

Lecture 8 Bose-Einstein condensation, Ultracold quantum gases

Learning goals

- To understand deeply the concept of Bose-Einstein condensation of non-interacting bosons; to be able to derive the result and understand the details of the calculation.
- To get an idea of how an interacting Bose-Einstein condensate can be described theoretically.
- To get a brief overview of ultracold quantum gases.

Literature: P. Törmä and K. Sengstock (Eds.), Quantum Gas Experiments – Exploring Many-Body States, Imperial College Press (available as an ebook at Aalto library!); C.J. Pethick and H. Smith, Bose-Einstein Condensation in Dilute Gases, Cambridge University Press

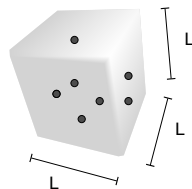
13 General remarks

Ultracold atomic Bose and Fermi gases are systems under intensive experimental and theoretical research at the moment. They provide an excellent setup to study many-body quantum physics. In the lectures 9-12, we will consider concepts like Bose-Einstein condensation, Fermi liquids, quantum phase transitions and superfluidity/superconductivity in the context of these ultracold gases. However, the concepts and the theoretical descriptions are of more general significance; they can be applied in various other fields of modern physics where many-body phenomena occur (condensed matter physics of solid state metallic, semiconductors, organic materials; nanophysics in general; nuclear physics; high energy physics). In addition to these general concepts, we will get a quick overview on issues specific to ultracold gases: trapping and manipulation of atoms by electromagnetic fields, imaging techniques, and recent experiments in the field.

14 Bose-Einstein condensation

14.1 Bose-Einstein condensation – a simple approach

Consider **non-interacting** particles (bosons) in a box



$$\hat{H} = \int d\mathbf{x} \psi^\dagger(\mathbf{x}) \left[-\frac{\hbar^2 \nabla^2}{2m} \right] \psi(\mathbf{x}). \quad (14.1)$$

For non-interacting particles, one does not have the usual interaction term

$$\left(+ \int d\mathbf{x}d\mathbf{x}' \psi^\dagger(\mathbf{x}) \psi^\dagger(\mathbf{x}') U(|\mathbf{x} - \mathbf{x}'|) \psi(\mathbf{x}') \psi(\mathbf{x}) \right). \quad (14.2)$$

For a particle in a box, the single particle wavefunction and energies are

$$\varphi_{\mathbf{n}}(\mathbf{x}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k}_{\mathbf{n}} \cdot \mathbf{r}} \quad (14.3)$$

$$\mathbf{k}_{\mathbf{n}} = \frac{2\pi}{L} (n_x, n_y, n_z) \quad n_i = 0, \pm 1, \pm 2, \dots \quad (14.4)$$

$$E_{\mathbf{n}} = \frac{\hbar^2 (2\pi)^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2). \quad (14.5)$$

We define \hat{N} , i.e. the particle number, in this basis. The field operators $\psi(\mathbf{x})$ can be expressed using this basis (see lectures on second quantization). The particle number is defined

$$\hat{N} = \sum_{\mathbf{n}} \hat{a}_{\mathbf{n}}^\dagger \hat{a}_{\mathbf{n}}. \quad (14.6)$$

The grand canonical density operator is

$$\hat{\rho} = \frac{1}{Z} e^{-\beta(\hat{H} - \mu\hat{N})}, \quad (14.7)$$

where $Z = Tr[e^{-\beta(\hat{H} - \mu\hat{N})}]$, $\beta = \frac{1}{k_B T}$, and μ is the chemical potential.

Now the expectation value (average number) of particles in the state (mode) \mathbf{n} is:

$$n_{\mathbf{n}} = \langle \hat{a}_{\mathbf{n}}^\dagger \hat{a}_{\mathbf{n}} \rangle = Tr \{ \hat{\rho} \hat{a}_{\mathbf{n}}^\dagger \hat{a}_{\mathbf{n}} \} = \frac{ze^{-\beta E_{\mathbf{n}}}}{1 - ze^{-\beta E_{\mathbf{n}}}}, \quad (14.8)$$

where $z = e^{\mu\beta}$. For more information see a course/book in statistical physics (e.g. the chapter 8.6 in Kerson Huang, Quantum Statistical Mechanics, Wiley, 2nd edition). Let us calculate the total density of the particles

$$\frac{N}{L^3} = \frac{1}{L^3} \sum_{\mathbf{n}} n_{\mathbf{n}} = \frac{1}{L^3} \sum_{\mathbf{n}} \frac{ze^{-\beta E_{\mathbf{n}}}}{1 - ze^{-\beta E_{\mathbf{n}}}} = \frac{1}{L^3} \frac{z}{1 - z} + \frac{1}{L^3} \sum_{\mathbf{n} \neq 0} \frac{ze^{-\beta E_{\mathbf{n}}}}{1 - ze^{-\beta E_{\mathbf{n}}}}. \quad (14.9)$$

