Bose–Einstein Condensation in Ultracold Atomic Gases

Branislav K. Nikolić
Department of Physics and Astronomy, University of Delaware, Newark, DE 19716, U.S.A.
http://wiki.physics.udel.edu/phys813
Is Quantum Degenerate Gas of Bosons Possible?

For a long time, it was thought that quantum degenerate gas is impossible

---

BEC of dilute gases is a **metastable state** within the **thermodynamically forbidden region** where a gas of atoms can come into kinetic equilibrium via two-body collisions, whereas it requires three-body collisions to achieve chemical equilibrium (i.e., to form molecules and stable solids).

**1978:** Search for gaseous BEC started with hydrogen atoms whose quantum spins are aligned (The atoms could not be cooled below about 100 mK because of collisions with the walls of the container. Solution to this problem led to "evaporative cooling" technique employed in all modern BECs and condensation of hydrogen in 1998)

**1995:** BEC in alkali atomic vapors

**1999:** quantum degenerate Fermi gas

**2003:** superfluid Fermi gas

Rev. Mod. Phys. 74, 875 (2002)
Parameter Estimates to Reach Metastable BEC in Realistic Systems

Credit: W. Ketterle, MIT

High Temperature $T$:
- thermal velocity $v$
- density $d^{-3}$
- "Billiard balls"

$\lambda_{dB} \sim n^{1/3}$

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"

"High" density:
- molecule/cluster formation, solidification and no BEC

$n_{\text{water}} \rightarrow T_c = 1 \text{ K}$

"Low" density:
- $n_{\text{water}}/10^9 \rightarrow T_c = 100 \text{ nK} - 1 \text{ \mu K}$
- seconds to minutes lifetime of the atomic gas and BEC possible
How Do We Know Which Atoms are Bosons?

On the Theory of Quantum Mechanics.
By P. A. M. Dirac, St. John’s College, Cambridge.

(Communicated by R. H. Fowler, F.R.S.—Received August 26, 1926.)

If now we adopt the solution of the problem that involves symmetrical eigenfunctions, we should find that all values for the number of molecules associated with any wave have the same a priori probability, which gives just the Einstein-Bose statistical mechanics.* On the other hand, we should obtain a different statistical mechanics if we adopted the solution with antisymmetrical eigenfunctions, as we should then have either 0 or 1 molecule associated with each wave. The solution with symmetrical eigenfunctions must be the correct one when applied to light quanta, since it is known that the Einstein-Bose statistical mechanics leads to Planck’s law of black-body radiation. The solution with antisymmetrical eigenfunctions, though, is probably the correct one for gas molecules, since it is known to be the correct one for electrons in an atom, and one would expect molecules to resemble electrons more closely than light-quanta.

Example: $^{23}$Na atom has 11 protons, 12 neutrons and 11 electrons.

Laser Cooling in Pictures

The Nobel Prize in Physics 1997 was awarded jointly to Steven Chu, Claude Cohen-Tannoudji and William D. Phillips “for development of methods to cool and trap atoms with laser light”.

Photos: Copyright © The Nobel Foundation

Doppler cooling:
Magnetic Trapping: “Thermos” for Nanokelvin Atoms

Credit: W. Ketterle, MIT

PHYS813: Quantum Statistical Mechanics BEC in ultracold atomic gases
Evaporative cooling consists in using a truncated confining magnetic potential, so that the fastest atoms are ejected from the trap. Due to elastic collisions, the remaining atoms reach a lower temperature.

In practice, the truncation of the potential is chosen 5 to 6 times larger than the instantaneous thermal energy $k_B T$, and one lowers this truncation continuously as the remaining atoms get colder.

Typically a reduction of the temperature by a factor 1000, and an increase of the density by a factor 30 is obtained through the evaporation of 99.9% of the atoms. One starts with $10^9$ atoms at a temperature of $\sim 1 \text{ mK}$, and ends up at the condensation point with $10^6$ atoms at $1 \mu\text{K}$. 

