Ultracold Quantum Gases

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Part 1: Bose-condensed Gases Part 2: Degenerate Fermi Gases

Ultracold quantum Gases Part 1 Bose-condensed gases

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Abstract

This is the first part of our lecturing course on ultracold quantum gases. It is dedicated to the gases of ultracold bosonic atoms and to the phenomenon of Bose-Einstein condensation. After the celebrated observation of Bose-Einstein condensation in trapped ultracold alkali atom gases in 1995, which got the Nobel Prize in 2001, the field of ultracold quantum gases is strongly expanding and it attracts scientists from atomic physics and quantum optics, condensed matter physics, nuclear physics, non-linear phenomena, and mathematical physics. The purpose of the lecturing course is to give an Introduction to the theory of ultracold quantum gases and to provide students and young researchers with necessary tools to work in this and related areas.

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Lecture 1. Key quantities. Elastic and inelastic interaction between atoms

1.1 Key quantities

What is an ultracold quantum gas? Let us consider a gas of atoms and introduce length scales for this system (see Fig. 1.1). First of all, there is a thermal de Broglie wavelength of the atoms, Λ_T , which is usually expressed in terms of the gas temperature T and atom mass m:

$$\Lambda_T = \left(\frac{2\pi\hbar^2}{mT}\right)^{1/2} \propto k_T^{-1},\tag{1.1}$$

and the thermal wavevector of the atoms, k_T , is inversely proportional to Λ_T . Second, there is a characteristic radius of interaction between atoms, R_e . The meaning of this quantity is that at interatomic distances much larger than R_e the motion of atoms is free, whereas at distances of the order of or smaller than R_e the shape of the wavefunction of the atoms is strongly influenced by the interaction between them. This brings us to the other important length scale, the mean interparticle separation $n^{-1/3}$, where n is the gas density.



Figure 1.1: The gas of atoms. Black circles denote atoms, and blue circles show the size of an atom plus the radius of interatomic interaction. The red line is the mean interatomic distance, and the brown curve shows the wave of the translational motion of an atom.

The gas is called *dilute* if the mean interatomic distance is much larger than the radius of interatomic interaction R_e , and this condition is commonly identified as the *dilute limit*:

$$n^{-1/3} \gg R_e \rightarrow nR_e^3 \ll 1$$
 dilute limit. (1.2)

Moreover, if $n^{-1/3} \leq R_e$, then the motion of atoms is not free anywhere in the coordinate space, and in most cases the system is no longer a gas. It is a liquid or solid.

The gas for which the thermal de Broglie wavelength Λ_T greatly exceeds R_e is called *ultracold*, and the inequality $\Lambda_T \gg R_e$ is usually identified as the *ultracold limit*:

$$\Lambda_T \gg R_e \rightarrow k_T R_e \ll 1$$
 ultracold limit. (1.3)

In a dilute ultracold gas we usually consider only pair interactions and collisions between the atoms, and the inequality (1.3) provides the leading role of *s*-wave collisions, i.e. collisions with zero orbital angular momentum. The latter issue will be discussed later in this lecture. The first ultracold dilute gas, the gas of spin-polarized atomic hydrogen ($H\uparrow$) was created in 1979 in Amsterdam by I.F. Silvera and J.T.M. Walraven, with temperatures of the order of hundreds of millikelvins and densities ranging from 10^{16} to 10^{19} cm⁻³. When the de Broglie wavelength Λ_T is much smaller than the mean interparticle separation, the gas can be considered as classical and it obeys the Boltzmann statistics:

$$n^{-1/3} \gg \Lambda_T \rightarrow n\Lambda_T^3 \ll 1$$
 Boltzmann statistics. (1.4)

When the temperature is made so low or the density so high that the inequality (1.4) is not satisfied and $n^{-1/3} \gtrsim \Lambda_T$, then the gas obeys quantum statistics and its macroscopic properties crucially depend on whether the atoms are bosons or fermions:

$$n\Lambda^3 \gtrsim 1 \rightarrow$$
 Quantum statistics. (1.5)

In this case the gas is called *quantum* and the quantity $n\Lambda^3$ is often called *degeneracy parameter*. The temperature at which $n\Lambda_T^3 \simeq 1$ is called *temperature of quantum degeneracy*. It is given by

$$T_d \simeq \frac{2\pi\hbar^2}{m} n^{2/3}.$$
(1.6)

The first quantum gases have been created in 1995 at JILA (E.A. Cornell and C.E. Wieman, ⁸⁷Rb), at MIT (W. Ketterle, Na), and at Rice (R. Hulet, ⁷Li). At present many tens of labs all over the world work with quantum gases of various types of atoms. The temperature is commonly ranging from 100 nK to 1 μ K, and the density is in the range from 10¹² to 10¹⁴ cm⁻³. The number of atoms in such a system is usually in the interval from 10⁵ to 10⁸. These parameters are achieved by optical and evaporative cooling in magnetic and optical traps. These methods are discussed in the course of J.T.M. Walraven.

1.2 Elastic interaction between atoms. Weakly interacting regime

An obvious energy scale in a gas is its temperature T. Another energy scale in an ultracold gas is the interaction energy per particle, and we now discuss how to calculate this quantity relying on the knowledge of the potential of interaction between atoms. We mean here the so-called elastic interaction between atoms, i.e. the interaction which does not change their internal states. In the dilute limit determined by the inequality (1.2) the total interaction energy in the system is the sum of all pair interactions:

$$E_{int} = \frac{N^2}{2} \epsilon_{int}, \qquad (1.7)$$

where $N \gg 1$ is the number of particles, $N^2/2$ is the number of pairs, and ϵ_{int} is the interaction energy for a pair of atoms. Equation (1.7) also assumes the regime of weak interactions, where the wavefunction of particles at the mean interparticle separation is not influenced by the interaction between them. The related criterion will be discussed later in this *Lecture*. Let us calculate ϵ_{int} assuming that atoms interact with each other via a potential U(r) (see Fig. 1.2).



Figure 1.2: The potential of interaction between two atoms, U(r), versus interatomic separation r. The brown line indicates the location of the characteristic radius of interaction, R_e . At $r \sim R_e$ the kinetic energy term in the Schroedinger equation (1.8) is $\sim \hbar^2/mR_e^2$ and it is of the order of the interaction term $|U(R_e)|$. Assuming that for $r \sim R_e$ the potential of interaction has the Van-der-Waals shape $U(r) = -C_6/r^6$, with C_6 being the Van-der-Waals constant, we obtain $R_e \approx (mC_6/\hbar^2)^{1/4}$. In alkali atom gases R_e ranges from 20Å for Li to 100Å for Cs, and it greatly exceeds the turning point for the zero-energy relative motion, R_0 .

The Schroedinger equation for the relative motion of a pair of atoms reads:

$$\left[-\frac{\hbar^2}{2m_r}\Delta_{\mathbf{r}} + U(r)\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}),\tag{1.8}$$

where $E = \hbar^2 k^2 / 2m_r$ is the energy of the relative motion, and we consider continuum states with a very low wavevector k. The quantity $m_r = m_1 m_2 / (m_1 + m_2)$ is the reduced mass, and for the case of atoms with equal masses (m) which we consider hereinafter one has $m_r = m/2$. We also introduced the usual notation for the Laplacian, $\Delta_{\mathbf{r}} = d^2/d\mathbf{r}^2$.

The calculation of ϵ_{int} is equivalent to calculating the shift of the energy of particles with mass m/2 in a large spherical box, due to their interaction via the potential U(r) with a force center at r = 0 (see Fig. 1.3). We now consider atoms with momenta $\hbar k$ satisfying the condition of the ultracold limit (1.3) and confine

ourselves to calculating their energy levels at zero orbital angular momentum (s-wave levels) in the box. Then the particle wavefunction ψ depends only on the distance r from the force center, and the Schroedinger equation (1.8) takes the form:

$$-\frac{\hbar^2}{m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)\psi(r) + U(r)\psi(r) = E\psi(r),\tag{1.9}$$

where the energy of an eigenstate with wavevector \mathbf{k} is $E = \hbar^2 k^2/m$, and we put the boundary condition

$$\psi(R) = 0 \tag{1.10}$$

at the boundary of the box.



