Bose-Einstein Condensation

– what we know, and what we would like to know –

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Topics

1. The concept of BEC
2. Ideal Bose gases
3. Dilute interacting gases

   3.1 $T = 0$

   3.2 $T > 0$
4. The hard core lattice gas

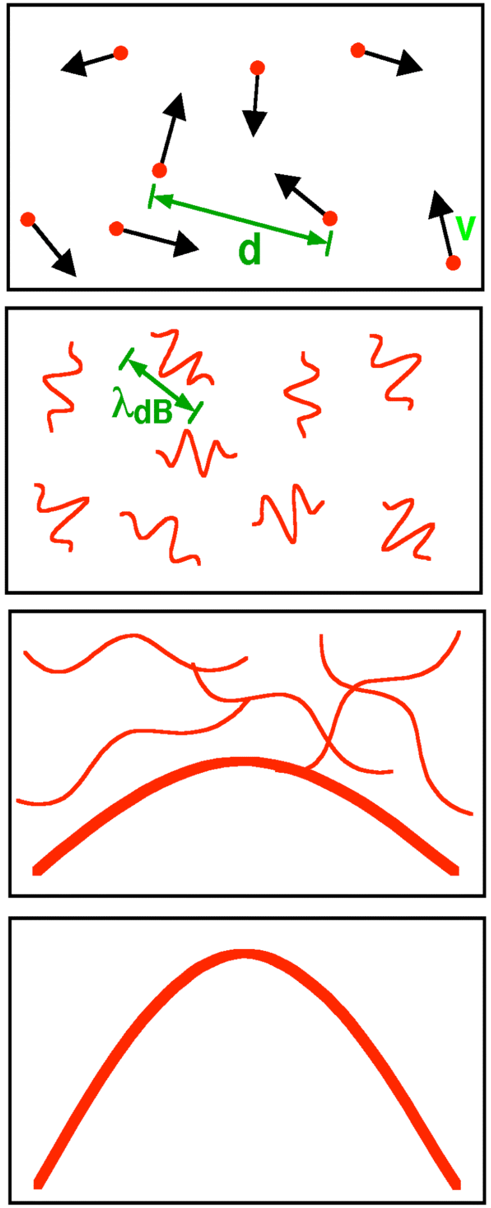
The concept of BEC

- Under normal conditions the atoms of a gas are distributed on very many quantum states so that every single state is only occupied by relatively few atoms.
- In BEC one quantum state is occupied by a macrosopic number of atoms. (Einstein 1924, for an ideal gas.)
- For BEC in dilute gases, where interactions can be ignored in first approximation, extremely low temperatures, of the order 10^{-8} K, are required. This was first achieved in 1995.
- Even for dilute gases, interactions *are* important. A mathematical proof of BEC for *interacting* bosons is a very hard problem! So far it has essentially only been achieved for:

  a) Trapped gases in dilute limits.

  b) A lattice gas of bosons with a hard core at exactly half filling.

What is Bose-Einstein condensation (BEC)?



High Temperature T:

thermal velocity v

density d^{-3}

"Billiard balls"

Low Temperature T:

De Broglie wavelength

$\lambda_{dB}=h/mv \propto T^{-1/2}$

"Wave packets"

$T=T_{crit}$: Bose-Einstein Condensation

$\lambda_{dB} \approx d$

"Matter wave overlap"

T=0: Pure Bose condensate

"Giant matter wave"

Notations

$\mathcal{H}_1$ single particle Hilbert space, $a^\dagger(\psi)$, $a(\phi)$ creation and annihilation operators on the *bosonic* Fock space $\mathcal{H} = \bigoplus_{n=0}^{\infty} \mathcal{H}_1^{\otimes_s^n}$.

$\langle\,\cdot\,\rangle$ a (pure or mixed) state on the algebra generated by the creation and annihilation operators; $\langle A\rangle = \mathrm{Tr}\, A\hat\rho$ with $\hat\rho \geq 0$, $\mathrm{Tr}\,\hat\rho = 1$.

If the *many-particle* system is in the state $\langle\,\cdot\,\rangle$, the average number of particles in a (normalized) *single-particle* state $\psi \in \mathcal{H}_1$ is

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

The average total particle number is

$$N = \sum_i \langle a^\dagger(\psi_i)a(\psi_i)\rangle$$

with $\{\psi_i\}$ an ON basis of $\mathcal{H}_1$.

Precise definition of BEC

The precise definition of BEC refers to a sequence of many-body states, $\langle\,\cdot\,\rangle_{(N)}$, with increasing (average) particle numbers $N \to \infty$, rather than one particular such state.

BEC means that for all large N the many-body state $\langle\cdot\,\rangle_{(N)}$ has a macroscopically occupied single particle state in the sense that

$$\sup_{\psi\in\mathcal{H}_1} N_\psi/N \geq C$$

with $C > 0$ independent of N.

One-particle density matrix

If $\mathcal{H}_1 = L^2(\mathbb{R}^d)$ (or $\ell_2(\mathbb{Z}^d)$), the one-particle density matrix $\gamma^{(1)}(x,y)$ of a state $\langle\,\cdot\,\rangle$ is defined by

$$\gamma^{(1)}(x,y) = \langle a^\dagger(x)a(y)\rangle.$$

For $\langle\cdot\,\rangle = \langle\cdot\,\rangle_{(N)}$ this is the integral kernel of a nonnegative operator with trace N. Spectral decomposition:

$$\gamma^{(1)}(x,y) = \sum_{i=0}^{\infty} N_i\,\psi_i(x)\psi_i(y)^*$$

with $\{\psi_i\}$ ON, $N_0 \geq \lambda_1 \geq \cdots \geq 0$, $\sum_i N_i = N$.

BEC means that

$$N_0 = O(N)$$

in the sense that $\limsup_{N\to\infty} N_0/N > 0$.

Off Diagonal Long Range Order

Often (but not always!) one deals with spatially homogeneous systems confined in a box Λ with side length L and volume $|\Lambda| = L^d$.

The thermodynamic limit means in this case that $L \to \infty$ as $N \to \infty$ with $\rho = N/|\Lambda|$ fixed.

Taking $\psi = |\Lambda|^{-1/2}\mathbb{1}_\Lambda$ as a trial state for γ we get

$$N_0 \geq \frac{1}{|\Lambda|}\int\int_{\Lambda\times\Lambda}\gamma(x,y)dxdy.$$

Thus a sufficient criterion for BEC in the thermodynamic limit is

Off Diagonal Long Range Order (ODLRO):

$$\lim_{|\Lambda|\to\infty}\frac{1}{|\Lambda|^2}\int\int_{\Lambda\times\Lambda}\gamma(x,y)dxdy > 0.$$

On the other hand, (exponential) decay of $\gamma(x,y)$ as $|x-y| \to \infty$ proves absence of BEC.