The second term in the above equation is, for large N ,

$$\frac{1}{L^3} \sum_{\mathbf{n} \neq 0} \frac{ze^{-\beta E_{\mathbf{n}}}}{1 - ze^{-\beta E_{\mathbf{n}}}} \approx \frac{1}{L^3} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dn_x dn_y dn_z \frac{ze^{-\beta \left(\frac{\hbar^2 (2\pi)^2}{2mL^2} \mathbf{n}^2 \right)}}{1 - ze^{-\beta \left(\frac{\hbar^2 (2\pi)^2}{2mL^2} \mathbf{n}^2 \right)}}. \quad (14.10)$$

Let $A = \beta \frac{\hbar^2 (2\pi)^2}{2mL^2}$. Let us make a variable transformation:

$$\mathbf{n} \rightarrow \frac{\mathbf{n}'}{\sqrt{A}}, \quad dn_x dn_y dn_z \rightarrow \frac{dn'_x dn'_y dn'_z}{A^{\frac{3}{2}}} \quad (14.11)$$

and let us use spherical coordinates in the variable \mathbf{n}' (and drop the prime). Then

$$\frac{1}{L^3} \sum_{\mathbf{n} \neq 0} \frac{ze^{-\beta E_{\mathbf{n}}}}{1 - ze^{-\beta E_{\mathbf{n}}}} \approx \int d\Omega \int_0^\infty dn \frac{ze^{-n^2} n^2}{1 - ze^{-n^2}} \frac{1}{L^3} \frac{1}{A^{\frac{3}{2}}} = \frac{1}{\lambda^3} g_{\frac{3}{2}}(z), \quad (14.12)$$

where

$$g_{\frac{3}{2}}(z) = \frac{4}{\sqrt{\pi}} \int_0^\infty dx x^2 \frac{ze^{-x^2}}{1 - ze^{-x^2}} = \sum_{l=1}^{\infty} \frac{z^l}{l^{\frac{3}{2}}} \quad (14.13)$$

and λ is the thermal de Broglie wavelength

$$\lambda = \sqrt{\frac{2\pi\hbar^2}{mk_B T}} = \lambda_{dB}. \quad (14.14)$$

Here $z = e^{\mu/\beta}$, therefore (for $\mu \leq 0$, which is the case now; in general, μ cannot exceed the energy of the lowest state since otherwise the Bose distribution function $f(E_n) = 1/(e^{(E_n - \mu)/(kT)} - 1)$ would be negative)

$$0 < z < 1 \Rightarrow \max \left(\frac{1}{L^3} \sum_{\mathbf{n} \neq 0} \frac{ze^{-\beta E_{\mathbf{n}}}}{1 - ze^{-\beta E_{\mathbf{n}}}} \right) = \max \left(\frac{1}{\lambda^3} g_{\frac{3}{2}}(z) \right) = \frac{1}{\lambda^3} g_{\frac{3}{2}}(1) = \frac{1}{\lambda^3} 2.612. \quad (14.15)$$

That is, the density of the particles in the states $\mathbf{n} \neq 0$ is bounded from above!! (at fixed T) The maximum density in other than the ground state is $2.612/\lambda^3$, and the maximum number of particles in those states is $2.612L^3/\lambda^3$.

\Rightarrow This must mean that, if particles are added, $\frac{z}{1-z}$ grows. Particles accumulate to $\mathbf{n} = 0$ state!!

$$\left. \begin{array}{l} \text{fixed } T, \quad N \text{ grows} \\ \text{or} \\ \text{fixed } N, \quad T \text{ decreases} \end{array} \right\} \Rightarrow \text{BEC} \quad (14.16)$$

Note: In reality, the bosons are always at least weakly interacting. Furthermore, they might be confined by a nontrivial potential, not just a box. The theoretical description then changes, but the above simple argument gives the basic idea of Bose-Einstein condensation.