Credit: W. Ketterle, MIT
## Summary of Multi-Stage Cooling to BEC

<table>
<thead>
<tr>
<th>Stage</th>
<th>Temp. $T$</th>
<th>Density $n$ [cm$^{-3}$]</th>
<th>Phase space density $nT^{-3/2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oven</td>
<td>500 K</td>
<td>$10^{14}$</td>
<td>$10^{-13}$</td>
</tr>
<tr>
<td>Laser cooling</td>
<td>50 $\mu$K</td>
<td>$10^{11}$</td>
<td>$10^{-6}$</td>
</tr>
<tr>
<td>Evap. cooling</td>
<td>500 nK</td>
<td>$10^{14}$</td>
<td>2.6</td>
</tr>
<tr>
<td>BEC</td>
<td>(10 - 100 nK)</td>
<td>$3 \cdot 10^{14}$</td>
<td>$10^7$</td>
</tr>
</tbody>
</table>

Credit: W. Ketterle, MIT
Experiment: Release

BEC in ultracold atomic gases

PHYS813: Quantum Statistical Mechanics

The number of atoms (~ $10^7$) that can be put into the traps is not truly macroscopic. As a consequence, the thermodynamic limit is never reached exactly. A first effect is the lack of discontinuities in the thermodynamic functions. Hence BEC in trapped gases is not, strictly speaking, a phase transition.

- **Density**: $10^{13}$ cm$^{-3}$
- **Typical distance between atoms**: 300 nm
- **Typical scattering length**: 10 nm
- **87Rb, 23Na, 7Li**

Scattering length is much smaller than characteristic interparticle distances so that interactions are weak.

The Nobel Prize in Physics 2001 was awarded jointly to Eric A. Cornell, Wolfgang Ketterle and Carl E. Wieman “for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates”.

Photos: Copyright © The Nobel Foundation
Criterions for BEC of Interacting Bosons

For a homogeneous fluid of particles in a box with periodic boundary conditions, the one-body reduced matrix, which is the $N$-body matrix traced over all but the variables corresponding to a single particle:

$$
\rho_1(r, r') = \frac{N}{Z_N} \int d r_2 \ldots d r_N \rho(r, r_2, \ldots, r_N; r', r_2, \ldots, r_N)
$$

has the property (C. N. Yang):

$$
\lim_{|r - r'| \to \infty} \rho_1(r, r') = f(r)f(r')
$$

For atoms in a trap $\rho_1(r, r')$ will approach zero, simply because of the nature of the potential, when $|r - r'| \to \infty$, and other criteria must then be found. For actual experiments, the condensate is recognized by its sudden appearance as a compact cloud of particles that forms at the center of the trap.

Eigenvalues of $\rho_1(r, r')$ (Penrose and Onsager):

→ if all eigenvalues are of order unity, the system is normal
→ if one eigenvalue is of order $N$, the rest of order unity, the system is a simple BEC

$$
\rho_1(r, r') = N_0 \Psi_0^*(r) \Psi_0(r') + \sum_{i \neq 0} n_i \Psi_i^*(r) \Psi_i(r'), \quad N_0 \sim N, \quad n_i \sim 1
$$

→ if two or more eigenvalues are of order $N$, the system is a fragmented BEC
For inhomogeneous systems the usual argument for the universal equivalence of different statistical ensembles needs to be reconsidered. Of course, there are special cases of inhomogeneous systems when the equilibrium system can be divided into essentially homogeneous layers, and each layer can be subjected to its own limiting process. This, requires that the volume of each homogeneous layer can be made infinite without changing the physical situation.

**Example:** In a constant gravitational field, the system can be divided into thin layers by planar equipotential surfaces. The thin layers between the planes can be made infinite in extent, enclosing regions of uniform density without altering the physics of the problem.

The diluted atomic gases confined in a trap exchange neither particles nor energy with a surrounding heat bath, after evaporative cooling is turned off, so that grand canonical ensemble (GCE) is inconsistent with experimental conditions → use MC ensemble.

The quantities used in the constructions of TD variables will in general fluctuate, and their statistics will be different for different ensembles. Should we associate the physically observed quantities with mean values, most probable values, or some other type of statistical average?

**TDL for GCE:**

\[ \frac{N}{R^3} \sim N\omega^3 \]

**Theory of BEC in Harmonic Potential: Grand Canonical Ensemble and Thermodynamic Limit**

\[ V(\mathbf{r}) = \frac{1}{2} V_0 \left( \frac{\mathbf{r}}{R} \right)^2 \]

\[ \omega = \sqrt{\frac{V_0}{R^2 m}} \]

\[ E = \hbar \omega (m_x + m_y + m_z + 1/2) \]

\[ N = \sum_{m_x, m_y, m_z} \frac{1}{\exp \beta[\hbar \omega (m_x + m_y + m_z + 3/2) - \mu] - 1} \]
Theory of BEC in Harmonic Trapping Potential: Critical Temperature

\[ N = n_0 + \left( \frac{kT}{\hbar \omega} \right)^3 \int_0^\infty du \int_0^\infty dv \int_0^\infty dw \frac{1}{1 - e^{-(u+v+w+\alpha)}} \]

where we have let \( u = \beta \hbar \omega m_x \), etc., and \( \alpha = \frac{3}{2} \beta \hbar \omega - \beta \mu \).