States and Hamiltonians

In practice, the states $\langle \cdot \rangle_{(N)}$ are canonical or grand canonical Gibbs states (thermal equilibrium states) corresponding to some Hamiltonian:

$$\langle A \rangle = \frac{1}{Z} \operatorname{Tr} A e^{-H/T}, \qquad \langle A \rangle = \frac{1}{\Xi} \operatorname{Tr} A e^{-(H-\mu \hat{N})/T}.$$

Ground states, corresponding to $T = 0$, are also important examples.

Typical N-particle Hamiltonians:

$$H_N = \sum_{j=1}^{N} \left(-\nabla_j^2 + V(x_j) \right) + \sum_{i<j} v(x_i - x_j).$$

operating on symmetric wave functions for spinless bosons.

The ideal Bose gas

If there is no interaction, $v = 0$, there is trivially BEC at $T = 0$; at fixed N the ground state of H_N is $\psi_0^{\otimes n}$ with ψ_0 the ground state of $-\Delta + V$.

The case $T > 0$ is often considered in a box: $V(x) = 0$ in a box Λ of side length L and ∞ outside the box.

The text-book grand-canonical treatment gives in the standard thermodynamic limit, $N \to \infty$, $\rho := N/L^3$ fixed:

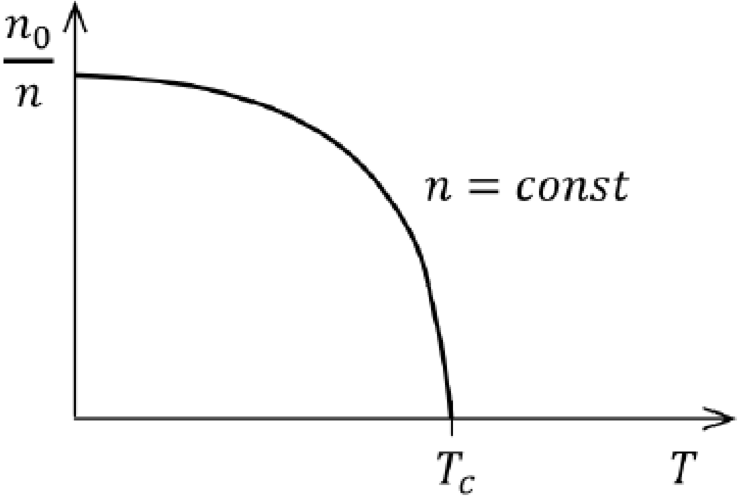
- No BEC in dimensions $d = 1$ or 2.
- For $d = 3$ BEC if

$$\rho > \rho_c(T) = C\,T^{3/2}$$

or equivalently,

$$T < T_c(\rho) = C' \rho^{2/3}$$

with $C = 2.612(mk_B/2\pi\hbar^2)^{3/2}$, $C' = C^{-2/3}$.



$\frac{n_0}{n}$
$n = const$
T_c
T

The ideal Bose gas (cont.)

REMARKS:

- The condition for BEC can also be written

$$\rho^{-1/3} < 0,7261\ \lambda_{\rm th}.$$

  with $\lambda_{\rm th} = (2\pi\hbar^2/mk_{\rm B})^{1/2}\, T^{-1/2}$.
- In a modified thermodynamic limit, where $N/(\ln NL^d)$ rather than N/L^d is kept fixed, there is BEC also in $d = 2$.
- In a harmonic trapping potential, $V(x) \sim \omega^2|x|^2$, one may consider a natural limit where $N\omega^d$ is kept fixed as $N \to \infty$.
  In this limit there is BEC for $d = 2$ and 3, but not for $d = 1$. If $N\omega/\ln N$ is kept fixed there is also BEC for $d = 1$.

This shows the importance of specifying precisely the conditions under which the limit $N \to \infty$ is taken.

Dilute, interacting gases

When we leave the realm of ideal gases and take the (unavoidable) interactions between the particles into account the situation changes drastically. The case $T = 0$, which is trivial for an ideal gas, already poses difficult challenges!

The mathematical theory of interacting Bose gases essentially started with the pioneering work of Bogoliubov in 1947. He wrote the Hamiltonian in terms of creation and annihilation operators in momentum space and introduced ingenious approximation methods. Refining these methods and making them rigorous has been a major theme in the mathematical physics work on the subject in the past few years.

On the other hand, this recent work was preceded by, and has an overlap with, some basic mathematical results that have been obtain since 1998 by working mainly in position space. The focus has been on gases which are dilute in a sense to be made precise soon.

The first quantity of interest at $T = 0$ is the many-body ground state energy in the standard thermodynamic limit.

Assume a spherically symmetric pair interaction potential $v \geq 0$ of short range. The *scattering length* of v, denoted by a, is defined by considering the zero energy scattering equation

$$-\nabla^2 f + \tfrac{1}{2} v f = 0$$

with $f \to 1$ at infinity. We have $0 \leq f \leq 1$, and for $r = |\mathbf{x}|$ larger than the range of v the solution has the form

$$f(r) = \left(1 - \frac{a}{r}\right)$$

which defines a. Partial integration, and $v \geq 0$, gives also

$$8\pi a = \int \{2|\nabla f|^2 + |f|^2 v\} = \int f v \leq \int v.$$

Consider now for $v \geq 0$ the Hamiltonian of N bosons in a box Λ of side length L with appropriate boundary conditions:

$$H_N = -\sum_{j=1}^{N} \nabla_j^2 + \sum_{1 \leq i < j \leq N} v(\mathbf{x}_i - \mathbf{x}_j)$$

Denote the ground state energy by $E^{\rm QM}(N, L)$.

Energy per particle in the limit $N \to \infty$, $L \to \infty$, $\rho = N/L^3$ fixed:

$$e_0(\rho) = \lim_{N \to \infty} E^{\rm QM}(N, L)/N$$

Ask for the *low density asymptotics* of $e_0(\rho)$. Low density means, by definition,

$$a \ll \rho^{-1/3}$$

Equivalently, $$a^3 \rho \ll 1.$$

The basic formula for the energy (leading order asymptotics for dilute gases) is

Theorem (Ground state energy, leading term)

For $a^3\rho \ll 1$

$$e_0(\rho) = 4\pi\, a\rho\,(1 + o(1)).$$

Heuristic argument for the formula:

"For a dilute gas only two body scattering matters", so

$$E^{\rm QM}(N,L) \approx \frac{N(N-1)}{2} E^{\rm QM}(2,L) \approx \frac{N^2}{2}\frac{8\pi a}{L^3} = N\, 4\pi a\rho.$$

This heuristic argument is, however, very far from a rigorous proof and it gives a wrong answer in two dimensions!

