

Hefei-Lectures 2015  
Forth Lesson: Bose-Einstein condensates

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## 4.1 Degenerate Quantum Gases

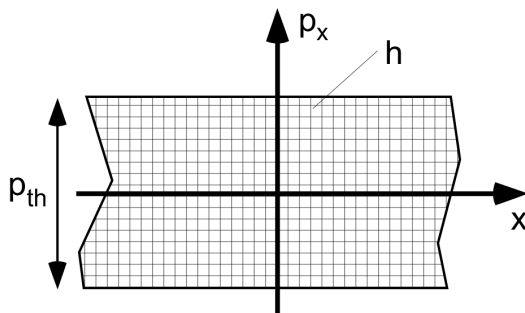
- phase space of a single particle

A single particle has 6 degrees of freedom: three components for the velocity and three for the position. In classical physics the state of the particle is a point in a 6 dimensional phase space. The particle changes the position in phase space either because it moves in position space according to its velocity or because it changes its momentum for instance via collisions.

In quantum physics we have to regard position-momentum-uncertainty and a particle occupies not a point in phase space but the 6D-volume

$$\Delta x \Delta y \Delta z \Delta p_x \Delta p_y \Delta p_z \simeq h^3$$

Phase space now consists of discrete cells of the size  $h^3$ . Here is a cross section through phase space in the  $x$ - $p_x$  direction:



If the particle can exchange energy with a reservoir of a given temperature its momentum covers a certain range given by

$$\frac{p_{th}^2}{2m} = k_B T.$$

- thermal wave length

If one cools the gas down the kinetic energy of the particle is limited to the range of the thermal energy.

$$\langle E_{kin} \rangle \simeq k_B T \simeq \frac{\langle p^2 \rangle}{2m}$$

Consequently also the momentum cannot exceed a certain amount of quantum fluctuations

$$p_{th} = \Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\langle p^2 \rangle} \simeq \sqrt{2m \langle E_{kin} \rangle} \simeq \sqrt{mk_B T}$$

(We use an inertial system where  $\langle p \rangle^2 = 0$  and  $\langle x \rangle^2 = 0$ ). At low temperatures the particle is squeezed into a smaller and smaller volume in momentum space. The position uncertainty is also affected via the uncertainty relation

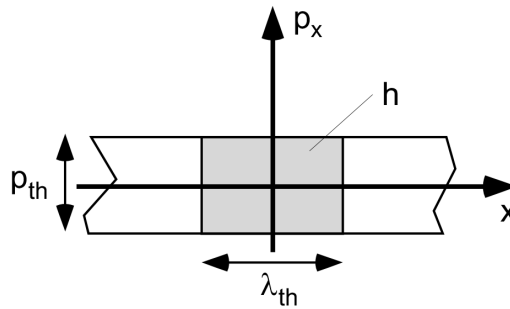
$$(\Delta p)^2 (\Delta x)^2 = \langle p^2 \rangle \langle x^2 \rangle > \frac{\hbar^2}{4}$$

and the particle gets smeared out in position space to a length  $\Delta x$

$$\Delta x := \sqrt{\langle \Delta x^2 \rangle} = \sqrt{\frac{\hbar^2}{4} \frac{1}{\langle p^2 \rangle}} \simeq \sqrt{\frac{1}{4} \frac{\hbar^2}{mk_B T}}$$

This motivates the definition of the "thermal wave length":

$$\lambda_{th} := \sqrt{2\pi \frac{\hbar^2}{mk_B T}} = \sqrt{8\pi} \Delta x$$



The estimation here regards only one dimension and there are prefactors to the thermal energy depending on the degrees of freedom of the particles i.e. on the dimension and on whether the particle is trapped or free. For an ideal and homogeneous gas the thermal wave length is used to describe the extension of the particles matter wave.

- degeneracy and macroscopic wave function

If we cool an atomic gas to very low temperatures the thermal wave length of the particle increases and at some point the single atom must share its phase space with other atoms. At a critical temperature  $T_c$  the average occupation number of a single cell in phase space exceeds one. Then the gas is called "degenerate". Below  $T_c$  more and more particles are squeezed into the same volume in phase space.

For indistinguishable particles the effect is dramatic. In the case of Fermions the Pauli principle forbids double occupancy and as many cells as particles are occupied some of those necessarily also at higher momenta. Therefore, even at  $T = 0$  there is still kinetic energy in the system which is called "Fermi energy".

For Bosons all atoms tend to assemble in the same cell. There is an increased population of the cell with lowest energy. The atoms in this cell are called "Bose-Einstein condensate". The total ensemble of all atoms is called "degenerate Bose gas". In a non-interacting gas at  $T = 0$  all atoms sit in the same cell in phase space.

In a condensate it is not possible to distinguish the atoms any more, not by their momentum and not by their position. The atoms lose their individuality and form what is called a macroscopic quantum state. Since all atoms behave exactly the same all atoms can be described together by a macroscopic wave function  $\psi(\vec{r})$  that is normalized to the number of atoms in the condensate.

- phase space density

In a given phase space volume  $\phi$  the number of cells  $N_z$  is given by

$$N_z = \frac{\phi}{h^3}$$

If we write the phase space volume as the product of the volume  $V$  in position space and the volume  $\phi_p$  in momentum space,

$$N_z = \frac{\phi_p V}{h^3},$$

the expression

$$n_z := \frac{N_z}{V} = \frac{\phi_p}{h^3},$$

is the density of cells in position space. Now we replace the word "cell" by the word "state" and talk about the "density of states" which means the same. Since the

$$\phi_p = p_{th}^3,$$

we get for the density of states

$$n_z = \frac{\Delta p^3}{h^3} \simeq \frac{1}{\lambda_{th}^3}.$$

To specify how many atoms have to share how many states one defines the "phase space density" as the ratio between the atomic number density and the density of states

$$\Lambda := \frac{n}{n_z} = \lambda_{th}^3 n.$$

The gas becomes degenerate if the atomic number density exceeds the density of states or phase space density exceeds one:

$$\begin{aligned} n_z &> n \\ \Lambda &> 1. \end{aligned}$$

With the average distance between two atoms  $d = n^{-1/3}$  we get

$$\lambda_{th} > d.$$

In the degenerate regime the distance is smaller than the thermal wave length.

- numbers

in a Doppler cooled gas with  $T = 100\mu K$ ,  $n = 10^{11}cm^{-3}$  the phase space density is  $\Lambda = 10^{-6}$  and the thermal wave length  $\lambda_{th} = 0.02\mu m$ .