Figure 1.3: Atoms (red points) in a large spherical box of radius R, interactiong with the force center (brown point) at the origin via the potential U(r).

At distances from the force center, $r \gg R_e$, we can drop the potential energy term $U(r)\psi$ from Eq. (1.9) and obtain the wavefunction

$$\psi \propto \frac{\sin(kr + \phi(k))}{kr},\tag{1.11}$$

where $\phi(k)$ is the (scattering) phase shift. The boundary condition (1.10) ensures a quantization relation for the wavevectors of the eigenstates:

$$kR + \phi(k) = \pi j, \tag{1.12}$$

with j being an integer. In order to express the phase shift ϕ through the parameters of the interaction potential U(r) we consider distances in the interval where $k^{-1} \gg r \gg R_e$. Then we can drop both U(r) and E from Eq. (1.9) which thus becomes an equation for the free motion at zero energy and gives the wavefunction

$$\psi \propto \left(1 - \frac{a}{r}\right). \tag{1.13}$$

The quantity a is called the scattering length and it is determined by the behavior of U(r) at distances $r \leq R_e$. For finding a one should solve Eq. (1.9) putting E = 0 and considering distances $r \gg k^{-1}$. The scattering length is then obtained by matching this exact solution for a given U(r), with ψ (1.13) at distances $r \gg R_e$. It is clear that a depends on a particular shape of the interaction potential U(r). In the case of a fairly deep potential well, where the relative motion in the region of the well is quasiclassical (WKB), the scattering length can be expressed through R_e and the WKB phase of the relative wavefunction (see Problem 1.1).

Considering distances $r \ll k^{-1}$ in Eq. (1.11) we obtain

$$\psi \propto \left(1 + \frac{\tan \phi}{kr}\right).$$
 (1.14)

Within the normalization coefficient, this expression should coincide with ψ (1.13). Assuming that $k|a| \ll 1$, this gives for the phase shift:

$$\phi = -ka. \tag{1.15}$$

Equation (1.15) allows us to reduce the quantization relation (1.12) to

$$k_j = \frac{\pi j}{R-a} = k_j^{(0)} + \frac{\pi j}{R^2}a,$$
(1.16)

where we assumed that certainly $R \gg |a|$ and put the subscript j for the wavevector of the eigenstate with a given quantum number j. The momentum $k_j^{(0)}$ in the right hand side of Eq. (1.16) determines the energy levels $E_j^{(0)} = \frac{\hbar^2 k_j^{(0)2}}{m}$ in the absence of interaction (a = 0), and the second term leads to the interaction-induced shift δE_j of the eigenenergies E_j . We thus obtain:

$$\delta E_j = E_j - E_j^{(0)} = \frac{\hbar^2}{m} (k_j^2 - k_j^{(0)2}) = \frac{\hbar^2 k_j^2}{m} \frac{2a}{R}.$$
 (1.17)

The interaction energy $\epsilon_{int}(k_j)$ for particles in the interval from \mathbf{k}_j to $\mathbf{k}_j + d\mathbf{k}_j$ is then related to the energy shift δE_j for particles in the momentum interval from \mathbf{k}_j to $\mathbf{k}_j + d\mathbf{k}_j$ is then related to the energy shift δE_j for particles in the interval of quantum numbers from j to j + dj as:

$$\frac{V4\pi k_j^2 dk_j}{(2\pi)^3} N(k_j) \epsilon_{int}(k_j) = \delta E_j N(j) dj, \qquad (1.18)$$

where V is the volume of the box, the occupation number $N(k_j) = N(j)$, and $dk_j/dj = \pi/R$. Equation (1.18) yields

$$\epsilon_{int} = \frac{g}{V},\tag{1.19}$$

where the quantity g is called the coupling constant and is given by

$$g = \frac{4\pi\hbar^2}{m}a.$$
 (1.20)

For the total interaction energy in the system, Eq. (1.7) then gives:

$$E_{int} = \frac{N^2}{2V}g,\tag{1.21}$$

and the interaction energy per particle is

$$\frac{\partial E_{int}}{\partial N} = ng. \tag{1.22}$$

The interaction energy ng is a very important quantity for ultracold bosons. This can be naively seen from the fact that at temperatures $T \ll ng$ the properties of the gas are mostly determined by the interactions.

Actually, for identical bosons in different momentum states the interaction energy per particle is 2ng, i.e. it is twice as large as the result of Eq. (1.22). This is because we have to symmetrize the wavefunction of the relative motion of two bosons with respect to their permutation. At large separations, where the interaction is not important, we have

$$\psi = \frac{1}{\sqrt{2}} [\exp(i\mathbf{q}\mathbf{r}) + \exp(-i\mathbf{q}\mathbf{r})],$$

where q is the relative wavevector. For $qr \ll 1$ the wavefunction is larger by a factor of $\sqrt{2}$ than without symmetrization, and this will also be the case at smaller distances where the interaction is already important. The interaction energy is proportional to $|\psi^2|$ and, as a result of symmetrization, it increases by a factor of 2. Note that the symmetrization is not needed for bosons with zero momenta, which is the case in a Bose-Einstein condensate that will be discussed later in the course, since their relative wavefunction is already symmetrical without interchanging the bosons. In this case the interaction energy per particle is given by Eq. (1.22).

What is the condition of the weakly interacting regime that allows us to confine ourselves to pair interactions between particles and use Eq. (1.7), which then leads to Eqs. (1.19), (1.21) and (1.22) ?. As we already said, in this regime the wavefunction of particles at the mean interparticle separation \bar{r} is not influenced by the interaction between them. Only under this condition one may omit many-body interactions and use Eq. (1.7). Let us consider a box of size \bar{r} :

$$\frac{4\pi\bar{r}^3}{3} = \frac{1}{n} \Rightarrow \ \bar{r} = \left(\frac{3}{4\pi n}\right)^{1/3}.$$
(1.23)

On average such a box contains one particle. In the limit of $T \rightarrow 0$, the particle kinetic energy in this box is $\sim \hbar^2/m\bar{r}^2$. The wavefunction of the particle is not influenced by its interaction with other particles, characterized by the energy ng, if

$$\frac{\hbar^2}{m\bar{r}^2} \gg n|g|. \tag{1.24}$$

Then, using Eq. (1.23) we immediately obtain the inequality

$$n|a|^3 \ll 1.$$
 (1.25)

Together with the condition of the dilute limit, $nR_e^3 \ll 1$, Eq. (1.25) gives the criterion of the weakly interacting regime. Note that Eqs. (1.20) and (1.22) and, hence Eq. (1.25), assume that characteristic particle momenta $\hbar k$ satisfy the inequality

$$k|a| \ll 1. \tag{1.26}$$

1.3 Two-body scattering problem

We now establish how the scattering length a is related to the parameters of the two-body elastic scattering problem. Again, the two-body scattering problem is equivalent to the scattering of a particle with mass m/2 from a force center, due to the particle-center interaction via the potential U(r). As a result of the interaction, an incident particle moving along the axis z with wavevector \mathbf{k} is scattered on an angle θ and acquires the momentum \mathbf{k}' (see Fig. 1.4). For elastic scattering we have $|\mathbf{k}'| = |\mathbf{k}|$.



Figure 1.4: Elastic scattering of an atom (red point) from the force center (brown point). The atom is initially moving along the z-axis with momentum \mathbf{k} and is scattered on an angle θ .