The formula has an interesting history and it took almost 70 years to establish it rigorously. (Lenz (1929), Bogoliubov (1947), Huang, Yang, ..., Lieb (50's and 60's), Dyson 1957, Lieb, JY 1998.)

A rigorous upper bound was given by Dyson in 1957 (for hard spheres), and also a lower bound, that was, however, a factor 1/14 off the mark. An asymptotically correct lower bound was not obtained until 40 years later by Lieb and JY.

Perhaps more important than the result itself was the method of proof in the LY paper. It implied a localization of the kinetic energy in the ground state, namely the fact that the ground state wave function is essentially flat except in the neighbourhood of configurations where pairs of points come close to each other. This was in particular employed for the proof of BEC in the so-called Gross-Pitaevskii (GP) limit by Lieb and Seiringer in 2002.

Improvements of the formula $e_0(\rho) = 4\pi a\rho(1 + o(1))$

In 1957 Lee, Huang and Yang used an ingenious, but non-rigorous, pseudopotential method to derive the formula

$$e_0(\rho) = 4\pi\, a\rho\, \left(1 + \frac{128}{15\sqrt{\pi}}(a^3\rho)^{1/2} + o(\sqrt{a^3\rho}\right) .$$

Proving it as a mathematical theorem was an open problem for many decades!

In certain special cases lower bounds of this type were obtained by Guiliani, Seiringer (2009), Lieb, Solovej (2009); and an upper bound for regular potentials by Yau, Yin (2009).

Finally, in 2019 Søren Fournais and Jan Philip Solovej succeeded in proving a lower bound including the Lee-Huang-Yang term, for short range L^1- potentials: *The energy of dilute bose gases*, Annals of Mathematics, **192**, 893–976, (2020).

Very recently the Yau-Yin proof of the upper bound has also been simplified and extended to include L^3-potentials: Giulia Basti, Serena Cenatiempo, Benjamin Schlein, arXiv:2101.06222

The long history of research of the ground state energy of a dilute Bose gas, starting with Lenz's paper of 1929 shows the complexity of the problem. It is therefore very interesting that a simplified approach exists which, although it has not yet been made completely rigorous, gives the correct formulas including the Lee-Huang-Yang term.

The "simple equation" of E.H. Lieb (1963)

Almost 60 years ago Elliott Lieb suggested a highly original approach to the ground state properties, including BEC, of dilute Bose gases in the infinite volume limit.

It is not completely rigorous because it rests on plausible, but so far unproven, assumptions about factorization of the ground state wave function ("Independence at Large Distances").

The starting point is the observation that the ground state wave function Ψ_0 is positive, so the function itself and not only its square defines a probability measure on configuration space.

Lieb then defines and studies the following "correlation function":

$$g_2(x_1 - x_2) = \lim_{N\to\infty, |\Lambda|/N=\rho} |\Lambda|^2 \frac{\int \Psi_0(x_1, x_2, x_3, \dots x_N) dx_3 \cdots dx_N}{\int \Psi_0(y_1, \dots y_N) dy_1 \cdots dy_N}$$

The ILD assumption is that g_2 tends to a constant at infinity, and more generally, the functions $g_n(x_1, \ldots, x_n)$ define in the same way as g_2 by integrating out all variables in Ψ_0 except the first n, tends to g_{n-1} if $x_n \to \infty$.

The ILD assumption reduces the ground state energy problem to a study of an integro-differential equation for this function on $\mathbb{R}^3$ instead of the Schrödinger equation for the full wave function on R^{3N}.

With $u(x) := 1 - g_2(x)$ and $e := \frac{1}{2}\rho \int (1 - u(x))v(x)$ the equation is

$$(-\nabla^2 + v(x) + 4e)u(x) = v(x) + 2e\rho(u * u)(x).$$

Already in 1963 Lieb showed how this equation gives the first terms for the ground state energy including the Lee-Huang-Yang term.

Very recently Lieb has come back to this approach in collaboration with E. Carlen, I. Jauslin and M. Holtzmann. They have both studied it both analytically and numerically and found very good agreement with Monte-Carlo calculation of energies and Bose Einstein condensation fraction for the full problem, not only at low densities.

Among these results is a formula, known from Bogoliubov's theory, for the depletion $\delta = \lim_{N\to\infty} 1 - (N_0/N)$ of the condensate

$$\delta = (8/3\sqrt{\pi})\sqrt{\rho a^3}\,(1 + o(1)).$$

In particular, it claims complete condensation in the ground state if $a^3\rho \to 0$.

Reference: E. Carlen, I. Jauslin, E.H. Lieb, and M. Holtzmann. *A fresh look at a simplified approach to the Bose gas*, ArXiv:2011.10869,

Gross-Pitaevskii Theory

Consider now the N-body Hamiltonian with an external Potential V, representing a confining trap,

$$H_N = \sum_{i=1}^{N} \{-\nabla_i^2 + V(\mathbf{x}_i)\} + \sum_{1\leq i<j\leq N} v(|\mathbf{x}_i - \mathbf{x}_j|).$$

The external potential comes with a natural length scale $L_V = e_V^{-1/2}$ where e_V is the spectral gap of $-\nabla^2 + V$.

Study the ground state properties of H_N and in particular BEC, in the *Gross-Pitaevskii (GP) limit* where $N \to \infty$ with a fixed value of the GP interaction parameter

$$g \equiv 4\pi N a / L_V \approx e_0(\rho)/e_V.$$

with $\rho = N/L_V^3$.

Fixing g has the physical meaning of fixing the ratio between the interaction energy per particle and the spectral gap in the trap.

Note also: $a^3\rho \sim g/N^2 = O(1/N^2)$ if g is fixed, so the GP limit is a special case of a dilute limit.

The GP limit can be achieved either by keeping a fixed and scaling the external potential V so that $L \sim N$, or, by keeping V fixed and taking $a \sim N^{-1}$. The latter can formally be regarded as a scaling of the interaction potential:

$$v(r) = N^2 v_1(Nr)$$

In the GP limit the N-particle ground state can be described by minimizing a functional of functions on $\mathbb{R}^3$, the *GP energy functional*

$$\mathcal{E}^{\mathrm{GP}}[\varphi] = \int_{\mathbb{R}^3} \left(|\nabla\varphi|^2 + V|\varphi|^2 + g|\varphi|^4\right) d^3\mathbf{x}$$

with the subsidiary condition $\int |\varphi|^2 = 1$.