In a degenerate gas we have  $T = 0.5\mu K$ ,  $n = 10^{15}cm^{-3}$ ,  $\Lambda > 1$ ,  $\lambda_{th} > 10\mu m$

## 4.2 Bose-Einstein Condensation of an Ideal Gas

We look at bosonic atoms without interaction

- thermal distributions of distinguishable particles (Boltzmann statistic)

Number of atoms in the energy interval  $(E, E + dE)$

$$\begin{aligned} \rho(\varepsilon)d\varepsilon &= \exp(-(\varepsilon - \mu)/kT) d\varepsilon = \exp(\mu/kT) \exp(-\varepsilon/kT) d\varepsilon \\ &= z \cdot \exp(-\varepsilon/kT) d\varepsilon \\ z &: = \exp(\mu/kT) \end{aligned}$$

Here, the "fugacity"  $z$  is just an abbreviation for  $\exp(\mu/kT)$ . The chemical potential  $\mu$  is used to fulfill by the normalization condition:

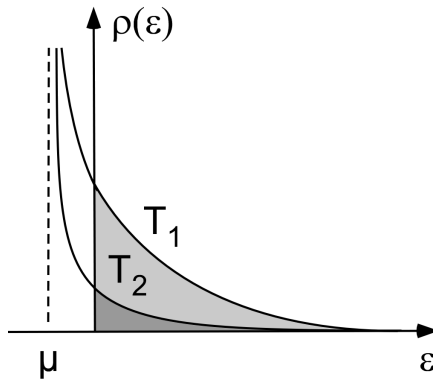
$$\bar{N} = \sum_j \rho(\varepsilon_j)$$

Sum is taken over all states (not energies! We see in a minute how this works.) If we look at the ratio for different energies we find that is only depends on temperature and not on the fugacity.

$$\frac{\rho(\varepsilon_i)}{\rho(\varepsilon_j)} = \frac{\exp(-\varepsilon_i/kT)}{\exp(-\varepsilon_j/kT)} = \exp(-(\varepsilon_i - \varepsilon_j)/kT)$$

- thermal distributions of indistinguishable particles (Bose-Einstein statistic)

$$\rho(\varepsilon)d\varepsilon = \frac{1}{\exp((\varepsilon - \mu)/kT) - 1} d\varepsilon = \frac{1}{z^{-1} \exp(\varepsilon/kT) - 1} d\varepsilon$$

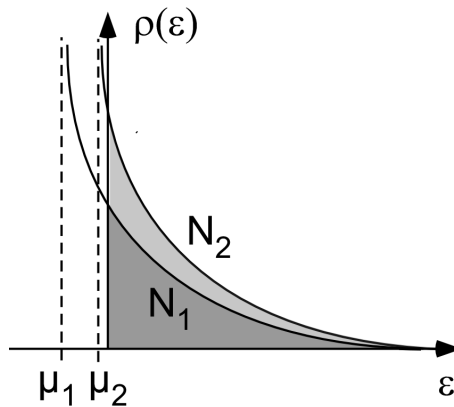


Now the ratio for different energies not only depends on temperature but also on the fugacity i.e. the number of particles.

$$\frac{\rho(\varepsilon_i)}{\rho(\varepsilon_j)} \neq \frac{\exp(-\varepsilon_i/kT)}{\exp(-\varepsilon_j/kT)}$$

- particle number at constant temperature

Increasing the particle number shifts the chemical potential and affect the ratio for the occupation at different energies.



The chemical potential cannot be larger than zero such that the largest occupation number are obtained for  $\mu = 0$ .

- Bose-Einstein condensate

What is the maximum particle density that can be described with Bose-Einstein distribution function for  $\mu = 0$ ? The particle density is given by the sum over the occupation numbers of all states and thus contains the integral of  $\rho(\varepsilon)$ . Since  $\rho(\varepsilon)$  has a pole at

$\varepsilon = 0$  one might think that also the integral is infinite. However, it turns out that this is not the case! Consequently, the thermal distribution only describes a finite density of atoms. If the density is increased the excess of atoms collect in the ground state and forms a new thermodynamic phase which is called "Bose-Einstein condensate" ("BEC"). We do the calculation not for a homogeneous gas but for atoms in a harmonic trap.

- critical number in a harmonic trap.

The particle number is given by the sum over the occupation in all states:

$$\bar{N} = \sum_j \frac{1}{z^{-1} \exp(\varepsilon_j/k_B T) - 1}$$

We can sum over the energy if we know how many states belong to the same energy class i.e. the degree of degeneracy  $g(\varepsilon_n)$ . If we know this function we can write

$$\bar{N} = \sum_{\varepsilon_n} g(\varepsilon_n) \frac{1}{z^{-1} \exp(\varepsilon_n/k_B T) - 1}.$$

The degree of degeneracy in harmonic trap is

$$g_n = \frac{1}{2} (n+1)(n+2) \approx \frac{1}{2} \left( \frac{\varepsilon}{\hbar\omega} \right)^2$$

Since the ground state at  $\varepsilon_0 = 0$  sits at the pole of the distribution function (for  $\mu = 0$ ) we treat it separately and remove it from the sum

$$\begin{aligned} \bar{N} &= N_0 + \sum_{\varepsilon_n \neq 0} \frac{g_n}{z^{-1} \exp(\varepsilon_n/k_B T) - 1} \\ N_0 &: = \frac{g_{n=0}}{z^{-1} \exp(0/k_B T) - 1} = \frac{1}{z^{-1} - 1} \end{aligned}$$

If the trap is not too small there are many bound energy levels and the energetic separation between the levels is small. We thus can replace the sum by an integral

$$\sum_{\varepsilon \neq 0} \rightarrow \frac{1}{\hbar\omega} \int_0^\infty d\varepsilon,$$

and for the sum we obtain

$$\begin{aligned} G(z) &: = \sum_{\varepsilon_n \neq 0} \frac{g_n}{z^{-1} \exp(\varepsilon_n/k_B T) - 1} \\ &= \frac{1}{\hbar\omega} \int_0^\infty \frac{1}{2} \left( \frac{\varepsilon}{\hbar\omega} \right)^2 \frac{1}{z^{-1} \exp(\varepsilon/k_B T) - 1} d\varepsilon \\ &= \left( \frac{k_B T}{\hbar\omega} \right)^3 \cdot \frac{1}{2} \int_0^\infty \frac{x^2}{z^{-1} \exp(x) - 1} dx \\ &= \left( \frac{k_B T}{\hbar\omega} \right)^3 \cdot \varsigma_3(z) \end{aligned}$$

with the function

$$\varsigma_3(z) := \frac{1}{2} \int_0^\infty \frac{x^2}{z^{-1} \exp(x) - 1} dx.$$

And

$$\bar{N} = N_0 + \left( \frac{k_B T}{\hbar \omega} \right)^3 \cdot \varsigma_3(z)$$

In the degenerate regime the chemical potential is zero and thus  $z = 1$ . We get

$$\bar{N} = N_0 + \left( \frac{k_B T}{\hbar \omega} \right)^3 \cdot \varsigma_3(1)$$