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14.2 How to describe the condensate of weakly interacting bosons – the Gross-Pitaevskii equation

Assume that the temperature is low enough so that the system has reached Bose-Einstein condensation. How can we describe the BEC of *weakly interacting* bosons in a simple way? One simple but yet powerful approach is the so called Gross-Pitaevskii equation. We derive it by starting from the full Hamiltonian for the many-body system, and we consider a Bose gas at $T = 0$:

$$\hat{H} = \hat{H}_0 + \hat{H}_I \quad (14.17)$$

$$\hat{H}_0 = \int d^3\mathbf{x} \psi^\dagger(\mathbf{x}) \left[\frac{\mathbf{p}^2}{2m} + V_T(\mathbf{x}) \right] \psi(\mathbf{x}) \quad (14.18)$$

$$\hat{H}_I = \frac{1}{2} \frac{4\pi a_s \hbar^2}{m} \int d^3\mathbf{x} \psi^\dagger(\mathbf{x}) \psi^\dagger(\mathbf{x}) \psi(\mathbf{x}) \psi(\mathbf{x}). \quad (14.19)$$

Here $V_T(\mathbf{x})$ describes the external confining potential for the particles (e.g., a harmonic trapping potential for the atoms, created by electric/magnetic/laser fields), and a_s is the scattering length.

To find the wave-function of the BEC using the variational principle, we want to calculate the expectation value of the Hamiltonian (the energy, or to be accurate, the Grand Potential) in the condensed state $|\phi\rangle$

$$\langle \phi | \hat{H} - \mu \hat{N} | \phi \rangle. \quad (14.20)$$

Consider the non-interacting case. The ground state of the system is N bosons in the lowest energy state of the potential V_T . In that case,

$$\left(\frac{\mathbf{p}^2}{2m} + V_T(\mathbf{x}) \right) \tilde{\varphi}_n(\mathbf{x}) = \varepsilon_n \tilde{\varphi}_n(\mathbf{x}) \quad (14.21)$$

$$|\tilde{\phi}\rangle = \frac{(a_0^\dagger)^N}{\sqrt{N!}} |vac\rangle \quad (14.22)$$

$$a_0^\dagger = \int d^3\mathbf{x} \tilde{\varphi}_0(\mathbf{x}) \psi^\dagger(\mathbf{x}). \quad (14.23)$$

However, now the interactions will change the wavefunctions of the states. We expand the field operators as

$$\psi(\mathbf{x}) = \sum_n a_n \varphi_n(\mathbf{x}) \quad (14.24)$$

where the wavefunctions $\varphi_n(\mathbf{x})$ are at the moment unknown. We now assume that the gas is condensed, that is, all the particles are in the lowest energy state:

$$|\phi\rangle = \frac{(a_0^\dagger)^N}{\sqrt{N!}} |vac\rangle = |N, 0, 0, \dots\rangle, \quad (14.25)$$

where in $|N, 0, 0, \dots\rangle$ the notation goes as $N(|N, 0, 0, \dots\rangle)$ is for $\varphi_0(\mathbf{x})$, $0(|N, 0, 0, \dots\rangle)$ is for $\varphi_1(\mathbf{x})$, and so on. (Remember that $a_0^\dagger = \int d^3\mathbf{x} \varphi_0(\mathbf{x}) \psi^\dagger(\mathbf{x})$.) We will then derive the Gross-Pitaevskii equation from which the condensate wave function $\varphi_0(\mathbf{x})$ can be solved. The expectation value of the Hamiltonian now becomes (**Exercise Set 9**)

$$\begin{aligned} \langle \phi | \hat{H} - \mu \hat{N} | \phi \rangle &= N \int d^3\mathbf{x} \varphi_0^*(\mathbf{x}) \left[\frac{\mathbf{p}^2}{2m} + V_T(\mathbf{x}) + (N-1) \frac{2\pi a_s \hbar^2}{m} |\varphi_0(\mathbf{x})|^2 - \mu \right] \varphi_0(\mathbf{x}) \\ &= N \int d^3\mathbf{x} \mathcal{L}(\mathbf{x}). \end{aligned} \quad (14.26)$$