Motivation for the term $g|\varphi|^4$: With $\rho(\mathbf{x}) = N|\varphi(\mathbf{x})|^2$ the local density, we have

$$Ng \int |\varphi|^4 = 4\pi a \int \rho(\mathbf{x})^2,$$

and $4\pi a\rho(\mathbf{x})^2$ is the interaction energy per unit volume by the previous analysis of the ground state energy of a homogeneous, dilute gas.

The minimizer of the GP functional is the unique, nonnegative solution of the (time independent) Gross-Pitaevskii equation

$$(-\nabla^2 + V + 2g|\varphi|^2)\varphi = \mu\,\varphi$$

with a Lagrange multiplier μ.

We denote the minimizer by $\varphi^{\mathrm{GP}}(\mathbf{x})$. The corresponding energy is

$$E_g^{\mathrm{GP}} = \mathcal{E}^{\mathrm{GP}}[\varphi^{\mathrm{GP}}] = \inf\{\mathcal{E}^{\mathrm{GP}}[\varphi] : \int |\varphi|^2 = 1\}.$$

The GP energy functional can be obtained formally from the many body Hamiltonian by replacing $v(\mathbf{x}_i - \mathbf{x}_j)$ by $8\pi a \delta(\mathbf{x}_i - \mathbf{x}_j)$ and making a Hartree type product ansatz for the many body wave function, i.e., writing

$$\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N) = \varphi(\mathbf{x}_1) \cdots \varphi(\mathbf{x}_N).$$

This is not a proof, however, and the true ground state is not of this form. In particular, if v is a hard sphere potential, $\langle \Psi, H\Psi \rangle = \infty$ for all such wave functions. Finite energy can in this case only be obtained for functions of the form

$$\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N) = \varphi(\mathbf{x}_1) \cdots \varphi(\mathbf{x}_N) F(\mathbf{x}_1, \dots, \mathbf{x}_N)$$

with $F(\mathbf{x}_1, \dots, \mathbf{x}_N) = 0$ if $|\mathbf{x}_i - \mathbf{x}_j| \leq a$ for some $i \neq j$. The upper bound on the energy is, in fact, proved by using trial functions of this form with a function F involving the zero-energy scattering solution of the two-body problem.

Basic results of GP theory are the following theorems (Lieb, Seiringer, JY (2000), Lieb, Seiringer (2002)):

Theorem (Energy asymptotics)

If $N \to \infty$ with g fixed (i.e., $a \sim N^{-1}L$), then

$$\frac{E^{\mathrm{QM}}(N,a)}{N E_g^{\mathrm{GP}}} \to 1$$

Theorem (BEC in GP limit)

If $N \to \infty$ with g fixed, then the 1-particle density matrix $\gamma^{(1)}$ converges to the projector on φ^{GP}:

$$\frac{1}{N}\gamma^{(1)}(\mathbf{x},\mathbf{x}') \to \varphi^{\mathrm{GP}}(\mathbf{x})\varphi^{\mathrm{GP}}(\mathbf{x}').$$

Sketch of the proof of BEC in a box Λ of side length L:

Notation: $\mathbf{X} = (\mathbf{x}_2, \dots, \mathbf{x}_N)$, $\psi_{\mathbf{X}}(\mathbf{x}) = \Psi_0(\mathbf{x}, \mathbf{X})$. The depletion of the condensate is

$$1 - N_0/N = 1 - (NL^3)^{-1} \int\int \gamma^{(1)}(\mathbf{x}, \mathbf{x}')d\mathbf{x}d\mathbf{x}' = \int d\mathbf{X} \|\psi_{\mathbf{X}} - \langle \psi_{\mathbf{X}} \rangle\|^2$$

Simple Poincaré inequality:

$$\|f - \langle f \rangle\|^2 \leq CL^2 \|\nabla f\|^2$$

where $\langle f \rangle = L^{-3} \int f$.

Generalized Poincaré inequality for $\Omega \subset \Lambda = \Omega \cup \Omega^c$:

$$\|f - \langle f \rangle\|^2 \leq C_1 L^2 \|\nabla f\|^2_{L^2(\Omega)} + C_2 |\Omega^c|^{2/3} \|\nabla f\|^2.$$

Localization of the kinetic energy:

While

$$\int d\mathbf{X}\|\nabla\psi_{\mathbf{X}}\|^2 \sim \rho a(1+o(1))$$

(by the energy estimate) it is implicit in the 1998 proof of LY that there is an $\Omega\subset\Lambda$ such that $|\Omega^c|/L^3=o(1)$ and

$$(\rho a)^{-1}\int d\mathbf{X}\|\nabla\psi_{\mathbf{X}}\|^2_{L^2(\Omega)}=o(1).$$

Hence:

$$1-N_0/N\leq L^2\rho a\times o(1)=\frac{Na}{L}\times o(1)\to 0$$

if $N\to\infty$ with $g=Na/L$ fixed.

An inspection of the estimates reveals in that the $o(1)$ factor is in fact $O(N^{-1/10})$. Hence it shows also BEC beyond the GP limit, namely for $a\sim N^{-1+\kappa}$ provided $\kappa<1/10$.

Refinements of the GP limit theorems

Since the first derivation of the GP equation for a BEC condensate from the many body Hamiltonian many new developments have taken place, in particular:

- Bose gases in rotating traps. (Lieb, Seiringer (2006), Nam, Rougerie, Seiringer (2016),...
- Time dependent equation: Erdös, Schlein, Yau (2006)...; Pickl (2008),...; Brennecke, Schlein (2017),...
- BEC beyond the GP limit: Lieb, Seiringer (2002); Adhikari, Brennecke, Schlein et al (2020); Fournais (2020); Hainzl (2020),...
- Optimal rates of convergence: (Boccato, Brennecke, Cenatiempo, Schlein, Schraven (2020-21); Nam, Napiórkowski, Ricaud, Triay (2020),...

The study of the GP equation for gases in rotating traps and the associated vortices is a research area of its own: (Aftalion (2006), Ignat, Millot (2008); Seiringer (2008), Correggi, Rougerie, JY, (2008...)

The study of time dependent problems employs different techniques from those for the time independent case

For rigorous Bogoliubov theory and its implications for GP see the notes of the lecture course of Benjamin Schlein!

One works here with the Hamiltonian in momentum space:

$$H = \sum_{p\in\mathbb{Z}^d} p^2 a_p^* a_p + \sum_{p,q,k\in\mathbb{Z}^2} \hat{v}(k) a_{p-k}^* a_{q+k}^* a_p a_q$$

and controlled approximations of it, separating out terms containing a_0^*, a_0 combined with sophisticated manipulations on the rest.