We can solve for the number of atoms in the ground state and get

$$N_0 = \bar{N} - \left( \frac{k_B T}{\hbar \omega} \right)^3 \cdot \varsigma_3(1)$$

with

$$\varsigma_3(1) = 1.202.$$

- critical temperature

At large temperature the number of atoms in the ground state it is zero (can not be negative). It becomes positive at the critical temperature when  $N_0$  just passes zero

$$0 = \bar{N} - \left( \frac{k_B T_c}{\hbar \omega} \right)^3 \cdot \varsigma_3(1)$$

solving for  $T_c$

$$\begin{aligned} k_B T_c &= \hbar \omega N^{1/3} \cdot (\varsigma_3(1))^{-1/3} \\ &= \hbar \omega N^{1/3} \cdot 0.941. \end{aligned}$$

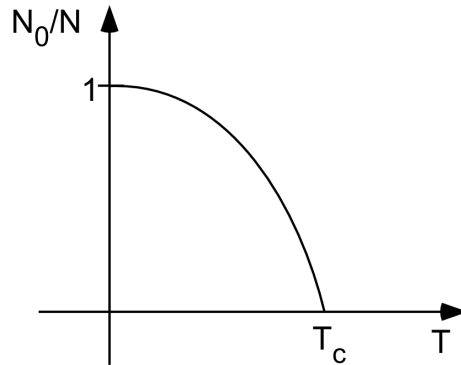
or

$$T_c = 0.941 \frac{\hbar \omega}{k_B} N^{1/3}$$

We can express the number of particle by using  $T_c$

$$\begin{aligned} \frac{N_0}{\bar{N}} &= 1 - \left( \frac{k_B T}{\hbar \omega} \right)^3 \cdot \varsigma_3(1) \frac{1}{N} \left( \frac{T_c}{T} \right)^3 \\ &= 1 - \left( \frac{T}{T_c} \right)^3. \end{aligned}$$





The number of atoms in the ground state increases dramatically for temperatures below  $T_c$ . At  $T = 0$  all atoms are in the ground state. At  $T_c$  a new phase (condensate) slowly appears and the number of thermal atoms is continuously reduced. (For the experts: the phase transition at  $T_c$  is a third order phase transition without interaction and a second order phase transition if collisions between the atoms are included.)

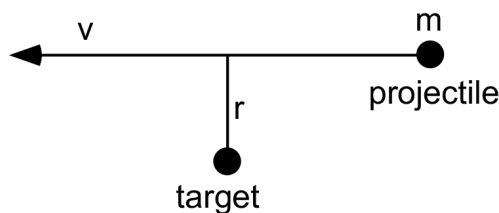
### 4.3 S-Wave Collisions

- angular momentum at low temperature

Classically the value of the angular momentum between two particles that pass each other along a straight line is

$$L_z = m \cdot v \cdot r,$$

with the (reduced) mass  $m$  the relative velocity  $v$  and the distance of closest approach  $r$ . (The vector  $\vec{L}$  has only one nonzero component  $L_z$  with the  $z$ -axis normal to the plane of the collision.)



The interaction between the atoms at long distances is due to the van der Waals force. The potential is a central potential and depends only on the distance between the atoms. We assume it has a characteristic length  $a$  which we call the scattering length. A collisional interaction is only possible if the two atoms approach each other to a distance closer than the  $a$ .

$$r < a,$$

which limits the possible values for the angular momentum

$$L_z < m \cdot v \cdot a.$$

In quantum physics the angular momentum is quantized

$$\begin{aligned} L_z &= m_l \hbar < m \cdot v \cdot a \\ m_l &< \frac{m \cdot v \cdot a}{\hbar} \end{aligned}$$

At low temperatures the velocity is getting smaller and at some point the right side of the equation is smaller than one. Angular momenta with  $m_l > 0$  are not affected by the interaction.

- angular momentum in a MOT

At the Doppler temperature of a MOT and a cloud size of a few  $100 \mu\text{m}$ , states with higher angular momenta are occupied but mainly s-waves are affected by the atomic interaction although p- and d-wave collisions can be observed.

- angular momentum in a BEC

In a BEC the extension of the cloud is less than  $100 \mu\text{m}$  and the velocity is effectively zero (besides some corrections due to the finite size). States with  $l > 0$  are not occupied. A target atom sees a projectile atom coming in from all directions with the same probability. There is no difference in the direction any more. "Direction" loses its meaning. Since all atoms are entirely indistinguishable, all atoms see all other atoms coming in from all directions with the same probability. Every single atom is a target atom and a projectile atom at the same time. This is hard to visualize but we will come back to that later.

- s-wave function

The relative motion of the two atoms is described by a wave function  $\psi(\vec{r})$  which obeys a Schrödinger equation. Since the potential is depending only on  $r$

$$U = V(|\vec{r}_1 - \vec{r}_2|) = V(r)$$

it is convenient to use polar coordinates. As in the analysis of hydrogen, the angular part of the wave function factors out

$$\psi_{k,l,m}(\vec{r}) = Y_{l,m}(\varphi, \theta) R_{k,l}(r).$$

The above argument shows that one can set  $l = 0$  and one obtains

$$\psi_{k,l,m}(\vec{r}) = Y_{00}(\varphi, \theta) R_{k,0}(r) = \frac{1}{\sqrt{4\pi}} R_{k,0}(r) =: \psi_k(r)$$

For the radial part of the wave function  $R_{k,0}(r)$  one obtains a radial Schrödinger equation which one needs to solve. The pair is unbound and the energy is slightly above the dissociation energy

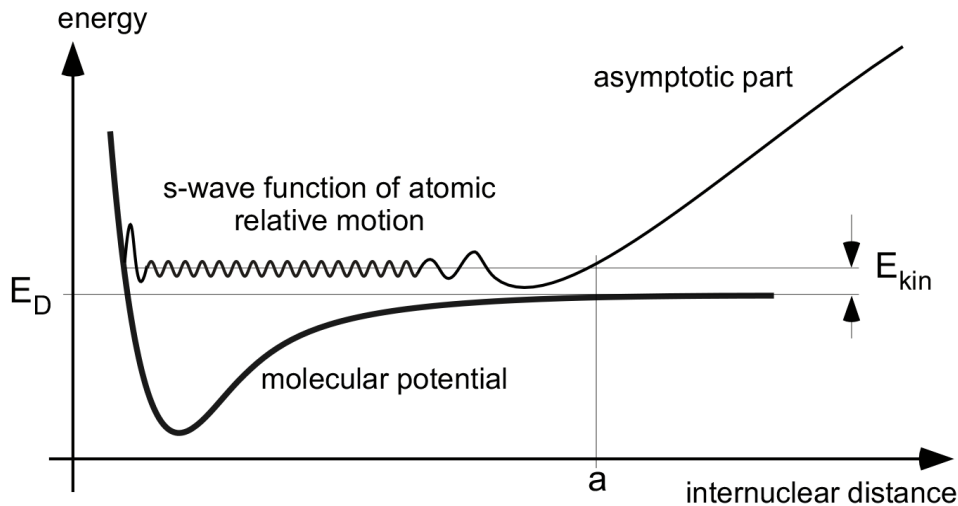
$$E > E_D.$$

That is why the principle quantum number  $n$  for bound states is replaced by the wave number  $k$ . Its a good quantum number since it describes the total energy of the relative motion which at large distances is totally kinetic

$$E_k = \lim_{r \rightarrow \infty} (E_{kin}) = \frac{\hbar^2 k^2}{2m}.$$

- radial wave function

At small distances the wave function  $\psi_k(r)$  rapidly oscillates because the relative motion acquires momentum when rolling down the potential.