The motion of the particle is governed by the Schroedinger equation (1.8) and at an infinite separation from the center the particle wavefunction is a superposition of the incident plane wave and scattered spherical wave:

$$\psi = \exp(i\mathbf{kr}) + \frac{f(\theta)}{r}\exp(ikr), \qquad (1.27)$$

where $f(\theta)$ is called the scattering amplitude, and the vector **r** is taken in the direction of **k'**. The probability $\alpha(k)$ for the scattered wave to pass through the surface of a sphere of radius r per unit time is equal to the intensity of the scattered wave $|f(\theta)|^2/r^2$ multiplied by $vr^2d\Omega$ and integrated over the solid angle Ω . Here $v = 2\hbar k/m$ is the velocity of the incident particle or, returning to the two-body scattering problem, the relative velocity of colliding atoms. We thus have:

$$\alpha(k) = \int \frac{|f(\theta)|^2 d\Omega}{r^2} r^2 v, \qquad (1.28)$$

The quantity $\alpha(k)$ is called the rate constant of elastic collisions. The number of scattering events per unit time and unit volume is given by $\bar{\alpha}N^2/2V$, where $\bar{\alpha}$ is the rate constant averaged over the momentum distribution of particles. The quantity

$$\sigma(k) = \frac{\alpha(k)}{v} = \int |f(\theta)|^2 d\Omega \qquad (1.29)$$

has a dimension of surface area and is called the elstic cross section.

For finding the scattering amplitude $f(\theta)$ one commonly expands it in Legendre polynomials:

$$f(\theta) = \sum_{l=0}^{\infty} (2l+1) f_l P_l(\cos\theta), \qquad (1.30)$$

where f_l is called the partial scattering amplitudes. It corresponds to the scattering with orbital angular momentum l. Using the same type of expansion for the plane wave in Eq. (1.27):

$$\exp(i\mathbf{kr}) = \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos\theta), \qquad (1.31)$$

where j_l are spherical Bessel functions, one then deduces from Eq. (1.8) a set of equations for a given orbital angular momentum l and finds the partial scattering amplitudes by solving these equations.

In the ultracold limit where the momentum $\hbar k$ satisfies the inequality $kR_e \ll 1$, the leading scattering channel is the one with the orbital angular momentum l = 0. It is called *s*-wave scattering and the corresponding scattering amplitude f_0 is independendent of θ . The scattering cross section then is $\sigma_0 = 4\pi f_0^2$, and for identical bosons we have to multiply it by a factor of 2 due to symmetrization of the wavefunction of colliding atoms with respect to their permutation as explained in the end of the previous subsection.

The wavefunction $\psi^{(0)}$ of the relative motion of atoms at l = 0 obeys the Schroedinger equation (1.9). At $r \to \infty$ it is given by the *s*-wave part of ψ (1.27), which is obtained straightforwardly by using Eqs. (1.30) and (1.31) in Eq. (1.27). This yields

$$\psi^{(0)} = \frac{\sin kr}{kr} + \frac{f_0}{r} \exp(ikr); \qquad r \to \infty$$
(1.32)

On the other hand, at $r \gg R_e$ one can drop U(r) in Eq. (1.9) and arrive at Eq. (1.11) for the relative wavefunction, which we now rewrite in the form:

$$\psi^{(0)} = \frac{1}{kr} (\cos\phi \sin kr + \sin\phi \cos kr). \tag{1.33}$$

Then, writing Eq. (1.32) as

$$\psi^{(0)} = \frac{1}{kr} \left[(1 + ikf_0) \sin kr + kf_0 \cos kr \right]; \quad r \to \infty$$
 (1.34)

and equalizing logarithmic derivatives of $\psi^{(0)}$ (1.33) and $\psi^{(0)}$ (1.34) we find:

$$f_0 = \frac{\tan \phi}{k(1 - i \tan \phi)} = \frac{\exp(2i\phi) - 1}{2ik}.$$
 (1.35)

As we already discussed in the previous subsection, at distances in the interval $R_e \ll r \ll k^{-1}$ one can drop both U(r) and $\hbar^2 k^2/m$ from Eq. (1.9) and reduce it to the equation for the free motion at zero energy. This leads to Eq. (1.13) for the wavefunction: $\psi \propto (1 - a/r)$. On the other hand, Eq. (1.33) at $r \ll k^{-1}$ leads to Eq. (1.14): $\psi \propto (1 + \tan \phi/kr)$. We thus immediately see that

$$\tan\phi = -ka,\tag{1.36}$$

and equation (1.35) reduces to

$$f_0 = -\frac{a}{1+ika}.$$
 (1.37)

For $k|a| \ll 1$ we have $f_0 = -a$ and clearly see that the scattering length is the amplitude of the s-wave scattering in the limit of $k \to 0$.

In most of the forthcoming discussions we will consider momenta $\hbar k$ of particles satisfying the inequality $k|a| \ll 1$. It is however instructive to briefly mention that a general expression for the cross section, following from Eqs. (1.29) and (1.37), reads:

$$\sigma_0 = \frac{4\pi a^2}{1 + k^2 a^2}.\tag{1.38}$$

For $k|a| \ll 1$ Eq. (1.38) reduces to $\sigma_0 = 4\pi a^2$ as we already discussed above. However, for $k|a| \gg 1$ we obtain $\sigma_0 = 4\pi k^2$. Note that Eq. (1.38) is obtained in the ultracold limit, i.e. it assumes that $kR_e \ll 1$. So, in order to have $k|a| \gtrsim 1$ we should have an anomalously large scattering length $|a| \gg R_e$. This case is called resonance scattering of slow particles.

What does this correspond to? Let us consider a weakly bound state with orbital angular momentum l = 0 (s-state) for two atoms in the potential U(r) (see Fig. 1.5). The term weakly bound means that the extention of the wavefunction ψ_b of this state greatly exceeds the radius of the potential, R_e . The wavefunction ψ_b obeys the Schroedinger equation (1.9) in which we should now replace a positive energy E by $-\epsilon_0$, where ϵ_0 is the binding energy of the considered *s*-state:

$$-\frac{\hbar^2}{m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)\psi_b(r) + U(r)\psi_b(r) = -\epsilon_0\psi_b(r).$$
(1.39)

For $r \gg R_e$ we drop U(r) from Eq. (1.39) and obtain

$$\psi_b(r) = \sqrt{\frac{\kappa}{2\pi}} \frac{1}{r} \exp(-\kappa r), \qquad (1.40)$$

where $\kappa^{-1} = \hbar/\sqrt{m\epsilon_0}$ is the extention of the wavefunction ψ_b . According to the definition of a weakly bound state, we should have the inequality $\kappa^{-1} \gg R_e$.



Figure 1.5: Weakly bound state of two atoms (red line), with the binding energy ϵ_0 , in the interaction potential U(r) (blue curve). The brown point shows the location of the characteristic radius of the potential, R_e , and the brown lines indicate possible deeply bound states.

At distances in the interval $R_e \ll r \ll \kappa^{-1}$ we can drop both U(r) and ϵ_0 from Eq. (1.39), which transforms it to an equation of free motion at zero energy. The resulting wavefunction is given by

$$\psi_b \propto \left(\frac{1}{r} - \kappa\right) \propto \left(1 - \frac{1}{\kappa r}\right)$$
 (1.41)

and it should coincide within a normalization coefficient with the wavefunction $\psi^{(0)}$ of the scattering problem at $k \to 0$ in the same potential U(r). As we already found above, $\psi^{(0)} \propto (1 - a/r)$ in the limit of vanishing energy. Thus,

comparing this expression with Eq. (1.41) we see that in the presence of a weakly bound *s*-state the scattering length is positive and large: $a = \kappa^{-1} \gg R_e$. The binding energy is related to the scattering length as

$$\epsilon_0 = \frac{\hbar^2 \kappa^2}{m} = \frac{\hbar^2}{ma^2}.$$
(1.42)

Let us now look at equations (1.19) and (1.20). They show that the energy of interaction between two particles in the continuum states with very low momenta is large and positive at a large and positive a. This means that such particles strongly repel each other. At the same time, we just arrived at the conclusion that they can form a weakly bound state. This is an interesting observation and it allows us to answer the frequently asked question: does a potential well supporting many bound states repel or attract an incident slow particle ? The answer is that in general it can be both. However, if there exists a weakly bound state of this particle in the well, then at particle wavevectors $k \to 0$ it is repelled by the well.

