = 1$. This gives

$$E_0^{\text{QM}} \leq N e_0$$

where $e_0 = \mathcal{E}^{\text{GP}}[\psi_0]$ is the g.s.e. of the GP functional.

- An **operator lower bound** for the many-body Hamiltonian H , up to controlled errors, in terms of the 1-particle **mean-field Hamiltonian**

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BEC follows from the upper and lower bounds and the fact that there is an **energy gap** between e_0 and the next lowest eigenvalue, e_1 , of the mean-field Hamiltonian h :

Let

$$N_0 = \langle \Psi_0 | a^\dagger(\psi_0) a(\psi_0) | \Psi_0 \rangle$$

be the **occupation number of the GP ground state** ψ_0 in the many-body ground state Ψ_0 . Then the energy bounds give

$$N_0 e_0 + (N - N_0) e_1 - o(1) N e_0 \leq E_0^{\text{QM}} \leq N e_0.$$

where the $o(1) = N^{-1/3} \min\{\gamma^{1/2}, \gamma\}$. Hence

Theorem (BEC).

$$\left(1 - \frac{N_0}{N}\right) \leq C \frac{e_0}{e_1 - e_0} N^{-1/3} \min\{\gamma^{1/2}, \gamma\}.$$

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Fragmented condensate for finite N

If $N_{<k}$ denotes the occupation of the k lowest eigenstates with eigenvalues e_0, \dots, e_{k-1} then more generally

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This can be useful for **finite** N because $e_k - e_0 \gg e_1 - e_0$ is possible, even if $k \ll N$.

Thus, if the gap $e_1 - e_0$ is very small and N not too large, the picture of a **fragmented condensate** may be more appropriate.

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The energy gap

Consider a one-dimensional Schrödinger operator $-\partial_z^2 + W(z)$ with Dirichlet boundary conditions and a nonnegative potential W .

Proposition (Gap).

Define $\eta > 0$ by $\eta^2 = \pi^2 + 3 \int_0^1 W(z) dz$. Then

$$e_1 - e_0 \geq \eta \ln(1 + \pi e^{-2\eta})$$

The proof is based on a modification of a result of Kirsch and Simon (1985), that involves the sup norm of W instead of the integral.

In our case $\eta = \eta_\omega = \sqrt{\pi^2 + 3m_\omega\sigma + 3\gamma}$ where m_ω is the number of obstacles in $[0, 1]$, that is almost surely equal to ν , in the limit $\nu \rightarrow \infty$.

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The wave function of the condensate

Analysis of the GP equation with the random potential leads to the following picture:

The random potential may lead to **localization** of the wave function of the condensate in subintervals. The interparticle interaction counteracts this effect, however, and can lead to **complete delocalization** (the condensate extends over the whole unit interval) if the interaction is strong enough.

When the three parameters, γ , ν and σ all tend to infinity in a certain way that guarantees that the GP energy becomes deterministic, a **transition between localization and delocalization** occurs when $\gamma \sim \nu^2$.

For $\gamma \lesssim \nu/(\ln \nu)^2$ the condensate is localized in a **fragmented subset** of the unit interval.

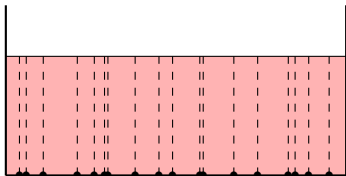
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Analysis of the GP equation with the random potential leads to the following picture:

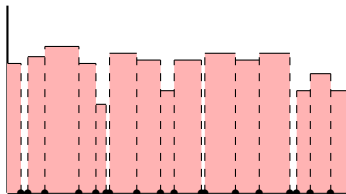
The random potential may lead to **localization** of the wave function of the condensate in subintervals. The interparticle interaction counteracts this effect, however, and can lead to **complete delocalization** (the condensate extends over the whole unit interval) if the interaction is strong enough.

When the three parameters, γ , ν and σ all tend to infinity in a certain way that guarantees that the GP energy becomes deterministic, a **transition between localization and delocalization** occurs when $\gamma \sim \nu^2$.

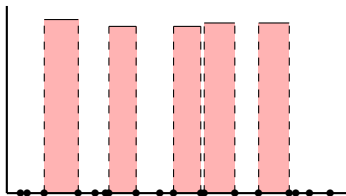
For $\gamma \lesssim \nu/(\ln \nu)^2$ the condensate is localized in a **fragmented subset** of the unit interval.



$$\gamma \gg \nu^2$$



$$\gamma \lesssim \nu^2$$



$$\gamma \lesssim \nu / (\ln \nu)^2$$

Loss of superfluidity

While there is complete BEC in the model in the limit considered, **superfluidity may get lost** due to gaps in the wave function.

An upper bound on the effect of twisting the boundary condition can be obtained with a trial function

$$\psi(x) = e^{i\phi(z)}\psi_0(z)$$

with ϕ real valued and $\phi(0) = 0$, $\phi(1) = \theta$. Then

$$\mathcal{E}^{\text{GP}}[\psi] - E^{\text{GP}}[\psi_0] = \int_0^1 |\nabla\phi(z)|^2 |\psi_0(z)|^2 dz.$$

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Now suppose $|\psi_0(z)|^2 \leq \varepsilon$ on a subinterval $[a, b]$ of length ℓ . Then, with

$$\phi(z) = \begin{cases} 0 & \text{if } z < a \text{ or } z > b \\ \frac{\theta}{\ell}(z - a) & \text{if } z \in [a, b] \end{cases}$$

we obtain

$$\mathcal{E}^{\text{GP}}[\psi] - E^{\text{GP}}[\psi_0] = \frac{\varepsilon}{\ell} \theta^2.$$

Hence, $n_{\text{SF}} \leq \varepsilon/\ell$, and if $\varepsilon/\ell < 1$, superfluidity is suppressed.

More generally, if there are k intervals where $|\psi_0(z)|^2 \leq \varepsilon$ one can divide the twist between the intervals and obtain

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If $\gamma \lesssim \nu^2$ the total length $k\ell$ of intervals where $|\psi_0|^2$ is small is $O(1)$, and ε can be estimated as $(\sigma\nu)^{-1}$ times the GP energy for $\sigma \rightarrow \infty$, which is $\nu^2/(\ln \nu)^2$. Hence, for $\gamma \lesssim \nu^2$,

$$n_{\text{SF}} \leq \frac{\nu}{\sigma(\ln \nu)^2}$$

which can be arbitrarily close to zero if σ is large. On the other hand we still have $n_{\text{BEC}} \rightarrow 1$ in the $N \rightarrow \infty$ limit, provided $\sigma\nu N^{-1/3}\gamma \rightarrow 0$. So, mathematically at least, a **Bose glass** is possible in this model as a limiting case.