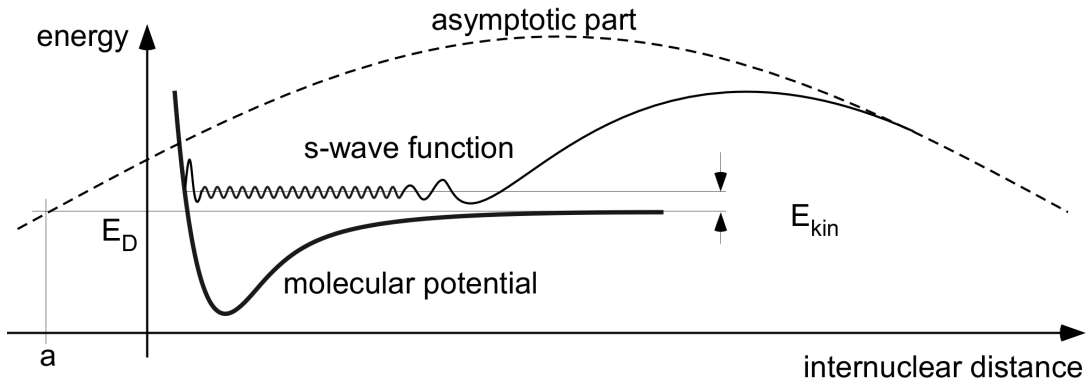
At large distances the kinetic energy is very small and one obtains a spherical wave with a very long wave length.

$$\lim_{r \rightarrow \infty} \psi_k(\vec{r}) = \psi_0 \frac{1}{r} \sin(k(r - a)) = \psi_0 \frac{1}{r} \sin(kr + \varphi)$$

$$\varphi : = -ka.$$

In the sketch above the "asymptotic part" is just the start of this oscillation. The effect of the interaction in the far field is nothing more than that the spherical wave does not start at the origin but is shifted by some offset  $a$ . This offset is called "scattering length". The phase shift  $\varphi$  is called the "s-wave scattering phase".

In the example above the "scattering length"  $a$  is positive but it is also possible that  $a$  is negative:



The value of the scattering length depends very sensitively on the details of the molecular potential.

- typical length scales in a BEC

$$(r_e \simeq a_0) \ll (a \simeq 100a_0) \ll (d \simeq 10^4 a_0) < (\lambda \simeq 10^5 a_0)$$

with the range of the van der Waals potential  $r_{vdW}$ , the scattering length  $a$ , the average distance between two atoms  $d$ , and the size of the condensate  $\lambda$  which is also the de Broglie wave length of the particles in the condensate.

#### 4.4 Interaction, Gross-Pitaevskii equation, and the Lorentz model in Optics

In a real condensate the atoms interact via collisions. The collisions lead to a phase shift of the wave function just as the phase of the light field is shifted if it interacts with atoms. There is obviously some analogy. We use it to derive a differential equation for the macroscopic wave function of the condensate.

- Lorentz-Model

We remember the Lorentz model from lesson 3 where we obtained an expression for the index of refraction of

$$n = 1 + \frac{K}{k^3} \cdot \rho$$

The dimensionless constant  $K = d_a^2 k^2 \varphi_D$  contains the details of the superposition of the dipoles in the dipole sheets,  $k$  is the wave number of the light field and  $\rho$  the density of dipoles and  $d_a$  the average distance between two atoms. The propagation of light in the dielectric media is described by the Helmholtz equation:

$$\nabla^2 E + \frac{n^2 \omega^2}{c^2} E = 0.$$

For  $n$  near 1 one can write approximately

$$n^2 = \left(1 + \frac{K}{k^3} \rho\right)^2 = 1 + 2\frac{K}{k^3} \rho + \left(\frac{K}{k^3} \cdot \rho\right)^2 \simeq 1 + 2\frac{K}{k^3} \rho$$

which results in

$$\begin{aligned} \nabla^2 E + \left(1 + 2\frac{K}{k^3} \rho\right) \frac{\omega^2}{c^2} E &= 0 \\ \nabla^2 E + \left(1 + 2\frac{K}{k^3} \rho\right) k^2 E &= 0 \\ \nabla^2 E + 2\frac{K}{k} \rho E &= -\frac{\omega^2}{c^2} E \end{aligned}$$

- Gross-Pitaevskii equation

A collision shifts the phase of the matter wave function by a scattering phase just as the light field is shifted in phase by the dipole sheet. We can make the connection to the Lorentz model if we regard each atom as part of a macroscopic wave function that takes over the role of the light. At the same time each atom is also part of the target that scatters the wave and shifts its phase just analogous to the dipole sheets that make up the dielectric material in the Lorentz model. We thus try the following substitution for the field

$$E \rightarrow \psi$$

and the for the density of dipoles which is analogous to the density of atomic scatterers

$$\rho \rightarrow |\psi|^2$$

Inserting in the Helmholtz equation yields

$$\nabla^2 \psi + 2\frac{K}{k} |\psi|^2 \psi = -\frac{\omega^2}{c^2} \psi$$

We multiply both sides with

$$-\frac{\hbar^2}{2m}$$

and obtain

$$\begin{aligned} \left(-\frac{\hbar^2}{2m} \nabla^2 - \frac{\hbar^2 K}{m k} |\psi|^2\right) \psi &= \frac{\hbar^2 \omega^2}{2m c^2} \psi. \\ \left(-\frac{\hbar^2}{2m} \nabla^2 + g |\psi|^2\right) \psi &= \mu \psi. \end{aligned}$$

$$\begin{aligned} g &: = -\frac{\hbar^2 K}{m k} \\ \mu &: = \frac{\hbar^2 \omega^2}{2m c^2} \end{aligned}$$

We identify the constant  $K$  with the scattering phase in the following way

$$K = 4\pi \cdot \varphi = -4\pi \cdot ka$$

such that

$$g = 4\pi \frac{\hbar^2}{m} a.$$

With this setting, we obtain the correct equation for an interacting BEC that can be strictly derived by starting with the many body hamiltonian (see below). It is called the "Gross-Pitaevskii equation". For the bizarre situation of s-wave scattering in a condensate, the constant  $K$  turns out to be just the s-wave scattering phase  $\varphi$  times  $4\pi$ .