1.4 Inelastic collisions

Besides elastic collisions, atoms of an ultracold gas can undergo inelastic collisions, i.e. the collisions changing their internal states. Consider a gas of bosonic atoms which are in an excited (hyperfuine) internal state A_2 . Then binary collisions between the can lead to their relaxation transition to the ground state A_1 . One may consider, for example, the following inelastic collisional processes:

$$A_2 + A_2 \Rightarrow A_1 + A_2 + \Delta E \tag{1.43}$$

$$A_2 + A_2 \Rightarrow A_1 + A_1 + 2\Delta E, \qquad (1.44)$$

with ΔE being the difference between energies of the internal states A_2 and A_1 .

In most of the ultracold gases (alkali atoms, atomic hydrogen, chromium, metastable triplet helium) the inelastic relaxation processes (1.43) and (1.44) are induced by the magnetic dipolar interaction, and the energy release ΔE greatly exceeds the gas temperature and interparticle elastic interaction so that the outgoing atoms are ejected from the gas sample. The Hamiltonian of the magnetic dipolar interaction reads

$$\hat{H}_d = \frac{(\hat{\mu}_1 \hat{\mu}_2)r^2 - 3(\hat{\mu}_1 \mathbf{r})(\hat{\mu}_2 \mathbf{r})}{r^5},$$
(1.45)

where $\hat{\mu}_1$ and $\hat{\mu}_2$ are operators of magnetic moments of the colliding atoms, and **r** is the interatomic distance. The product $\mu_1\mu_2$ is of the order of μ_B^2 , where μ_B is the Bohr magneton, so that the magnetic dipolar interaction is rather weak and can be treated within the perturbation theory by using the Fermi Golden rule. In this sense the magnetic dipolar relaxation belongs to the class of *weak inelastic processes*. For the number of relaxation events per unit time, due to the process (1.43) we have:

$$W_{rel} = \frac{2\pi}{\hbar} \sum_{f} |\langle i|H_d|f \rangle|^2 \delta(E_f - E_i) \frac{N^2}{2}.$$
 (1.46)

Here $N^2/2$ is the number of pairs of A_2 -state atoms, and the subscripts *i* and *f* label the initial and final states of the relaxation transition. Omitting the small initial kinetic energy of colliding atoms the energy conservation law for the relaxation process (1.43) becomes

$$E_f - E_i = \frac{\hbar^2 k_f^2}{m} - \Delta E = 0, \qquad (1.47)$$

where $k_f = (m\Delta E/\hbar^2)^{1/2}$ is the wavevector of the relative motion in the final state. The transition matrix element $\langle i|H_d|f \rangle$ should be calculated with the initial and final wavefunctions of the relative motion of the atoms, which behave at large interatomic separations as $(1/\sqrt{V}) \exp(i\mathbf{k}_{i,f}\mathbf{r})$, where V is the volume of the system.

Consider for simplicity bosonic atoms with electron spin 1/2 and omit the effect of nuclear spins. For example, this is justified if ΔE is related to the change in the Zeeman energy and is much larger than the energy of hyperfine interaction. Let us discuss the process (1.43) in which A_1 is the lower Zeeman internal atomic state, let say spin- \downarrow , and A_2 is the upper Zeeman state spin- \uparrow . Then we have $\hat{\mu}_1 = 2\mu_B \hat{\mathbf{S}}_1$, $\hat{\mu}_2 = 2\mu_B \hat{\mathbf{S}}_2$, and $\Delta E = 2\mu_B B$, with B being the magnetic field and $\hat{\mathbf{S}}_1$, $\hat{\mathbf{S}}_1$ the spin operators of the atoms.

Let us then assume that the relative kinetic energy in the final state, $\hbar^2 k_f^2/m = \Delta E$, is still much smaller than the typical atomic energy \hbar^2/mR_e^2 . In this case inelastic transitions occur at interatomic distances $k_f^{-1} \gg R_e$ and the transition matrix element $\langle i|H_d|f \rangle$ can be found simply using plane waves for the initial and final wavefunctions. Putting $\mathbf{k}_i = 0$ we have

$$\langle i|H|f \rangle = \int d^3r \,\tilde{H}_d(\mathbf{r}) \exp(i\mathbf{k}_f \mathbf{r}),$$
 (1.48)

and the matrix element over the spin variables $\hat{H}_D(\mathbf{r})$ is easily obtained taking into account that the relaxation transitions change the internal state A_2 from spin- \uparrow tp spin- \downarrow and do not change the internal state A_1 (spin- \downarrow). The interaction Hamiltonian (1.45) leads to

$$\tilde{H}_d(\mathbf{r}) = -\sqrt{\frac{24\pi}{5}} \frac{\mu_B^2}{r^3} Y_{21}(\theta, \varphi), \qquad (1.49)$$

where the spherical harmonic $Y_{21}(\theta, \varphi) = \sqrt{15/8\pi} \cos \theta \sin \theta \exp i\varphi$, and θ, φ are the polar and azimuthal angles of the vector **r** with respect to the direction of the magnetic field. Using the expansion (1.31) for the plane wave $\exp(i\mathbf{k}_f \mathbf{r})$, completed by the known relation

$$P_l(\cos\theta_{\mathbf{kr}}) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_{lm}\left(\frac{\mathbf{r}}{r}\right) Y_{lm}^*\left(\frac{\mathbf{k}_f}{k_f}\right),$$

from equations (1.48) and (1.49) we obtain

$$< i|H|f> = -4\pi \sqrt{\frac{24\pi}{5}} \,\mu_B^2 Y_{21}^* \left(\frac{\mathbf{k}_f}{k_f}\right) \int_0^\infty \frac{j_2(x)}{x} \, dx = 8\pi \sqrt{\frac{54\pi}{5}} \,\mu_B^2 Y_{21} \left(\frac{\mathbf{k}_f}{k_f}\right). \tag{1.50}$$

In a thermal gas we have to symmetrize the initial wavefunction of colliding A_2 state atoms with respect to their permutation, which increases the transition probabilitry by a factor of 2. Then equation (1.46) immediately gives

$$W_{rel} = 2\alpha_{rel} \frac{N^2}{2V},\tag{1.51}$$

with the relaxation rate constant:

$$\alpha_{rel} = \frac{432\pi}{5} \frac{\mu_B^4 m k_f}{\hbar^3} \tag{1.52}$$

and the final wavevector k_f following from the energy conservation law (1.47).

Assuming that in the relaxation process both atoms are ejected from the sample, for the atom loss rate we obtain:

$$\frac{dn}{dt} = -2\alpha_{rel}n^2. \tag{1.53}$$

The atom density decreases with increasing time t as

$$n(t) = \frac{1}{1 + t/\tau_{rel}},$$
(1.54)

where the quantity $\tau_{rel} = (2\alpha_{rel}n(0))^{-1}$ is a characteristic relaxation time and it determines the life-time of the gas. In many cases the relaxation rate constant is small and the inelastic process of collisional relaxation can be neglected. For example, in an ultracold gas of ⁸⁷Rb atoms one has $\alpha_{rel} \sim 10^{-16}$ cm³/s, and the relaxation time is $\tau_{rel} \sim 100$ s at commonly used densities $n \sim 10^{14}$ cm⁻³. Note that the life-time of the order of seconds is already sufficiently large for performing detailed investigations of ultracold gases in experiments. At the same time, the relaxation rate constant strongly depends on a particular system and in some cases the relaxation process is very important, for example in a gas of chromium atoms which have a magnetic moment of $6\mu_B$.