GP limit at $T > 0$ in a harmonic trap

The first experiments exhibiting BEC in dilute gases were carried out in harmonic traps at very low, but still nonzero, temperatures. It is important to develop GP theory and prove BEC also in such traps for $T > 0$.

A combination of a GP limit and a thermodynamic limit at $T > 0$ was studied in the paper: A. Deuchert, R. Seiringer, JY, *Bose–Einstein Condensation in a Dilute, Trapped Gas at Positive Temperature*, Commun. Math. Phys. **368**, 723–776 (2019).

The trapping potential is here $V(x) = \omega^2|x|^2 - \frac{3}{2}\omega$ with length scale $L_{\rm osc} = \omega^{-1/2}$. The thermodynamic limit is the one appropriate for harmonic traps meaning that $N \to \infty$, but

$$\frac{N}{(L_{\rm osc}^2 T)^3} = \text{const.}$$

With $\beta := 1/T$ and $\omega = L_{\rm osc}^{-2}$ this means $N(\beta\omega)^3 = \text{const.}$

Explanation of thermodynamic limit: While the 1-particle ground state and the GP minimizer have an extension $\sim L_{\rm osc} = \omega^{-1/2}$, the thermal cloud has an extension $R_{\rm th} \gg L_{\rm osc}$, determined by $R_{\rm th}^2 L_{\rm osc}^{-4} \sim T$. This gives $R_{\rm th} \sim L_{\rm osc}^2 T^{1/2}$. The average particle distance in the thermal cloud, $\sim N^{-1/3} R_{\rm th}$, is comparable to the thermal length, $T^{-1/2}$, precisely under the condition $N/(L_{\rm osc}^2 T)^3 = \text{const}$. Note also that this implies

$$R_{\rm th}/L_{\rm osc} \sim N^{1/6}.$$

For the GP limit we assume the the interaction potential v is scaled so that its scattering length a satisfies

$$aN/L_{\rm osc} = \text{const.}$$

Goal: Prove this picture

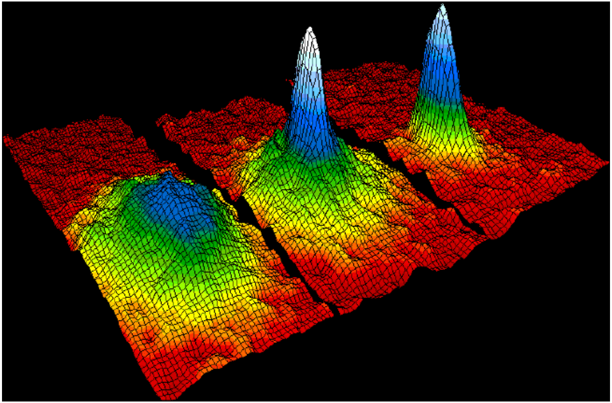
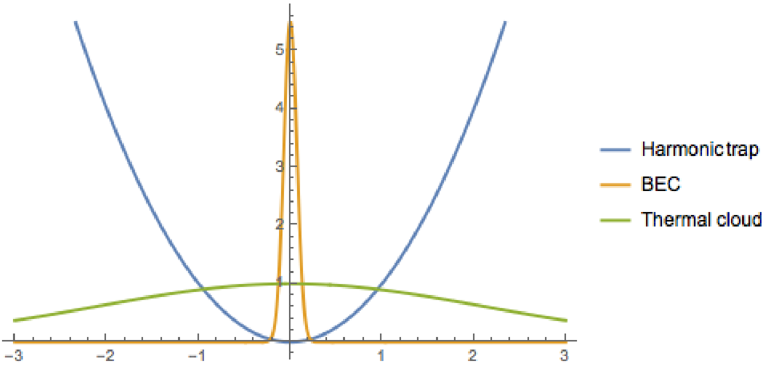


Figure: Emergence of BEC inside the thermal cloud of Rubidium atoms

Anderson et al., Observation of bose-einstein condensation in a dilute atomic vapor, Science 269, 198 (1995)

Length scales



- Length scale condensate: $\omega^{-1/2}$
- Length scale thermal cloud: $\omega^{-1/2}\frac{1}{(\beta\omega)^{1/2}} \gg \omega^{-1/2}$

The main results concern the free energy

$$F(\beta, N, a, \omega) = -\tfrac{1}{\beta} \ln \left(\mathrm{Tr}\, e^{-\beta H_N} \right),$$

and the 1-particle density matrix

$$\gamma^{(1)}(x_1, x_2) = \frac{1}{Z} \mathrm{Tr} \left(\hat{a}^*(x_1) \hat{a}(x_2) e^{-\beta H_N} \right)$$

in a combination of the GP and the thermodynamic limit. They show in particular complete BEC with the same transition temperature as for the ideal gas.

We denote the free energy and 1-particle density matrix for the ideal gas by F_0 and $\gamma_0^{(1)}$ respectively, and the normalized ground state wavefunction of the harmonic oscillator by φ_0. Also, $N_0(N, \beta, \omega)$ denotes the particle number in the condensate for the ideal gas.

Theorem (GP+thermodynamic limit)

$$\lim \tfrac{1}{\omega N} \left| F(\beta, N, a, \omega) - F_0(\beta, N, \omega) - E^{\mathrm{GP}}(N_0, a, \omega) \right| = 0.$$

$$\lim \tfrac{1}{N} \left\| \gamma_N^{(1)} - \left(\gamma_{N,0}^{(1)} - N_0 |\varphi_0\rangle\langle\varphi_0| + |\phi^{\mathrm{GP}}_{N_0,a_N}\rangle\langle\phi^{\mathrm{GP}}_{N_0,a_N}| \right) \right\|_1 = 0.$$

$$\lim \tfrac{1}{N} \left\| \gamma_N^{(1)} - |\phi^{\mathrm{GP}}_{N_0,a_N}\rangle\langle\phi^{\mathrm{GP}}_{N_0,a_N}| \right\| = 0$$

The proof makes essential use of the separation of scales expressed by $R_{\mathrm{th}} \sim N^{1/6} L_{\mathrm{osc}}$ which leads to the following expectations in the combined limit:

- The thermal cloud of the ideal gas remains essentially intact.
- BEC takes place for $T < T_{\mathrm{c}}^0$ and the condensate can be described by the GP minimizer, residing close to the center of the trap.

Although the separation of scales and the diluteness simplifies the problem the proof still requires some work! Besides the techniques for the ground state energy one employs i.a.

- The Gibbs variational principle for the free energy,
  $F = \min_\Gamma \mathrm{Tr}\,[H\Gamma + \Gamma \ln \Gamma]$
- IMS localization and localization in Fock space to separate the region of extension $O(L_{\rm osc})$ from the thermal cloud
- Estimates for relative entropies

Remark: The fact that the transition temperature for BEC and the condensate fraction for the interacting gas stay the same as for the ideal gas relies essentially on the diluteness of the system. Otherwise deviation from these values can be expected and have been seen in experiments. Capturing these effects mathematically is an open problem.