Different to the plane wave geometry of the Lorentz mode there is no pre factor  $d_a^2 k^2 = (2\pi d_a/\lambda)^2$ . In a condensate the ratio  $d_a/\lambda$  makes little sense since the average separation between the atoms  $d_a$  is no good quantity for particles that are fully indistinguishable also in respect to their position in space. However, we may look at a quantum gas above  $T_c$  and interpret  $\lambda$  as the thermal wavelength  $\lambda_{th}$  and  $d_a$  as the distance between two distinguishable particles. That means that the two particles have to be in different cells in phase space. The distance for two neighboring cells is just  $\lambda_{th}$  such that  $d_a/\lambda = \lambda_{th}/\lambda_{th} = 1$ . This could explain the vanishing pre factor in our model where the "wave length" and "particle separation" are quantities of the same physical object (quantum gas) rather than quantities of two different physical objects (light and atoms).

- chemical potential

In the original Helmholtz equation the energy term on the right side contains the photon energy. If we follow the analogy, the photon energy should vanish at zero energy in the limit for  $T \rightarrow 0$ . However, in a dielectric material the photon is "dressed" by the atoms, and also contains the energy of the electric field which sits in the dipoles. If we make the transition to zero temperature its the dressed energy  $\hbar\omega_d = \hbar c n k$  which should become zero:

$$\omega_d^2 = c^2 n^2 k^2 = c^2 k^2 \left(1 + \frac{K}{k^3} \rho\right)^2 \simeq c^2 k^2 \left(1 + 2\frac{K}{k^3} \rho\right) = 0$$

From the last equation we obtain

$$\begin{aligned} k^2 &= -2\frac{K}{k}\rho \\ \omega^2 &= c^2 k^2 = -c^2 2\frac{K}{k}\rho. \end{aligned}$$

Inserting in the expression for  $\mu$  yields

$$\mu = \frac{\hbar^2}{2m} \frac{\omega^2}{c^2} = -\frac{\hbar^2}{2m} 2\frac{K}{k}\rho = \frac{4\pi\hbar^2}{m} a\rho$$

The energy  $\mu$  is called the "chemical potential" of the BEC.

- collapse of a condensate

In a trap the condensate forms a spherical, lens like object. For negative scattering length,  $K$  is positive and the index of refraction in the analogous Lorentz model larger than 1. The BEC acts as focusing lens for its own matter wave and the radius of the BEC is getting smaller. This further reduces the focal length and the BEC is even further compressed. In fact, in a trap a BEC with negative scattering length becomes unstable if the atom number exceeds a critical value. It collapses until, at high enough density three body collisions set in. They lead to molecule formation and the BEC gets lost. This is very similar to self-focussing of light in a nonlinear material where the index of refraction is intensity dependent due to the Kerr effect. Above a critical power the incident beam creates it own lens which reduces the beam waist until a catastrophic intensity is reached and the dielectric material is destroyed.

- expansion

For positive scattering length  $K < 0$  and the index of refraction smaller than 1. The lens is now defocussing and the condensate tries to expand. In the trap this is counterbalanced by the restoring force of to the trapping potential. The balance between trapping and self-defocussing determines the size of the condensate in the trap (see next section). If the trap is turned off the condensate falls down under gravity. During this fall it can now expand until the density is so small that the index of refraction is 1. One can observe this expansion by taking images of the condensate after some time of flight. This technique is routinely used to detect the properties of the condensate in the trap.

## 4.5 Properties of a trapped condensate

- stationary GP-equation

As for the Schrödinger equation we use the ansatz which separates the space and the time variables. With

$$\phi(\vec{r}, t) = e^{-i\mu/\hbar t} \phi(\vec{r})$$

we obtain the stationary GP-equation

$$\left( -\frac{\hbar^2 \nabla^2}{2m} + V_{trap}(\vec{r}) + g |\phi(\vec{r})|^2 \right) \phi(\vec{r}) = \mu \phi(\vec{r})$$

- energy

What is the energy of a BEC. We calculate the expectation value:

$$\int \phi^*(\vec{r}) \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{trap}(\vec{r}) + g |\phi(\vec{r})|^2 \right) \phi(\vec{r}) d\vec{r} = \int \phi^*(\vec{r}) \mu \phi(\vec{r}) d\vec{r}$$

$$E_{kin} + E_{trap} + 2E_{WW} = \mu N$$

The factor 2 in front of  $E_{ww}$  takes care the fact that each atom is wave and target at the same time. It can be strictly derived.

- chemical potential in a homogeneous gas

Lets look at a condensate in a box potential with Volume  $V$ . Inside the box there is no potential and we have

$$V_{trap}(\vec{r}) = 0.$$

Its reasonable to assume that the macroscopic wave function is homogenous inside the box. It has a constant phase which we set zero and an Amplitude which is given by normalization

$$\phi(\vec{r}) = \sqrt{\frac{N}{V}}.$$

We obtain no contribution from kinetic energy and no contribution from the potential energy

$$\begin{aligned} E_{kin} &= - \int \phi^*(\vec{r}) \frac{\hbar^2 \nabla^2}{2m} \phi(\vec{r}) d\vec{r} = - \int \sqrt{\frac{N}{V}} \frac{\hbar^2 \nabla^2}{2m} \sqrt{\frac{N}{V}} d\vec{r} = 0 \\ E_{pot} &= \int \phi^*(\vec{r}) V_{trap}(\vec{r}) \phi(\vec{r}) d\vec{r} = 0. \end{aligned}$$

All we have is interaction energy

$$\begin{aligned} U &: = E_{int} = \frac{1}{2} \int \phi^*(\vec{r}) g |\phi(\vec{r}, t)|^2 \phi(\vec{r}) d\vec{r} = \frac{1}{2} g \int \sqrt{\frac{N}{V}} |\phi(\vec{r}, t)|^2 \sqrt{\frac{N}{V}} d\vec{r} \\ &= \frac{1}{2} g \frac{N}{V} \int |\phi(\vec{r}, t)|^2 d\vec{r} = \frac{gN^2}{2V} \end{aligned}$$

We thus obtain

$$\begin{aligned} 2E_{int} &= \mu N \\ 2 \left( \frac{gN^2}{2V} \right) &= \mu N \\ \mu &= g \frac{N}{V} \end{aligned}$$

In thermodynamics the chemical potential is defined as

$$\frac{dU}{dN} = \frac{d}{dN} \left( \frac{gN^2}{2V} \right) = g \frac{N}{V} = \mu$$

The variable  $\mu$  is in fact the chemical potential for a homogenous condensate.