Binary inelastic processes occuring with a fairly large probability at short interparticle distances (strong inelastic processes) require rather involved numerical calculations. An example of such a process is Penning ionization in pair collisions of metastable triplet helium atoms: one of them goes to the ground state and the other one gets ionized. However, for a qualitative analysis of this type of processes, instead of a direct solution of the problem one may put a perfectly absorbing wall at a certain (short) interparticle distance r_0 . The presence of this wall means that there is only an incoming spherical flux at $r = r_0$. In other words, once the particles approach each other at the distance r_0 they necessirily undergo the inelastic transition (see Problem 1.2).

The inelastic collisional decay of an ultracold gas is present even if all atoms are in the lowest energy state. The reason is that the interaction potential between two atoms, U(r), in most cases supports many bound (molecular) states. Therefore, there exists a process of three-body recombination. Namely, three atoms collide, two of them form a bound molecular state, and the third one



Figure 1.6: The process of three-body recombination. Brown lines indicate bound molecular states in the interaction potential U(r) (blue curve). Red balls show three colliding atoms: the two atoms connected with the black arrow collide with each other and form a bound molecular state, and the third one should be inside a sphere of radius ~ R_e around them in order to carry away the binding energy.

carries away the binding energy ϵ (see Fig. 1.6). This is one of the very few cases where one consideres three-body interactions in ultracold gases.

In order to obtain a dimensional estimate for the rate of three-body recombination we follow the ideas of the Thompson model developed for the formation of neutral atoms in electron-electron-ion collisions (J.J. Thomson, Phil,. Mag., **47**, 337 (1924)). We assume that two atoms collide and form a bound molecular state, and for carrying away the binding energy the third atom should be inside a sphere of radius ~ R_e around them. The probability that it is there is approximately equal to (nR_e^3) , where n is the atom density. Then the rate of three-body recombination, i.e. the number of recombination events per unit time, is roughly the rate of two-body collisions multiplied by (nR_e^3) :

$$W_{rec} \sim \sigma \tilde{v} (nR_e^3) \frac{N^2}{V},$$
 (1.55)

and a more detailed analysis shows that we should put \tilde{v} of the order of the velocity of particles in the outgoing channel of the recombination process. Since the binding energy of the formed molecular state is $\epsilon \sim \hbar^2/mR_e^2$, we have $\tilde{v} \sim \hbar/mR_e$. Then, writing the number of recombination events per unit time

in the form:

$$W_{rec} = \alpha_{rec} \frac{N^3}{V^2},\tag{1.56}$$

from Eq. (1.55) we obtain an estimate for the recombination rate constant α_{rec} :

$$\alpha_{rec} \sim \sigma \tilde{v} R_e^3 \sim \frac{4\pi\hbar}{m} R_e^2, \tag{1.57}$$

where we implicitly assumed that $\sigma \sim \pi R_e^2$. The binding energy ϵ is much larger than any other energy scale in the system. Therefore, the molecule formed in the recombination process and the third atom acquire a high kinetic energy and are ejected from the gas sample. Thus, in each recombination event the gas looses three atoms, and the rate of recombination determines the life-time of the gas.

The decrease of the atom density due to three-body recombination is governed by the equation:

$$\frac{dn}{dt} = -\alpha_{rec} n^3, \tag{1.58}$$

and a characteristic recombination time is $\tau_{rec} \sim (\alpha_{rec} n^2)^{-1}$. For most ultracold gases, α_{rec} ranges from 10^{-28} to 10^{-30} cm⁶/s and the recombination life-time of the gas, τ_{rec} , is of the order of seconds or tens of seconds at commonly achieved densities $n \sim 10^{14}$ cm⁻³.

In the forthcoming lectures we will omit both the three-body recombination and collisional relaxation, having in mind that they can be made rather slow by decreasing density or selecting proper internal atomic states. Therefore, we will use the Hamiltonian of the many-body bosonic system, which for identical bosons in first quantization can be written as

$$H = -\frac{\hbar^2}{2m} \sum_{\alpha} \Delta_{\mathbf{r}_{\alpha}} + \frac{1}{2} \sum_{\alpha \neq \beta} U(\mathbf{r}_{\alpha} - \mathbf{r}_{\beta}), \qquad (1.59)$$

where particles are labeled by indeces α and β . Note that Eq. (1.59) assumes the weakly interacting regime where one can also omit many-body elastic interactions between particles.

Problems 1

1.1 Consider the interaction potential U(r) which has a deep potential well and Van der Waals tail as shown in Fig. 1.2. The zero-energy relative motion of atoms in the region of the well is quasiclassical (WKB) and it remains WKB at distances $(r \ll R_e)$ where the interaction potential acquires the Van der Waals shape $U(r) = -C_6/r^6$. Express the s-wave scattering length through the characteristic radius of the potential, $R_e = (mC_6/\hbar^2)^{1/4}$, and the WKB phase $\Phi = \int_{R_0}^{\infty} \sqrt{m|U(r)|}/\hbar^2 dr$. (G.F. Gribakin and V.V. Flambaum, Phys. Rev. A, 48, 546 (1993); G.V. Shlyapnikov, J.T.M. Walraven, and E.L. Surkov, Hyperfine Interactions, 76, 31 (1993)).

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The wavefunction of the s-wave relative motion with wave vector \mathbf{k} obeys Eq. (1.9):

$$-\frac{\hbar^2}{m}\left[\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr}\right]\psi(r) + U(r)\psi(r) = \frac{\hbar^2k^2}{m}\psi(r).$$

In the ultracold limit, $kR_e \ll 1$, at distances $r \ll k^{-1}$ we may put k = 0 in this Schroedinger equation.

In the inner region, $r \ll R_e$, the relative motion is quasiclassical and we have the WKB expression for the wavefunction:

$$\psi \propto \frac{1}{r\sqrt{p(r)}} \sin\left(\frac{1}{\hbar} \int_{R_0}^r p(r')dr' + \frac{\pi}{4}\right),\tag{1.60}$$

where $p(r) = \sqrt{m|U(r)|}$ is the classical momentum of the motion. At distances where the interaction potential acquires the Van der Waals form $U(r) = -C_6/r^6$, but the motion is still quasiclassical, we have $p(r) = \hbar R_e^2/r^3$ and equation (1.60) can be written as

$$\psi \propto \sqrt{r} \sin\left(\frac{R_e^2}{2r^2} - \frac{\pi}{4} - \Phi\right),$$
(1.61)

with $\Phi = \int_{R_0}^{\infty} [p(r)/\hbar] dr$ being the WKB phase.

On the other hand, for the Van der Waals potential, Eq. (1.9) with k = 0 becomes

$$-\frac{\hbar^2}{m} \left[\frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} \right] \psi(r) - \frac{C_6}{r^6} \psi(r) = 0.$$
(1.62)

Representing the wavefunction as $\psi(r) = r^{-1/2}\phi(r)$ and turning to a new variable $y = R_e^2/2r^2$ we reduce Eq. (1.62) to the Bessel equation:

$$\frac{d^2\phi}{dr^2} + \frac{1}{r}\frac{d\phi}{dr} + \left(1 - \frac{1}{16r^2}\right)\phi = 0.$$

The solution of this equation is expressed through the Bessel functions with indeces 1/4 and -1/4:

$$\phi \propto [J_{-1/4}(y) + AJ_{1/4}(y)], \tag{1.63}$$

and the coefficient A should be obtained by matching $\psi \propto r^{-1/2}\phi$ with ψ (1.61) at distances $r \ll R_e$ $(y \gg 1)$ where the motion is quasiclassical. For $y \gg 1$ we have

$$J_{1/4}(y) = \sqrt{\frac{2}{\pi y}} \cos\left(y - \frac{3\pi}{8}\right); \quad y \gg 1.$$

$$J_{-1/4}(y) = \sqrt{\frac{2}{\pi y}} \cos\left(y - \frac{\pi}{8}\right); \quad y \gg 1.$$