GP limit at $T > 0$ in a box (homogeneous gas)

Recently it has become experimentally feasible to confine cold Bose gases in box-like traps where the gas is approximately homogeneous. The theoretical analysis of the GP limit is more complicated than in the harmonic trap because the condensate and the thermal cloud are not spatially separated.

It could nevertheless be carried out by A. Deuchert and R.Seiringer: *Gross–Pitaevskii Limit of a Homogeneous Bose Gas at Positive Temperature*, Arch. Rational Mech. Anal. 236 (2020) 121–1271.

The results are analogous to those for a harmonic trap, but the methods of proof are different. They build partly on techniques from earlier theorems about the free energy of a dilute, homogeneous gas in a thermodynamic limit. (Lower bound: Seiringer, 2008, using coherent states, upper bound Yin, 2010.)

Comments:

- Besides coherent states a new bound for relative entropies is derived and used.
- The upper bound is simpler than in Yin's paper (5 pages instead of 55!) because the in GP limit the gas is much more dilute than in the general dilute case considered by Yin ($\rho a^3 \sim N^{-2}$ rather than just $\ll 1$.)
- The BEC is proved by considering bounds for a the Hamiltonian perturbed by the projector on the free ground state

$$H_N \to H_N + \lambda|\psi_0^{\otimes N}\rangle\langle|\psi_0^{\otimes N}|$$

and differentiating at $\lambda = 0$.

Optical lattices

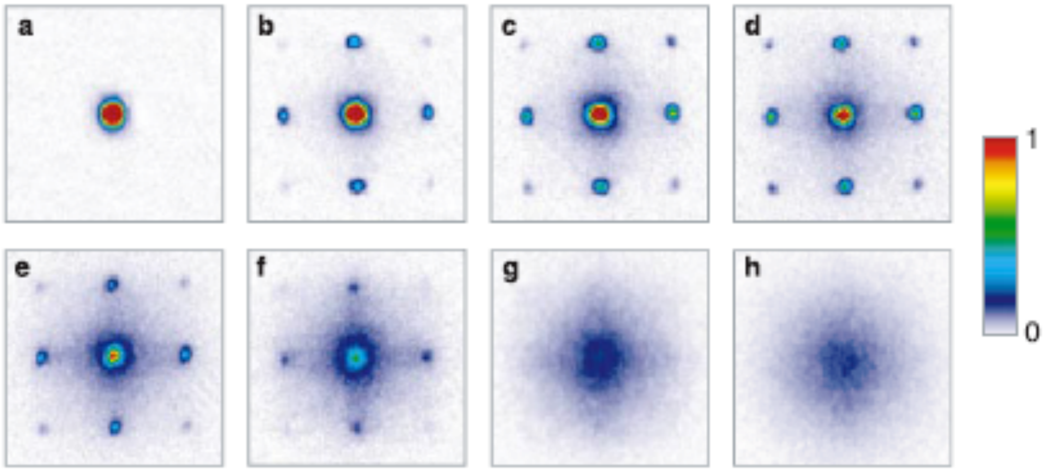
Since about 20 years it has become possible to trap cold atoms in optical lattices consisting of the intersection points of crossing laser beams.

In this way artificial lattice gases have been created. A remarkable development was the observation of a reversible transition from a Bose-Einstein condensate to a state with localized atoms as the strength of the periodic, optical trapping potential was varied. This is an example of a quantum phase transition.

This has been studied theoretically within the so-called Bose-Hubbard model, but not yet on the level of a rigorous mathematical theorem. Rigorous results can, however, be proved for a hard core lattice gas.

BEC as a quantum phase transition

Figure 9 Experimental observation of the quantum phase transition from a superfluid to a Mott insulator in a Rb BEC[59]. When the gas was released from the optical lattice the atoms from the more than 100,000 lattice sites overlapped. In the superfluid state, an interference pattern of multiple peaks formed as a result of the phase coherence. When the lattice potential was increased, strong number squeezing in the insulating state suppressed the interference. From **a** to **g**, the lattice potential was increased from zero to twenty recoil energies.



Hard core lattice gas

A lattice gas of bosons with a hard core interactions can approximately be realized experimentally in optical lattices. The grand canonical Hamiltonian for this model is

$$H - \mu\hat{N} = -\tfrac{1}{2}\sum_{\langle\mathbf{xy}\rangle}(a^\dagger_{\mathbf{x}}a_{\mathbf{y}} + a_{\mathbf{x}}a^\dagger_{\mathbf{y}}) - \mu\sum_{\mathbf{x}\in\Lambda} a^\dagger_{\mathbf{x}}a_{\mathbf{x}}.$$

Here $\langle\mathbf{xy}\rangle$ denotes nearest neigbours in a periodic box $\Lambda\subset\mathbb{Z}^d$.
The creation and annihilation operators $a^\#_{\mathbf{x}}$ and $a^\#_{\mathbf{y}}$ commute for $\mathbf{x}\neq\mathbf{y}$ but for $\mathbf{x}=\mathbf{y}$ satisfy the CAR

$$a^2_{\mathbf{x}} = {a^\dagger_{\mathbf{x}}}^2 = a^\dagger_{\mathbf{x}}a_{\mathbf{x}} + a_{\mathbf{x}}a^\dagger_{\mathbf{x}} = 0$$

reflecting the hard core condition.

Grand canonical state

The Hilbert Hilbert space is $\mathcal{H} = \bigotimes_{\mathbf{x}\in\Lambda} \mathbb{C}^2$. and the grand canonical state is

$$\langle \cdot \rangle \equiv \langle \cdot \rangle_{\Lambda,\mu} = \frac{1}{\Xi}\mathrm{tr}\left(\cdot \, e^{-[H-\mu\hat{N}]/T}\right).$$

The creation and annihilation operators can be represented as 2×2 matrices with

$$a^\dagger_{\mathbf{x}} \leftrightarrow \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad a_{\mathbf{x}} \leftrightarrow \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad a^\dagger_{\mathbf{x}} a_{\mathbf{x}} \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

for each $\mathbf{x}\in\Lambda$. More precisely, these matrices are tensored with the unit matrix at the other lattice sites than $\mathbf{x}$.