- equation of state for a homogenous condensate.

Pressure is defined as

$$p = -\frac{dU}{dV} = -\frac{d}{dV} \left( \frac{gN^2}{2V} \right) = \frac{g}{2} \left( \frac{N}{V} \right)^2$$

$$V^2 p = \frac{g}{2} N^2$$

This is the equation of state for the homogenous condensate.

- compressibility and speed of sound

The adiabatic compressibility at constant entropy is defined

$$\kappa := -\frac{1}{V} \frac{dV}{dp}$$

We find

$$\frac{dV}{dp} = \frac{1}{2} \sqrt{\frac{g}{2}} N p^{-3/2} = \frac{1}{2} \sqrt{\frac{g}{2}} N \left( \frac{g}{2} \left( \frac{N}{V} \right)^2 \right)^{-3/2} = \frac{1}{g} \frac{V^3}{N^2}$$

and for the compressibility

$$\kappa = \frac{1}{g} \left( \frac{V}{N} \right)^2 = \frac{1}{gn^2}.$$

The speed of sound is related to the compressibility via

$$c = \frac{1}{\sqrt{\kappa \rho}},$$

with the density of mass

$$\rho = m \frac{N}{V}.$$

Thus

$$c = \frac{1}{\sqrt{\frac{1}{g} \left( \frac{V}{N} \right)^2 m \frac{N}{V}}} = \sqrt{\frac{g}{m} \frac{N}{V}}$$

Density fluctuations propagate inside the condensate at a constant speed which does not depend on the wave length (no dispersion)

- healing length

At the edge of the box potential the condensate density cannot suddenly drop to zero. There is a typical length scale at which the condensate reacts to changes in the potential shape. It called the "healing length". We assume an exponential drop along the x-direction as we approach the wall placed at  $x = 0$ .

$$\phi(\vec{r}) = \phi_0 e^{-x/x_0},$$

Such a function leads to a kinetic energy which increases for short decay length  $x_0$

$$\begin{aligned}\langle \varepsilon_{kin} \rangle &= \phi_0 e^{-x/x_0} \frac{\hbar^2 \nabla^2}{2m} \phi_0 e^{-x/x_0} \\ &= \frac{\hbar^2}{2m} |\phi_0|^2 e^{-x/x_0} \frac{1}{x_0^2} e^{-x/x_0} \\ &= \frac{\hbar^2}{2m} \frac{1}{x_0^2} |\phi(\vec{r})|^2.\end{aligned}$$

The interaction energy tries to get all atoms as far apart as possible by filling the whole box.

$$\langle \varepsilon_{int} \rangle = g \phi_0 e^{-x/x_0} |\phi_0 e^{-x/x_0}|^2 \phi_0 e^{-x/x_0} = g |\phi(\vec{r})|^4.$$

Steady state is reached if both energy parts are in balance:

$$\begin{aligned}\langle \varepsilon_{kin} \rangle &= \langle \varepsilon_{int} \rangle \\ \frac{\hbar^2}{2m} \frac{1}{x_0^2} |\phi(\vec{r})|^2 &= g |\phi_0 e^{-x/x_0}|^4 \\ x_0 &= \sqrt{\frac{\hbar^2}{2gm |\phi(\vec{r})|^2}} = \sqrt{\frac{1}{8\pi a \cdot |\phi(\vec{r})|^2}}\end{aligned}$$

If we substitute the density  $|\phi(\vec{r})|^2$  by its maximum value  $|\phi_0|^2$  in the middle of the box we get the healing length

$$\xi := \frac{1}{\sqrt{8\pi a \cdot |\phi_0|^2}}$$

This is the shortest range at which a condensate can follow. Typical values are on the order of 100 nm. If a condensate is forced in smaller potentials such as optical lattices it breaks apart and the gas has to be described by another model. (Bose-Hubbard model).

- Thomas Fermi approximation

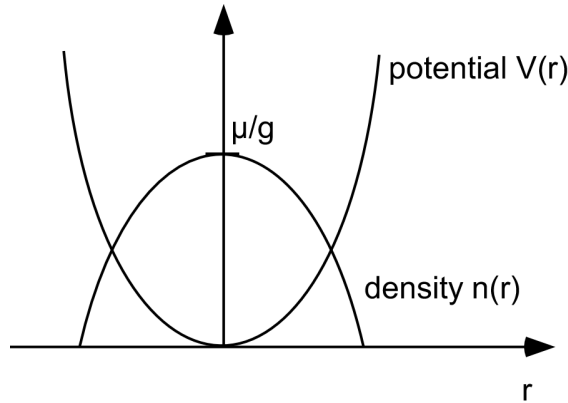
For an increasing number of atoms with positive scattering length  $a > 0$  in a harmonic trap, the atoms creep up the potential well and the total potential energy increases as well as the interaction energy. The kinetic energy stays constant. At some point one can neglect the kinetic energy and gets

$$(V_{trap}(\vec{r}) + g |\phi(\vec{r})|^2) \phi(\vec{r}) \simeq \mu \phi(\vec{r}).$$

This algebraic equation can directly be solved for the density:

$$|\phi(\vec{r})|^2 \simeq \frac{1}{g} (\mu - V_{trap}(\vec{r})).$$

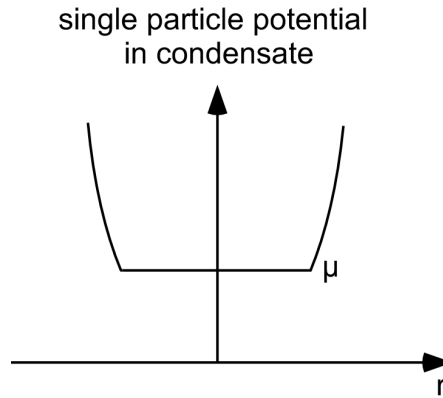
This is the "Thomas Fermi approximation". The density is a direct image of the trapping potential. For a harmonic trap one obtains an inverted parabola.



At the edge of the condensate the density suddenly ends. This is an artefact due to the approximation. If we include the kinetic energy we expect that the density decays on a length scale given by the healing length. The phase is constant across the condensate. This approximation is very good for typical condensate.

- single particle

A single particle moves in the combined potential of the trap and the interaction potential of all other particles. IN the Thomas Fermi approximation both potentials just cancel such that a single particle can move freely inside the condensate.