Then, using $\phi(y)$ from Eq. (1.63) the wavefunction of the relative motion becomes

$$\psi \propto \sqrt{r} \left\{ (1+A) \cos \frac{\pi}{8} \cos \left(y - \frac{\pi}{4}\right) + (1-A) \sin \frac{\pi}{8} \sin \left(y - \frac{\pi}{4}\right) \right\}.$$
 (1.64)

Rewriting Eq. (1.63) in the form:

$$\psi \propto \sqrt{r} \left\{ \cos \Phi \sin \left(y - \frac{\pi}{4} \right) - \sin \Phi \cos \left(y - \frac{\pi}{4} \right) \right\},$$
 (1.65)

and equalizing logarithmic derivatives ψ'/ψ of wavefunctions (1.64) and (1.65) we obtain:

$$A = -\frac{\cos\left(\Phi - \frac{\pi}{8}\right)}{\cos\left(\Phi + \frac{\pi}{8}\right)}.$$
(1.66)

We now consider the solution (1.63) in the limit of $r \gg R_e$ ($y \ll 1$). For $y \ll 1$ we have

$$J_{1/4}(y) = \left(\frac{y}{2}\right)^{1/4} \frac{1}{\Gamma(5/4)} = \left(\frac{R_e}{2r}\right)^{1/2} \frac{1}{\Gamma(5/4)}; \quad y \ll 1.$$
$$J_{-1/4}(y) = \left(\frac{2}{y}\right)^{1/4} \frac{1}{\Gamma(3/4)} = \left(\frac{2r}{R_e}\right)^{1/2} \frac{1}{\Gamma(3/4)}; \quad y \ll 1.$$

Thus, in the interval of distances where $k^{-1} \gg r \gg R_e$, the wavefunction $\psi = r^{-1/2}\phi(r)$ acquires an asymptotic form:

$$\psi \propto \left(1 + \frac{AR_e}{2r} \frac{\Gamma(3/4)}{\Gamma(5/4)}\right). \tag{1.67}$$

At the same time, in this range of distances we may drop both U(r) and $\hbar^2 k^2/m$ in Eq. (1.9). The solution of the resulting equation of the free motion at zero energy is given by Eq. (1.13):

$$\psi \propto \left(1 - \frac{a}{r}\right)$$

This is how we introduced the scattering length a, showing later that it is related to the s-wave scattering phase shift and scattering amplitude in the limit of $k \to 0$. Comparing Eq. (1.67) with Eq. (1.13) we see that

$$a = -\frac{AR_e}{2} \frac{\Gamma(3/4)}{\Gamma(5/4)}.$$

Then, using equation (1.66) for the coefficient A, we obtain the final expression for the scattering length in terms of R_e and the WKB phase Φ :

$$a = \frac{R_e \Gamma(3/4)}{2\Gamma(5/4)} \frac{\cos\left(\Phi - \frac{\pi}{8}\right)}{\cos\left(\Phi + \frac{\pi}{8}\right)}.$$
(1.68)

The scattering length depends on Φ as shown in Fig .1.7. It is zero for $\Phi = 5\pi/8 + \pi j$, where j is a non-negative integer, and reaches $\pm \infty$ for $\Phi = 3\pi/8 + \pi j$. In the latter case there appears a new bound state in the potential U(r). For $5\pi/8 + \pi j < \Phi < 11\pi/8 + \pi j$ we have a > 0, and for $3\pi/8 + \pi j < \phi < 5\pi/8 + \pi j$



Figure 1.7: The scattering length a as a function of the WKB phase Φ .

the scattering length is negative. Thus, positive values of a are met in a wider interval of Φ (by a factor of 3) than negative values.

1.2 Consider the same interaction potential U(r) as in *Problem 1.1*, but put a perfectly absorbing wall at a distance $r = r_0$ (see Fig. 1.9). The term perfectly absorbing means that at $r \to r_0$ there is only an incoming flux and the wavefunction behaves as $\psi \propto \exp[-ip_0(r-r_0)/\hbar]$, with $p_0 = \sqrt{m|U(r_0)|}$. This assumes the validity of the WKB approximation for $r \to r_0$. Calculate the scattering amplitude and the rate constant of inelastic losses in the limit of $k \to 0$.

Lecture 2. Second quantization. Bose-Einstein condensation in an ideal gas

2.1 Second quantization. Main relations

Let us now introduce a method of second quantization for a many-body system of bosons. Consider N identical spinless bosons in a very large (but finite) volume V and assume first that they do not interact with each other. In free space quantum numbers of individual particles are their wavevectors $\mathbf{k}_1, \mathbf{k}_2, \dots \mathbf{k}_N$. We then write the many-body wavefunction of the system as

$$\Psi \propto \sum_{P} \psi_{\mathbf{k}_1}(\mathbf{r}_1) \psi_{\mathbf{k}_2}(\mathbf{r}_2) \dots \psi_{\mathbf{k}_N}(\mathbf{r}_N).$$
(2.1)



Figure 1.8: The scattering potential U(r) with a perfectly absorbing wall at $r = r_0$.

The single-particle wavefunction is $\psi_{\mathbf{k}_i}(\mathbf{r}_i) = (1/\sqrt{V}) \exp(\mathbf{k}_i \mathbf{r}_i)$, and the sum in Eq. (2.1) is taken over all possible permutations of the bosons. Note that some of the values \mathbf{k}_i can be equal to each other.

For two particles in two different momentum states, \mathbf{k}_1 and \mathbf{k}_2 , we have

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}V} \left[\exp(i\mathbf{k}_1\mathbf{r}_1 + i\mathbf{k}_2\mathbf{r}_2) + \exp(i\mathbf{k}_2\mathbf{r}_1 + i\mathbf{k}_1\mathbf{r}_2) \right].$$
(2.2)

In the case of N particles we can write:

$$\Psi = \left(\frac{N_1!N_2!\dots}{N!}\right)^{1/2} \sum_{P'} \psi_{\mathbf{k}_1}(\mathbf{r}_1)\psi_{\mathbf{k}_2}(\mathbf{r}_2)\dots$$
 (2.3)

Here N_i is the number of bosons in the state with the wavevector \mathbf{k}_i , and the sum is taken only over the permutations of different wavevectors \mathbf{k}_i . One certainly has

$$\sum_{i} N_i = N. \tag{2.4}$$

In the presence of interaction between particles, Ψ (2.3) is not a stationary eigenstate, since the momenta of individual particles are not conserved. Nevertheless, we can still use the wavefunctions (2.3) as a set of basic functions.

We now consider an operator of the form

$$\hat{\mathcal{H}}^{(1)} = \sum_{\alpha} \hat{h}^{(1)}_{\alpha}, \qquad (2.5)$$

with the operator $\hat{h}_{\alpha}^{(1)}$ acting only on a single particle α . This can be, for example, an external potential acting on individual particles. Let us find matrix

elements of the operator $\hat{\mathcal{H}}^{(1)}$ between the states described by the wavefunctions (2.3). Since each of $\hat{h}^{(1)}_{\alpha}$ acts only on a single particle, non-zero matrix elements can only exist between the states with the same N_1, N_2, \ldots or between the states in which one of these numbers increases by 1 and another one decreases by 1.