The Hamiltonian as an XY model

The Hamiltonian can alternatively be written with aid of of the spin 1/2 operators

$$S^1 = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S^2 = \frac{1}{2}\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad S^3 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

because $a^\dagger_{\mathbf{x}} = S^1_{\mathbf{x}} + \mathrm{i}S^2_{\mathbf{x}} \equiv S^+_{\mathbf{x}}, \quad a_{\mathbf{x}} = S^1_{\mathbf{x}} - \mathrm{i}S^2_{\mathbf{x}} \equiv S^-_{\mathbf{x}}$.

When written in terms of the spin operators the grand canonical Hamiltonian (up to a constant) has the form of the "XY model"

$$H_{\Lambda,\mu} = -\sum_{\langle\mathbf{xy}\rangle}(S^1_{\mathbf{x}}S^1_{\mathbf{y}} + S^2_{\mathbf{x}}S^2_{\mathbf{y}}) - \mu\sum_{\mathbf{x}\in\mathbf{\Lambda}} S^3_{\mathbf{x}}.$$

Gauge symmetry

The grand canonical state is invariant under rotations of the spin operators in the 12-plane. This continuous $U(1)$ symmetry correspond to the gauge transformations

$$a_{\mathbf{x}}^{\dagger} \mapsto e^{\mathrm{i}\theta} a_{\mathbf{x}}^{\dagger}, \quad a_{\mathbf{x}}^{\dagger} \mapsto e^{-\mathrm{i}\theta} a_{\mathbf{x}}^{\dagger}$$

and reflects the fact that the Hamiltonian conserves the particle number.

It is an important fact that BEC is equivalent to spontaneous breaking of gauge symmetry in the thermodynamic limit. Continuous symmetries are notoriously hard to break because of thermal fluctuations that tend to restore the symmetry. This partly explains why proofs of BEC are so difficult to achieve.

Gauge symmetry breaking

The standard way to test for symmetry breaking is to add to the Hamiltonian a symmetry breaking term multiplied by a parameter that is taken to zero after the thermodynamic limit.

In the case at hand we can take the "magnetization" in some direction $\vec{n}$ in the 12-plane, i.e, add a term

$$\varepsilon\,\vec{n}\cdot\vec{S} = \varepsilon\,|\Lambda|^{1/2}\vec{n}\cdot\widetilde{\vec{S}}_{\mathbf{0}}$$

with

$$\vec{S} = \sum_{\mathbf{x}\in\mathbf{\Lambda}} (S^1_{\mathbf{x}}, S^2_{\mathbf{x}}).$$

and the Fourier transformed operators

$$\widetilde{S}^{1,2}_{\mathbf{p}} = |\Lambda|^{-1/2} \sum_{\mathbf{x}\in\mathbf{\Lambda}} S^{1,2}_{\mathbf{x}} \exp(\mathrm{i}\mathbf{p}\cdot\mathbf{x}).$$

Gauge symmetry breaking (cont.)

Let $\langle \cdot \rangle \equiv \langle \cdot \rangle_{\Lambda,\mu,\varepsilon}$ denote the state with the symmetry breaking term. For finite Λ and $\varepsilon > 0$ we have

$$\langle \vec{n} \cdot \vec{S} \rangle_{\Lambda,\mu,\varepsilon} \neq 0$$

but, because $\langle \cdot \rangle_{\Lambda,\mu,\varepsilon=0}$ is rotationally symmetric for Λ fixed,

$$\lim_{\varepsilon \to 0} \langle \vec{n} \cdot \vec{S} \rangle_{\Lambda,\mu,\varepsilon} = 0.$$

Spontanous breaking of the symmetry means that

$$\lim_{\varepsilon \to 0} \lim_{\Lambda \to \mathbb{Z}^d} \frac{1}{|\Lambda|} \langle \vec{n} \cdot \vec{S} \rangle_{\Lambda,\mu,\varepsilon} \neq 0.$$

Gauge symmetry breaking (cont.)

In the particle picture it is natural to express the symmetry breaking term through the creation and annihilation operators:

$$\varepsilon\, |\Lambda|^{1/2} \left(e^{\mathrm{i}\theta}\, \widetilde{a}_{\mathbf{0}}^{\dagger} + e^{-\mathrm{i}\theta}\, \widetilde{a}_{\mathbf{0}} \right).$$

Gauge symmetry breaking is thus equivalent to

$$\lim_{\varepsilon\to 0} \lim_{\Lambda\to\mathbb{Z}^d} |\Lambda|^{1/2} \langle \widetilde{a}_{\mathbf{0}} \rangle_{\Lambda,\mu,\varepsilon} \neq 0$$

BEC and gauge symmetry breaking

ODLRO, implying BEC, means on the other hand that

$$\lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|^2} \sum_{\Lambda} \sum_{\Lambda} \gamma(\mathbf{x}, \mathbf{y}) = \lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|} \langle \widetilde{a}_{\mathbf{0}}^{\dagger} \widetilde{a}_{\mathbf{0}} \rangle_{\Lambda,\mu,\varepsilon=0} > 0.$$

By Cauchy-Schwarz

$$|\langle \widetilde{a}_{\mathbf{0}} \rangle|^2_{\Lambda,\mu,\varepsilon} \leq \langle \widetilde{a}_{\mathbf{0}}^{\dagger} \widetilde{a}_{\mathbf{0}} \rangle_{\Lambda,\mu,\varepsilon}$$

so symmetry breaking implies BEC.

But also the converse is true! This is a general fact that would be obvious if $\widetilde{a}_{\mathbf{0}}$ were a c-number but a complication arises because the symmetry breaking term does not commute with the Hamiltonian. Using coherent states a rigorous proof is, however, possible so

BEC $\leftrightarrow$ breaking of gauge symmetry

Reflection positivity

The value $\mu = 0$ corresponds to $N = \langle \hat{N} \rangle = |\Lambda|/2$, i.e., half filling. At this special value (and only for this value!) the grand canonical state has the property of reflection positivity which can be utilized to study BEC.

So far it is the only known method for proving ODLRO in the thermodynamic limit for interacting systems with a continuous symmetry.

Since reflection positivity is not stable under perturbations the method applies only to special models and parameter values.

Reflection positivity was originally introduced in relativistic quantum field theory by Osterwalder and Schrader in 1973. In 1976 Fröhlich, Simon and Spencer used it to prove ODLRO in some classical spin systems. This was generalized to quantum spin systems by Dyson, Lieb, Simon in 1977.

To define RP we split Λ into two equally large parts Λ_{L} and Λ_{R} ("left" and "right") by means of a hyperplane cutting through bonds between lattice points.

Let $\mathcal{A}_{\mathrm{L}}$ and $\mathcal{A}_{\mathrm{R}}$ be the algebras of observables localized in Λ_{L} and Λ_{R} respectively. There is a natural involution Θ mapping $\mathcal{A}_{\mathrm{L}}$ into $\mathcal{A}_{\mathrm{R}}$.