- negative scattering length

We use the Gross-Pitaevskii equation to estimate the critical atom number for the collapse of a condensate at negative scattering length. We assume a wave function  $\phi(r)$  that describes a spherical condensate with a radius  $\Delta r$ . We estimate the kinetic energy as the localization energy required to compress the atoms to the size given by the radius.

$$\left\langle -\frac{\hbar^2 \nabla^2}{2m} \right\rangle \simeq -\frac{\hbar^2}{2m \Delta r^2}.$$

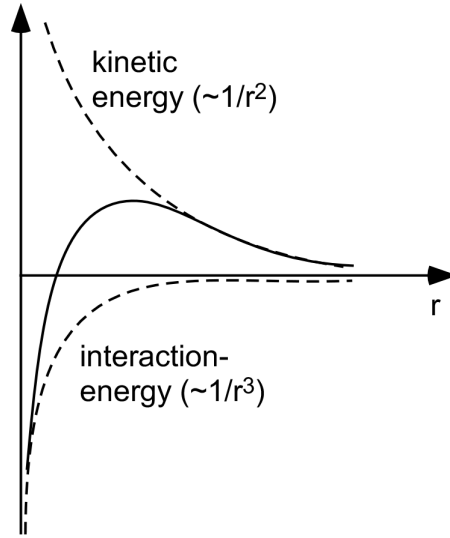
Similarly we estimate the interaction energy by assuming a constant density inside the sphere.

$$\langle g |\psi(r, t)|^2 \rangle = gn(r) \simeq g \frac{N}{V} = g \frac{N}{\frac{4}{3}\pi \Delta r^3}$$

The total energy is

$$\langle E \rangle \simeq -\frac{\hbar^2}{2m} \frac{1}{\Delta r^2} + N \frac{g}{\frac{4}{3}\pi \Delta r^3}.$$

It contains a term which increases with decreasing radius as  $r^{-2}$  and a term which decreases as  $-r^{-3}$ . The sum has a critical radius where the energy is maximum.



Below this critical radius the condensate can gain energy if it is reducing the radius. We calculate the maximum

$$\frac{d\langle E \rangle}{d\Delta r} \simeq 2 \frac{\hbar^2}{2m\Delta r^3} - 3N \frac{|g|}{\frac{4}{3}\pi \Delta r^4},$$

and solve for the atom number

$$0 = 2 \frac{\hbar^2}{2m\Delta r^3} - \frac{9}{4\pi} N \frac{|g|}{\Delta r^4}$$

$$N = \frac{4\pi \Delta r \hbar^2}{9 |g| m}.$$

The initial radius before the collapse is given by the radius of the single particle wave function in a harmonic trap

$$\Delta r = \sqrt{\frac{\hbar}{m\omega}}.$$

With this we obtain an estimate for the critical atom number

$$\begin{aligned} N_c &= \frac{4\pi}{9} \frac{\hbar^{5/2}}{\omega^{1/2} |g| m^{3/2}} \\ &= \frac{2\pi}{9} \frac{1}{|a|} \sqrt{\frac{\hbar}{\omega m}}, \end{aligned}$$

For  ${}^7\text{Li}$  with a scattering length of  $a = -28a_0$  in a trap with  $\omega = 2\pi \cdot 150\text{Hz}$  one obtains  $N_c = 1542$ . The experimental observation is  $N < 1300$ . For more shallow traps the critical number increases and one gets larger condensates.

## appendix: Hamilton Operator and Bogoliubov Approximation

- many body hamiltonian

In second quantization the many body hamiltonian is

$$H = \int \hat{\Psi}^+(\vec{r}, t) \left[ -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{trap}}(\vec{r}) + \frac{1}{2} \int \hat{\Psi}^+(\vec{r}', t) U(\vec{r}' - \vec{r}) \hat{\Psi}(\vec{r}', t) d\vec{r}' \right] \hat{\Psi}(\vec{r}, t) d\vec{r}$$

with the particle mass  $m$  and the trapping potential  $V(\vec{r})$ . The interaction is described by the two particle interaction potential  $U(\vec{r}' - \vec{r})$ . The factor  $1/2$  before the integral regards double counting of the interaction between two particles. The field operator

$$\hat{\Psi}(\vec{r}, t) := \sum \hat{\Psi}_n(\vec{r}, t) = \sum \hat{a}_n(t) \Psi_n(\vec{r}, t)$$

is the sum of the single particle operators  $\hat{\Psi}_n(\vec{r}, t)$  and obeys

$$\begin{aligned} \left[ \hat{\Psi}(\vec{r}, t), \hat{\Psi}^+(\vec{r}', t) \right] &= \delta(\vec{r} - \vec{r}') \\ \left[ \hat{\Psi}(\vec{r}, t), \hat{\Psi}(\vec{r}', t) \right] &= \left[ \hat{\Psi}^+(\vec{r}, t), \hat{\Psi}^+(\vec{r}', t) \right] = 0 \end{aligned}$$

The  $\hat{a}_n(t)$  are the annihilation operators.

- Heisenberg-equation

The equation of motion is given by

$$i\hbar \frac{\partial}{\partial t} \hat{\Psi}(\vec{r}, t) = \left[ \hat{\Psi}(\vec{r}, t), H \right]$$

We write

$$\begin{aligned} H &= \int \hat{\Psi}^+(\vec{r}', t) H_0 \hat{\Psi}(\vec{r}', t) d\vec{r}' + \int \hat{\Psi}^+(\vec{r}', t) \hat{\Psi}^+(\vec{r}'', t) U(\vec{r}'' - \vec{r}') \hat{\Psi}(\vec{r}'', t) \hat{\Psi}(\vec{r}', t) d\vec{r}' d\vec{r}'' \\ H_0 &: = -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{trap}}(\vec{r}) \end{aligned}$$

and calculate the commutator for the first term

$$\begin{aligned}
& \left[ \hat{\Psi}(\vec{r}, t), \int \hat{\Psi}^+(\vec{r}', t) H_0 \hat{\Psi}(\vec{r}', t) d\vec{r}' \right] \\
&= \int \left[ \hat{\Psi}(\vec{r}, t), \hat{\Psi}^+(\vec{r}', t) H_0 \hat{\Psi}(\vec{r}', t) \right] d\vec{r}' \\
&= \int \hat{\Psi}(\vec{r}, t) \hat{\Psi}^+(\vec{r}', t) H_0 \hat{\Psi}(\vec{r}', t) d\vec{r}' - \int \hat{\Psi}^+(\vec{r}', t) H_0 \hat{\Psi}(\vec{r}', t) \hat{\Psi}(\vec{r}, t) d\vec{r}' \\
&= \int \hat{\Psi}(\vec{r}, t) \hat{\Psi}^+(\vec{r}', t) H_0 \hat{\Psi}(\vec{r}', t) d\vec{r}' - \int \hat{\Psi}^+(\vec{r}', t) \hat{\Psi}(\vec{r}, t) H_0 \hat{\Psi}(\vec{r}', t) d\vec{r}' \\
&= \int \left[ \hat{\Psi}(\vec{r}, t), \hat{\Psi}^+(\vec{r}', t) \right] H_0 \hat{\Psi}(\vec{r}', t) d\vec{r}' = \int \delta(\vec{r} - \vec{r}') H_0 \hat{\Psi}(\vec{r}', t) d\vec{r}' \\
&= H_0 \hat{\Psi}(\vec{r}, t).
\end{aligned}$$

In the third line we used  $\left[ \hat{\Psi}(\vec{r}', t), \hat{\Psi}(\vec{r}, t) \right] = 0$  and that  $H_0$  acts on  $r'$  but not on  $r$ .