Integration can be avoided by performing discrete sum exactly

\[ N = \sum_{l=1}^{\infty} \frac{e^{-a_l}}{(1 - e^{-l\beta \hbar \omega})^3} \]

The original sum does not vary uniformly around \( u + v + w = 0 \) (where it can have a very sharp peak), so that the integral approximation miscounts \( n_0 = N_0 \)

\[ N = n_0 + \left( \frac{kT}{\hbar \omega} \right)^3 \int_0^\infty du \int_0^\infty dv \int_0^\infty dw \sum_{l=1}^{\infty} e^{-l(u+v+w+\alpha)} \]

\[ = n_0 + \left( \frac{kT}{\hbar \omega} \right)^3 \sum_{l=1}^{\infty} e^{-l\alpha} \left( \int_0^\infty du e^{-lu} \right)^3 \]

\[ = n_0 + \left( \frac{kT}{\hbar \omega} \right)^3 F_3(\alpha), \]

\[ F_3(\alpha) = \sum_{l=1}^{\infty} e^{-l\alpha} \frac{1}{l^3} \]

\[ \hbar \omega = \hbar \sqrt{\frac{U_0}{m} \left( \frac{d}{N} \right)^{1/3}} = \frac{k_B T_0}{N^{1/3}} \]

\[ d = \frac{N}{R^3} \]

\[ T_c = T_0 \zeta(3)^{-1/3} \]

\[ N = N_0 + N \left( \frac{T}{T_0} \right)^3 F_3(\alpha) \]

Correct TDL ensures properly extensive expression for the number of noncondensed particles
Condensate Fraction as a Function of Temperature: Theory vs. Experiment

Physics Today 52(12), 37 (1999)

**Figure 2.** The condensate fraction as a function of temperature is affected by both finite-size and interaction effects. Here are the predictions of three different models for the fraction of atoms that is in the condensate when the JILA trap is loaded with 2000 rubidium-87 atoms. The dotted line shows the thermodynamic result of equation 2. The dashed line is the result of incorporating finite-size effects, distributing 2000 atoms according to the Bose–Einstein distribution. The Popov theory (solid red line) includes both a finite number of atoms and atom–atom interactions, and gives very good agreement with observed condensate fractions.

\[
N = N_0 \left[ 1 - \left( \frac{T}{T_c} \right)^3 \right]
\]

BEC in spherically symmetric harmonic oscillator trapping potential

\[
N = N_0 \left[ 1 - \left( \frac{T}{T_c} \right)^{3/2} \right]
\]

BEC in textbook homogeneous gas

finite-size corrections:

\[
\frac{N_0}{N} = 1 - \left( \frac{T}{T_c^0} \right)^3 - \frac{3 \omega \zeta(2)}{2 \omega_{10} \zeta(3)} \left( \frac{T}{T_c^0} \right)^2 N^{-1/3}
\]
Density Matrix of BEC in Harmonic Trapping Potential

$$\rho_1(r, r') = \sum_{l=1}^{\infty} e^{\beta \mu l} \left\{ \sum_m e^{-l\beta E_m} \psi_m(r) \psi_m^*(r') \right\}$$

$$d_i(r, r') = \left( \frac{m \omega}{\hbar \sinh(l \beta \omega)} \right)^{3/2} \times \prod_{i=x, y, z} \exp\left\{ - \frac{m \omega}{2\hbar \sinh(l \beta \omega)} \times [(r_i^2 + r_i'^2) \cosh(l \beta \omega) - 2 r_i r_i'^2] \right\}$$

$$\rho(r) = \sum_{l=1}^{\infty} e^{\beta \mu l} \left( \frac{m \omega}{\hbar \sinh(l \beta \omega)} \right)^{3/2} \rho_c(0) = \left( \frac{2\pi m kT_c}{\hbar^2} \right)^{3/2} \sum_{l=1}^{\infty} \frac{1}{l^{3/2}} = \left( \frac{2\pi m kT_c}{\hbar^2} \right)^{3/2} \zeta(3/2)$$

$$kT_c = \frac{2\pi \hbar^2}{m} \left( \frac{\rho_c(0)}{\zeta(3/2)} \right)^{2/3}$$

By coincidence, trapped gas, which has its BEC localized near the origin, has a condensate there under just the same conditions as the homogenous gas of density $\rho_c(0)$.