Note that in quantum theory the Lagrangian density $\mathcal{L}(\mathbf{x})$ is proportional to $\hat{H} - \mu\hat{N}$ in the way stated in the above equation. This is in contrast to classical mechanics where the Lagrangian equals the kinetic energy minus the potential energy. The difference is because in quantum theory one uses the variational principle to find the wavefunction (or quantum field) rather than the particle trajectory as in classical mechanics. Using the Euler-Lagrange equations

$$\frac{\delta\mathcal{L}}{\delta\varphi_0} - \frac{\partial}{\partial x_1} \frac{\delta\mathcal{L}}{\delta\frac{\partial\varphi_0}{\partial x_1}} - \frac{\partial}{\partial x_2} \frac{\delta\mathcal{L}}{\delta\frac{\partial\varphi_0}{\partial x_2}} - \frac{\partial}{\partial x_3} \frac{\delta\mathcal{L}}{\delta\frac{\partial\varphi_0}{\partial x_3}} = 0 \quad (14.27)$$

(same for the complex conjugate)

one obtains (**Exercise Set 9**) the Gross-Pitaevskii equation:

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V_T(\mathbf{x}) + N \frac{4\pi a_s \hbar^2}{m} |\varphi_0(\mathbf{x})|^2 \right) \varphi_0(\mathbf{x}) = \mu \varphi_0(\mathbf{x}). \quad (14.28)$$

This equation determines the *ground state* wavefunction of the BEC, $\varphi_0(\mathbf{x})$. The *excitations* of the condensate can be described, e.g., by using the Bogoliubov theory, as was discussed in Lecture 4 for bosons. In Lecture 10, the Bogoliubov theory will be considered again but in the context of Fermions.

15 Ultracold atoms: alkali and others

The research on ultracold atoms started with alkali atoms:

Only one electron at the outermost shell; existence of suitable electronic transitions for laser cooling and trapping.

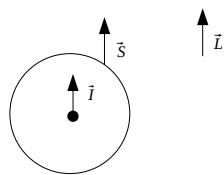
Typically: Li, Na, K, Rb, Cs (bosonic or fermionic isotopes)

More recently, also other atoms have been trapped and cooled to quantum degeneracy:

Sr, Cr, Yb, Er, Dy, etc.

Note: also ultracold molecules can be produced.

The relevant electronic states of the (alkali) atoms are determined by the quantum number n related to the state of the outermost electron, the angular momentum L and the spin S of that electron, and the nuclear spin I .



Good and useful quantum numbers are obtained by combining them

$$\mathbf{J} = \mathbf{S} + \mathbf{L} \quad (15.1)$$

$$\mathbf{F} = \mathbf{J} + \mathbf{I}. \quad (15.2)$$

This gives the basis

$$|n, J, F, m_F\rangle \quad (15.3)$$

The different F states are called the hyperfine states. The states corresponding to different m_F are called Zeeman sublevels of the hyperfine states. Atoms in ultracold gases can be prepared into one internal state, that is, one hyperfine state (and even to a certain Zeeman sublevel, whose degeneracy is lifted in a magnetic field). Also gases where part of the atoms are in internal state (e.g. Zeeman sublevel) and the rest of the particles in some other(s) can be prepared. The particles in different internal states are distinguishable. Therefore they can be understood as particles with a different "pseudospin". One can also talk about a gas with many "components". Particles in these different pseudospin states can be used to simulate, for instance, electrons with different spins that feel a certain lattice potential and interactions.

The atoms (and nowadays also simple molecules) can be trapped with magnetic, electric and light fields, and cooled with laser cooling and evaporative cooling (confining potential is not infinitely high and can be lowered: the hottest atoms can escape) down to nanokelvin temperatures.

As a result, one can obtain trapped and ultracold gases! If you wish to learn more (not part of the course) about basics of ultracold quantum gases, Chapter 2 of the book P. Törmä and K. Sengstock (Eds.), *Quantum Gas Experiments – Exploring Many-Body States*, Imperial College Press (available as an ebook at Aalto library) is recommended.