For example, return to the case of two particles and consider the transition between the state

$$\frac{1}{\sqrt{2}} \left[\psi_1(\mathbf{r}_1) \psi_2(\mathbf{r}_2) + \psi_2(\mathbf{r}_1) \psi_1(\mathbf{r}_2) \right] \ (N_1 = 1; N_2 = 1)$$

and the state

$$\psi_1(\mathbf{r}_1)\psi_1(\mathbf{r}_2) \ (N_1=2; N_2=0).$$

Then, with the normalization condition $\int d^3 \mathbf{r} |\psi_{1,2}(\mathbf{r})|^2 = 1$, we have:

$$\langle N_2 = 1, N_1 = 1 | \hat{\mathcal{H}}^{(1)} | N_2 = 0, N_1 = 2 \rangle = \sqrt{2} h_{12}^{(1)},$$
 (2.6)

where

$$h_{12}^{(1)} = \int \psi_1^*(\mathbf{r}) \hat{h}^{(1)}(\mathbf{r}) \psi_2(\mathbf{r}) d^3 r.$$
(2.7)

In a general case of N particles, using Eq. (2.3) we find:

$$\langle N_i, N_k - 1 | \hat{\mathcal{H}}^{(1)} | N_i - 1, N_k \rangle = h_{ik}^{(1)} \sqrt{N_i N_k}.$$
 (2.8)

For the diagonal matrix element we have:

$$\bar{\mathcal{H}}^{(1)} \equiv \langle N_1, N_2, \dots N_i, \dots | \hat{\mathcal{H}}^{(1)} | N_1, N_2, \dots N_i, \dots \rangle = \sum_i h_{ii}^{(1)} N_i.$$
(2.9)

Let us now consider operators $\hat{a}_i \equiv \hat{a}_{\mathbf{k}_i}$ which act not on the particle coordinates but on the occupation numbers, decreasing the occupation number of the state with a given \mathbf{k}_i by 1:

$$\hat{a}_i | N_1, N_2, ..., N_i ... \rangle = \sqrt{N_i} | N_1, N_2, ..., N_i - 1, ... \rangle.$$
 (2.10)

The operators \hat{a}_i are called annihilation operators of particles, since an operator \hat{a}_i annihilates a particle in the state *i* (the state with the wavevector \mathbf{k}_i). On the basis of Eq. (2.10) we have for the corresponding matrix element:

$$\langle N_i - 1 | \hat{a}_i | N_i \rangle = \sqrt{N_i}.$$
(2.11)

In a similar way, we introduce operators \hat{a}_i^{\dagger} called creation operators of particles:

$$\hat{a}_{i}^{\dagger}|N_{1}, N_{2}, ...N_{i}...\rangle = \sqrt{N_{i}+1}|N_{1}, N_{2}, ...N_{i}+1, ...\rangle.$$
 (2.12)

The operator \hat{a}_i^{\dagger} creates a particle in the state *i*, and the corresponding matrix element is

$$\langle N_i + 1 | \hat{a}_i^{\dagger} | N_i \rangle = \sqrt{N_i + 1}.$$
(2.13)

The product $\hat{a}_i^{\dagger} \hat{a}_i$ does not change the occupation numbers N_i . It has only diagonal matrix elements and can be written as

$$\hat{a}_i^{\dagger} \hat{a}_i = N_i. \tag{2.14}$$

Similarly, we can write

$$\hat{a}_i \hat{a}_i^{\dagger} = N_i + 1,$$
 (2.15)

and there is a commutation relation

$$\hat{a}_i \hat{a}_i^{\dagger} - \hat{a}_i^{\dagger} \hat{a}_i = 1.$$
(2.16)

Other commutation relations read:

$$\hat{a}_i \hat{a}_k - \hat{a}_k \hat{a}_i = 0 \tag{2.17}$$

$$\hat{a}_i \hat{a}_k^{\dagger} - \hat{a}_k^{\dagger} \hat{a}_i = 0; \quad i \neq k$$
 (2.18)

So, in a compact form we can write:

$$\hat{a}_i \hat{a}_k^{\dagger} - \hat{a}_k^{\dagger} \hat{a}_i = \delta_{ik}.$$
 (2.19)

One can easily check that all matrix elements of the operator

$$\hat{\mathcal{H}}^{(1)} = \sum_{i,k} h_{ik}^{(1)} \hat{a}_i^{\dagger} \hat{a}_k.$$
(2.20)

coincide with matrix elements of the operator $\hat{\mathcal{H}}^{(1)}$ (2.5). Thus, one can always write (2.5) in the form of (2.20) which is called the secondly quantized form.

This result is straightforwardly generalized to the case of the operator

$$\hat{\mathcal{H}}^{(2)} = \frac{1}{2} \sum_{\alpha,\beta} \hat{h}^{(2)}_{\alpha,\beta}, \qquad (2.21)$$

with $\hat{h}_{\alpha,\beta}^{(2)}$ acting on the coordinates of two particles, α and β . This type of operator describes pair interactions between particles. The secondly quantized form of this operator is

$$\hat{\mathcal{H}}^{(2)} = \frac{1}{2} \sum_{i,k,l,m} h_{ik}^{(2)lm} \hat{a}_k^{\dagger} \hat{a}_i^{\dagger} \hat{a}_l \hat{a}_m, \qquad (2.22)$$

with

$$h_{ik}^{(2)lm} = \int \psi_i^*(\mathbf{r}_1) \psi_k^*(\mathbf{r}_2) h^{(2)}(\mathbf{r}_1, \mathbf{r}_2) \psi_l(\mathbf{r}_1) \psi_m(\mathbf{r}_2) d^3 r_1 d^3 r_2.$$
(2.23)

2.2 Secondly quantized Hamiltonian in terms of momentumspace operators

We now return to the Hamiltonian (1.59) which describes particles in free space and write it in the secondly quantized form. The operator of the kinetic energy of particles is

$$\hat{K} = -\frac{\hbar^2}{2m} \sum_{\alpha} \Delta_{\mathbf{r}_{\alpha}}, \qquad (2.24)$$

and each Laplacian term of the sum can be treated as the operator $\hat{h}_{\alpha}^{(1)}(\mathbf{r}_{\alpha})$. It has only diagonal matrix elements and we have :

$$\sum_{\mathbf{k}} K_{\mathbf{k}\mathbf{k}} = \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} N_k.$$
(2.25)

Then, according to Eq. (2.20) one can write the kinetic energy operator \hat{K} as

$$\hat{K} = \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} \hat{a}^{\dagger}_{\mathbf{k}} \hat{a}_{\mathbf{k}}.$$
(2.26)

In order to write the secondly quantized form for the operator of the energy of interaction between particles,

$$\hat{P} = \frac{1}{2} \sum_{\alpha \neq \beta} U(\mathbf{r}_{\alpha} - \mathbf{r}_{\beta}), \qquad (2.27)$$

we use Eqs. (2.22) and (2.23) and the fact that in free space the basic set of wavefunctions is $\psi_{\mathbf{k}_i}(\mathbf{r}) = (1/\sqrt{V}) \exp(i\mathbf{k}_i \mathbf{r})$. This yields:

$$\hat{P} = \frac{1}{2} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} U_{12}^{34} \hat{a}^{\dagger}_{\mathbf{k}_1} \hat{a}^{\dagger}_{\mathbf{k}_2} \hat{a}_{\mathbf{k}_3} \hat{a}_{\mathbf{k}_4}, \qquad (2.28)$$

where

$$U_{12}^{34} = \frac{1}{V^2} \int d^3 r_1 d^3 r_2 U(\mathbf{r}_1 - \mathbf{r}_2) \exp[i(-\mathbf{k}_1 \mathbf{r}_1 - \mathbf{k}_2 \mathbf{r}_2 + \mathbf{k}_3 \mathbf{r}_1 + \mathbf{k}_4 \mathbf{r}_2)]. \quad (2.29)$$

Turning to the variables $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ we reduce Eq. (2.29) to the form

$$U_{12}^{34} = \frac{1}{V^2} \int d^3 r \, d^3 R \, U(\mathbf{r}) \exp[i(\mathbf{k}_3 + \mathbf{k}_4 - \mathbf{k}_1 - \mathbf{k}_2)\mathbf{R}) + i(\mathbf{k}_3 + \mathbf{k}_2 - \mathbf{k}_1 - \mathbf{k}_4)\mathbf{r}/2)]. \quad (2.30)$$