Reflection positivity of a state means, by definition, that for $F \in \mathcal{A}_{\mathrm{L}}$

$$\langle F \Theta \bar{F} \rangle \geq 0.$$

BEC; infrared bounds

Utilizing reflection positivity one can prove for the hard core lattice gas:

- BEC for sufficiently low T if $d \geq 3$, no BEC for high T.
- BEC in the ground state if $d = 2$, no BEC for $T > 0$.

(Dyson, Lieb, Simon (1977); Kennedy, Lieb, Shastry (1988)).

For $d = 1$ there is no BEC (Lenard (1964))

The role of reflection positivity in the proof is that the associated Cauchy-Schwarz inequalities (for reflexions w.r.t. different hyperplanes in Λ) lead to bounds for the occupation of states with momenta $\neq 0$ ("infrared bounds"). For sufficiently low temperatures these bounds show that the state with momentum 0 must be macroscopically occupied.

A quantum phase transition

The Hamiltonian can be modified by a periodic external potential

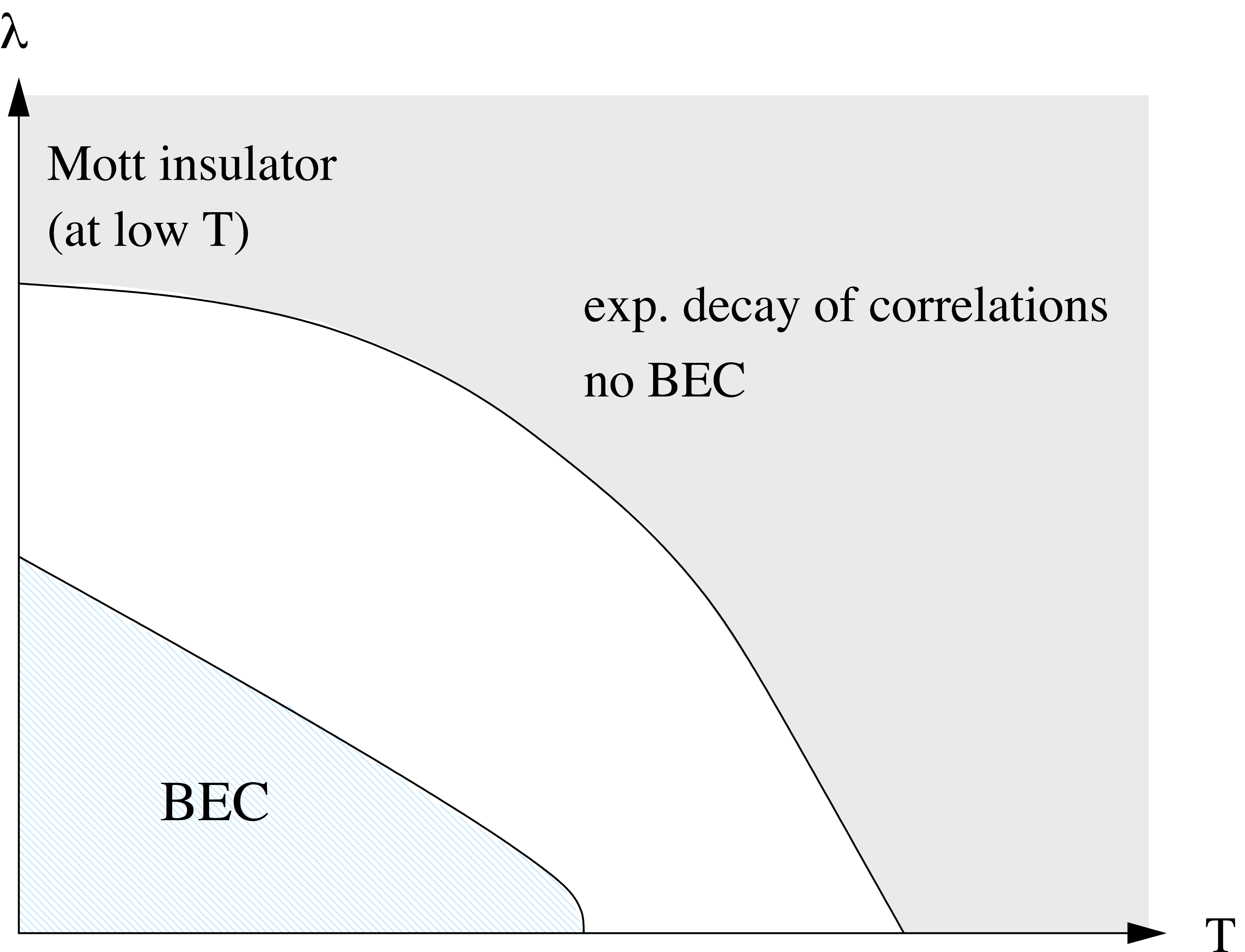
$$\lambda \sum_{\mathbf{x}\in\Lambda} (-1)^{\mathbf{x}} a^\dagger_{\mathbf{x}} a_{\mathbf{x}} = \lambda \sum_{\mathbf{x}\in\Lambda} (-1)^{\mathbf{x}} S^3_{\mathbf{x}}$$

still maintaining reflection positivity.

By varying λ it is possible to mimic a reversible quantum transition between BEC and localized atoms in an optical lattice. In 2003 Aizenman, Lieb, Seiringer, Solovej and JY proved:

- For small λ BEC survives.
- For large λ there is exponential decay of correlations and BEC is destroyed.

For the proof of the latter statement a representation of the 1-particle density matrix in terms of an imaginary-time path integral à la Feynman-Kac was employed.


λ
Mott insulator
(at low T)
exp. decay of correlations
no BEC
BEC
T

Concluding remarks

The focus in this lecture has been on results on BEC that have been proved as mathematical theorems.

For this reason I have essentially said nothing about the very remarkable path integral approach to BEC and superfluidity that Feynman introduced in 1953. Although mathematical physicists have certainly taken notice of it, it has so far not led to a proof of BEC for a dense system like liquid Helium.

Its standing in the community of computational physics is, however, very high as can be seen from the following quote:

“The quantum mechanics of many-body systems is usually presented as a difficult subject, and the phenomena of Bose condensation and superfluidity are often characterized as ill understood. One of Feynman’s early successes with path integrals is often neglected, his mapping with pathe integrals of a quantum system onto a classical model of interacting “polymers”. . . . This gives us a simple classical picture of a superfluid. Not only is it simple but it is exact for all thermodynamic properties.”

D. M. Ceperley, *Path integrals in the theory of condensed helium*, Reviews of Modern Physics **67**, 279 (1995).

I would really love to see a rigorous mathematical implementation of this vision!