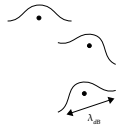
16 Quantum gases of alkali atoms

16.1 What is a quantum gas?

Gas:



Actually, each particle is associated with a wavefunction:



The spatial scale of the wavefunction is given by the thermal deBroglie wavelength

$$\lambda_{dB} = \sqrt{\frac{2\pi\hbar^2}{mk_B T}}. \quad (16.1)$$

If the particles are so close to each other that the wavefunctions start to overlap, it begins to matter whether the particles are bosons or fermions! **Quantum statistics** starts to play a role.



To achieve this, the gas should be either **very cold** or **very dense**.

Normally we do not see quantum gases because when matter gets colder or denser, it usually forms molecules, liquids and solids.

However, the quantum gases realized by alkali atom gases are **metastable** systems, living long enough (before solidifying etc.) in order to make experiments.

The gases are *extremely dilute*: 10^{13} atoms/cm³ - 10^{18} atoms/cm³ (c.f. density of molecules in normal air is around 10^{21} atoms/cm³).

How cold should the gas then be to observe effects of quantum statistics? **ULTRA-cold!!!**

$$\text{Interparticle distance} = 1/(\text{density})^{\frac{1}{3}} = \frac{1}{\sqrt[3]{n}}. \quad (16.2)$$

The interparticle distance should become comparable to the deBroglie wavelength to have overlap of quantum wavefunctions and thereby the effect of the quantum statistics:

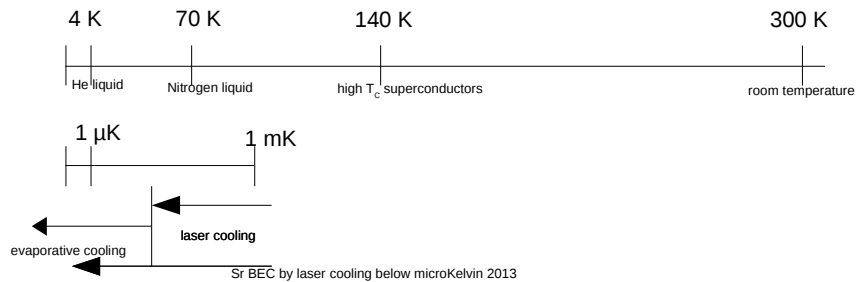
$$\frac{1}{\sqrt[3]{n}} \sim \sqrt{\frac{2\pi\hbar^2}{mk_B T}} \quad (16.3)$$

$$n \sim \left(\frac{mk_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} \quad (16.4)$$

e.g. (in SI units)

$$\left. \begin{array}{l} m = 100 m_p \\ \hbar = 10^{-34} \\ k_B = 10^{-23} \\ n = 10^{15} \frac{1}{\text{cm}^3} \end{array} \right\} \Rightarrow T \sim 1\mu\text{K} \quad (16.5)$$

Typically in the experiments, $T \sim 10\text{nK} - 100\mu\text{K}$.



16.2 Interactions in ultracold atomic gases

The interactions between the atoms are basically van der Waals interactions (the electron clouds of two atoms are interacting). Now, because the gases are very cold, the deBroglie wavelengths of the atoms are much larger than the range of the van der Waals potential, thus the collisions are very low energy collisions, i.e. the relevant momenta k are very small. Due to this, some important approximations can be done, and one can show that: *The s-wave scattering contribution, i.e. the partial wave with orbital angular momentum $l = 0$, is the dominant one, and it is possible to describe the whole scattering process by one number, the s-wave scattering length a_s , that is, $f(\theta) \sim -a_s$.* This argument is true in most atomic systems studied so far, however, with the research expanding beyond alkali atoms, cases where it is not any more valid start to emerge, such as ultracold erbium.

The scattering length can often be calculated from the detailed shape of the van der Waals potential, and also measured experimentally. One can then write the many-body Hamiltonian of the interacting system using the scattering length only and assuming contact interactions. This approximation is possible because the gases are so cold, and in most cases the approximation provides a sufficient description of the system.

Important:

There are also ways to **tune** the scattering length a_s , for instance by using the phenomenon of **Feshbach resonance**. Using a Feshbach resonance (related to the Fano resonance), the change of magnetic field can change the scattering length from positive to negative and from weak to strong. If you wish to learn more (not part of the course) about Feshbach resonances, Chapter 4 of the book P. Törmä and K. Sengstock (Eds.), *Quantum Gas Experiments – Exploring Many-Body States*, Imperial College Press (available as an ebook at Aalto library) is recommended.

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