For the second term

$$\int \left[ \hat{\Psi}(\vec{r}, t), \hat{\Psi}^+(\vec{r}', t) \hat{\Psi}^+(\vec{r}'', t) \right] U(\vec{r}'' - \vec{r}') \hat{\Psi}(\vec{r}'', t) \hat{\Psi}(\vec{r}', t) d\vec{r}' d\vec{r}''$$

the commutator is

$$\begin{aligned}
& \left[ \hat{\Psi}(\vec{r}, t), \hat{\Psi}^+(\vec{r}', t) \hat{\Psi}^+(\vec{r}'', t) \right] \\
&= \hat{\Psi}(\vec{r}, t) \hat{\Psi}^+(\vec{r}', t) \hat{\Psi}^+(\vec{r}'', t) - \hat{\Psi}^+(\vec{r}', t) \hat{\Psi}^+(\vec{r}'', t) \hat{\Psi}(\vec{r}, t) \\
&= \left( \delta(\vec{r} - \vec{r}') + \hat{\Psi}^+(\vec{r}', t) \hat{\Psi}(\vec{r}, t) \right) \hat{\Psi}^+(\vec{r}'', t) - \hat{\Psi}^+(\vec{r}', t) \hat{\Psi}^+(\vec{r}'', t) \hat{\Psi}(\vec{r}, t) \\
&= \delta(\vec{r} - \vec{r}') \hat{\Psi}^+(\vec{r}'', t) + \hat{\Psi}^+(\vec{r}', t) \left( \hat{\Psi}(\vec{r}, t) \hat{\Psi}^+(\vec{r}'', t) - \hat{\Psi}^+(\vec{r}'', t) \hat{\Psi}(\vec{r}, t) \right) \\
&= \delta(\vec{r} - \vec{r}') \hat{\Psi}^+(\vec{r}'', t) + \hat{\Psi}^+(\vec{r}', t) \delta(\vec{r} - \vec{r}'')
\end{aligned}$$

and the integral becomes

$$\begin{aligned}
& \int \delta(\vec{r} - \vec{r}') \hat{\Psi}^+(\vec{r}'', t) U(\vec{r}'' - \vec{r}') \hat{\Psi}(\vec{r}'', t) \hat{\Psi}(\vec{r}', t) d\vec{r}' d\vec{r}'' \\
&+ \int \hat{\Psi}^+(\vec{r}', t) \delta(\vec{r} - \vec{r}'') U(\vec{r}'' - \vec{r}') \hat{\Psi}(\vec{r}'', t) \hat{\Psi}(\vec{r}', t) d\vec{r}' d\vec{r}'' \\
&= \int \hat{\Psi}^+(\vec{r}'', t) U(\vec{r}'' - \vec{r}) \hat{\Psi}(\vec{r}'', t) d\vec{r}'' \hat{\Psi}(\vec{r}, t) \\
&+ \int \hat{\Psi}^+(\vec{r}', t) U(\vec{r} - \vec{r}') \hat{\Psi}(\vec{r}, t) \hat{\Psi}(\vec{r}', t) d\vec{r}'
\end{aligned}$$

Since the particles are indistinguishable  $U(\vec{r} - \vec{r}') = U(\vec{r}' - \vec{r})$  and the integral is

$$2 \int \hat{\Psi}^+(\vec{r}', t) U(\vec{r} - \vec{r}') \hat{\Psi}(\vec{r}', t) d\vec{r}' \hat{\Psi}(\vec{r}, t),$$

Finally, the equation of motion reads

$$i\hbar \frac{\partial}{\partial t} \hat{\Psi}(\vec{r}, t) = \left( -\frac{\hbar^2 \nabla^2}{2m} + V(\vec{r}) + \int \hat{\Psi}^\dagger(\vec{r}', t) U(\vec{r}' - \vec{r}) \hat{\Psi}(\vec{r}', t) d\vec{r}' \right) \hat{\Psi}(\vec{r}, t).$$

- Bogoliubov approximation

For a gas with increasing particle number the commutator for the field operator gets less and less important. For instance, the expectation value  $\int \langle \hat{\Psi}^\dagger(\vec{r}, t) \hat{\Psi}(\vec{r}, t) \rangle d\vec{r} = N$  differs from  $\int \langle \hat{\Psi}(\vec{r}, t) \hat{\Psi}^\dagger(\vec{r}, t) \rangle d\vec{r}$  only by the commutator  $\int \langle \delta(\vec{r} - \vec{r}') \rangle d\vec{r} = 1$ . One thus makes the ansatz

$$\hat{\Psi}(\vec{r}, t) = \phi(\vec{r}, t) + \Delta \hat{\Psi}(\vec{r}, t).$$

with a complex function

$$\phi(\vec{r}, t) = \sqrt{n(\vec{r}, t)} e^{i\varphi(\vec{r}, t)} = \langle \hat{\Psi}(\vec{r}, t) \rangle$$

which is the expectation value of the field operator for the state of the system (which of course is unknown). The second term is an operator and describes the rest fluctuations due to the commutator. In the Bogoliubov approximation it is neglected.

The total number of particles is given by

$$\begin{aligned} \int \langle \hat{\Psi}^\dagger(\vec{r}, t) \hat{\Psi}(\vec{r}, t) \rangle d\vec{r} &= N \\ \int |\phi(\vec{r}, t)|^2 d\vec{r} &= N \end{aligned}$$

and the absolute square of  $\phi(\vec{r}, t)$  is interpreted as particle density

$$n(\vec{r}, t) = |\phi(\vec{r}, t)|^2.$$

- contact potential

The interaction potential can be written as

$$\begin{aligned} U(r - r') &= g\delta(\vec{r} - \vec{r}') \\ g &= \frac{4\pi\hbar^2}{m}a \end{aligned}$$

This is not obvious and in order to understand this expression one has to understand the concept of "pseudo potentials" which we do not discuss here. For the equation of motion we obtain now the Gross-Pitaevskii equation

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \phi(\vec{r}, t) &= \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{trap}(\vec{r}) + g \int \phi^\dagger(\vec{r}', t) \delta(\vec{r} - \vec{r}') \phi(\vec{r}', t) d\vec{r}' \right) \phi(\vec{r}, t) \\ &= \left( -\frac{\hbar^2 \nabla^2}{2m} + V_{trap}(\vec{r}) + g |\phi(\vec{r}, t)|^2 \right) \phi(\vec{r}, t) \end{aligned}$$