Gross-Pitaevskiiii Equation for the Condensate Wavefunction

\[ \frac{\hbar}{\partial t} \Psi_0(r, t) = \left( \frac{\hat{P}^2}{2m} + V_{\text{trap}}(r) \right) \Psi_0(r, t) + N_0 U_0 |\Psi_0(r, t)|^2 \Psi_0(r, t) \]

Each atom feels an additional potential due to the mean field of all the other atoms present, which is proportional to the local atomic density.

\[ U_0 = \frac{4\pi \hbar^2 a}{m} \]

Since the atoms are extremely cold, only head-on, or the so-called s-wave collisions in quantum-mechanical description of scattering are important.

\( a > 0 \) repulsive, \( a < 0 \) attractive

large \( |a| \) → strong interactions

Bose-Einstein condensation is reached when the interparticle separation is comparable to the de Broglie wavelength of the atoms. For evaporatively cooled gases, the de Broglie wavelength of the atoms is enormous, compared to the range of the interatomic forces. We can therefore model binary scattering using an effective contact interaction: \( V(r - r') = U_c \delta(r - r') \). Here, \( U_c \) is given in terms of the binary s-wave scattering length \( a \) by \( U_c = 4\pi\hbar^2 a/m \), which appears in equation 3, the Gross-Pitaevskii equation. This interaction gives the exact low-energy scattering amplitude \((-a)\) when used in the simplest, first-order perturbation theory approximation (the Born approximation).

To see how the contact interaction changes the energy of the gas, one can consider the relative wavefunction of a pair of alkali atoms scattering off one another. For ultralow scattering energies, the effect of the interatomic potential is equivalent to that of a hard sphere of radius \( a \). When the scattering energy is zero, the relative wavefunction has the form \( \phi(r) = \chi(1 - a/r) \). Here, \( a \) is the scattering length and \( \chi \) is the asymptotic value of the wavefunction. Written in this way, the zero-energy wavefunction clearly has a node at \( a \). (The above wavefunction is valid only outside the range of the atomic potential; for smaller distances, the wavefunction depends on the details of the interatomic potential.)

In the dilute gas, the scattering length provides all of the information needed to calculate the change in the energy of the gas due to the interactions between the particles. In the limit of low scattering energies, this additional energy is stored in the increased kinetic energy of the particles produced by the boundary condition of a node at \( r = a \). This extra kinetic energy in the wavefunction is given by

\[ \int_a^\infty dr \left( 4\pi r^2 \right) \frac{\hbar^2}{m} \left\{ \chi \sqrt{1 - \frac{a}{r}} \right\}^2 = U_0 \chi^2. \]

If one takes \( \chi^2 \) as the density of the other particles, one obtains the needed expression for the energy of one particle in the presence of others.
Density Profile of BEC: GP Theory vs. Experiment

Usage of classical field (order parameter) for the condensate in GP theory is due to the large particle number which renders the non-commutivity of the original field operators in second quantization not important. This replacement is analogous to the transition from quantum electrodynamics to the classical description of electromagnetism in the case of a large number of photons.

Ansatz to solve GP equation:

\[ \Psi_0(r, t) = e^{-\mu t/\hbar} \phi(r) \]

Thomas-Fermi approximation for repulsive interactions:

\[ \frac{\hat{p}^2}{2m} \Psi_0(r, t) \ll N_0 U_0 |\Psi_0(r, t)|^2 \Psi_0(r, t) \]

\[ |\phi(r)|^2 \approx \frac{\mu - V_{\text{trap}}(r)}{N_0 U_0} \]
Condensate wave function from GPE at $T=0$ for Attractive and Repulsive Interactions

FIG. 8. Condensate wave function, at $T=0$, obtained by solving numerically the stationary GP Eq. (39) in a spherical trap and with attractive interaction among the atoms ($a<0$). The three solid lines correspond to $N|a|/a_{ho}=0.1,0.3,0.5$. The dashed line is the prediction for the ideal gas. Here the radius $r$ is in units of the oscillator length $a_{ho}$ and we plot $(a_{ho}^3/N)^{1/2}\phi(r)$, so that the curves are normalized to 1 [see also Eq. (40)].

FIG. 9. Same as in Fig. 8, but for repulsive interaction ($a>0$) and $Na/a_{ho}=1,10,100$.

Applications: Atoms in Optical Lattices to Simulate Condensed Matter Systems


superfluid state with phase coherence

bosonic Mott insulator with no coherence

superfluid state after restoring coherence

Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms

Marina Gruner, Oul Mandel, Tilman Esslinger, Theodor W. Hänsch & Immanuel Bloch

PHYS813: Quantum Statistical Mechanics

BEC in ultracold atomic gases