We then immediately see that there is a momentum conservation law:

$$\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4, \tag{2.31}$$

and obtain

$$U_{12}^{34} = \frac{1}{V} \int d^3 r \, U(\mathbf{r}) \exp[i(\mathbf{k}_3 - \mathbf{k}_1)\mathbf{r}].$$
(2.32)

For the interaction potential U(r) satisfying the condition $|U(r)| \ll \hbar^2/mr^2$ at distances where the potential acts, we may use the Born approximation for calculating the scattering amplitude f. In the limit of particle momenta tending to zero we have:

$$f = -a = -\frac{m}{4\pi\hbar^2} \int U(r) \, d^3r.$$
 (2.33)

Then, using equations (2.28), (2.32), and (2.33), in this (ultracold) limit we write the secondly quantized operator of the interaction energy as

$$\hat{P} = \frac{g}{2V} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3} \hat{a}^{\dagger}_{\mathbf{k}_1} \hat{a}^{\dagger}_{\mathbf{k}_2} \hat{a}_{\mathbf{k}_3} \hat{a}_{\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3}, \qquad (2.34)$$

where $g = 4\pi \hbar^2 a/m$ is the coupling constant introduced in *Lecture 1*.

Actually, one can also write Eq. (2.34) for the interaction potential U(r) which does not satisfy the condition of the Born approximation. This is because the interaction between two particles can lead to transitions:

$$\begin{split} & \mathbf{k}_3, \mathbf{k}_4 \Rightarrow \mathbf{k}_1, \mathbf{k}_2; \\ & \mathbf{k}_3, \mathbf{k}_4 \Rightarrow \mathbf{k}_1', \mathbf{k}_2' \Rightarrow \mathbf{k}_1, \mathbf{k}_2; \\ & \mathbf{k}_3, \mathbf{k}_4 \Rightarrow \mathbf{k}_1'', \mathbf{k}_2'' \Rightarrow \mathbf{k}_1', \mathbf{k}_2' \Rightarrow \mathbf{k}_1, \mathbf{k}_2; \end{split}$$

etc. This is equivalent to the summation of all vacuum "diagrams" and eventually leads to Eq. (2.34) if the scattering amplitude is momentum independent.

We can also act differently since we saw that the interaction energy for two particles is $\epsilon_{int} = g/V$. We replace the potential U(r) by a potential $U_{eff}(r)$ which satisfies the condition of the Born approximation and, at the same time, leads to the same scattering length a. Thus, assuming that the scattering amplitude is momentum independent and using Eqs. (2.26) and (2.34), we have the following secondly quantized form of the Hamiltonian (1.59):

$$\hat{H} = \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}} + \frac{g}{2V} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3} \hat{a}_{\mathbf{k}_1}^{\dagger} \hat{a}_{\mathbf{k}_2}^{\dagger} \hat{a}_{\mathbf{k}_3} \hat{a}_{\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3}.$$
 (2.35)

2.3 Secondly quantized Hamiltonian in terms of coordinatespace operators

Another form of second quantization is based on the use of field operators in the coordinate space, $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^{\dagger}(\mathbf{r})$. They are related to the annihilation and creation operators, $\hat{a}_{\mathbf{k}}$ and $\hat{a}_{\mathbf{k}}^{\dagger}$ by

$$\hat{\psi}(\mathbf{r}) = \sum_{\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r}) \hat{a}_{\mathbf{k}}, \qquad (2.36)$$

$$\hat{\psi}^{\dagger}(\mathbf{r}) = \sum_{\mathbf{k}} \psi_{\mathbf{k}}^{*}(\mathbf{r}) \hat{a}_{\mathbf{k}}^{\dagger}, \qquad (2.37)$$

with $\psi_{\mathbf{k}}(\mathbf{r}) = (1/\sqrt{V}) \exp(i\mathbf{kr})$ being a basic set of single-particle eigenfunctions. The operator $\hat{\psi}(\mathbf{r})$ annihilates a particle at the point \mathbf{r} , and the operator $\psi^{\dagger}(\mathbf{r})$ creates a particle at this point. Using commutation relations (2.17) and (2.19), from Eqs. (2.36) and (2.37) we obtain the following commutation relations:

$$\hat{\psi}(\mathbf{r})\hat{\psi}^{\dagger}(\mathbf{r}') - \hat{\psi}^{\dagger}(\mathbf{r}')\hat{\psi}(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}'), \qquad (2.38)$$

$$\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}') - \hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}) = 0.$$
(2.39)

Using equations (2.36) and (2.37) and the completeness theorem

$$\sum_{i} \psi_i^*(\mathbf{r}) \psi_i(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}'),$$

we straightforwardly express the operator $\hat{\mathcal{H}}^{(1)}$ (2.20) in terms of the field operators $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^{\dagger}(\mathbf{r})$:

$$\hat{\mathcal{H}}^{(1)} = \sum_{i,k} h_{i,k}^{(1)} \hat{a}_i^{\dagger} \hat{a}_k = \int d^3 r \, \hat{\psi}^{\dagger}(\mathbf{r}) \hat{h}^{(1)}(\mathbf{r}) \hat{\psi}(\mathbf{r}).$$
(2.40)

Accordingly, the operator of the kinetic energy of particles given by Eq. (2.24) can be written as

$$\hat{K} = \int d^3r \left[-\frac{\hbar^2}{2m} \hat{\psi}^{\dagger}(\mathbf{r}) \Delta_{\mathbf{r}} \hat{\psi}(\mathbf{r}) \right].$$
(2.41)

In a similar way we can write the secondly quantized form in terms of $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^{\dagger}(\mathbf{r})$ for the operator $\hat{\mathcal{H}}^{(2)}$ (2.21):

$$\hat{\mathcal{H}}^{(2)} = \frac{1}{2} \int d^3 r \, \hat{\psi}^{\dagger}(\mathbf{r}_1) \hat{\psi}^{\dagger}(\mathbf{r}_2) \hat{h}^{(2)}(\mathbf{r}_1, \mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) \hat{\psi}(\mathbf{r}_2)$$
(2.42)

and represent the operator of the energy of interaction between particles, \hat{P} (2.34) as

$$\hat{P} = \frac{g}{2} \int d^3 r \, \hat{\psi}^{\dagger}(\mathbf{r}) \hat{\psi}^{\dagger}(\mathbf{r}) \hat{\psi}(\mathbf{r}).$$
(2.43)

In case there is an external potential $V(\mathbf{r})$ acting on single particles, we may use equation (2.40) with $\hat{h}^{(1)}(\mathbf{r}) = V(\mathbf{r})$ and write the secondly quantized form for the energy of interaction of particles with this external field as

$$\hat{V} = \int d^3 r \, \hat{\psi}^{\dagger}(\mathbf{r}) V(\mathbf{r}) \hat{\psi}(\mathbf{r}).$$
(2.44)

We thus arrive at the following secondly quantized form of the Hamiltonian $\hat{H} = \hat{K} + \hat{V} + \hat{P}$ in terms of the field operators $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^{\dagger}(\mathbf{r})$:

$$\hat{H} = \int d^3r \left[-\frac{\hbar^2}{2m} \hat{\psi}^{\dagger}(\mathbf{r}) \Delta_{\mathbf{r}} \hat{\psi}(\mathbf{r}) + \hat{\psi}^{\dagger}(\mathbf{r}) V(\mathbf{r}) \hat{\psi}(\mathbf{r}) + \frac{g}{2} \hat{\psi}^{\dagger}(\mathbf{r}) \hat{\psi}^{\dagger}(\mathbf{r}) \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r}) \right].$$
(2.45)

We will use the secondly quantized Hamiltonian in the form (2.45) or in the form (2.35) throughout the entire lecturing course.

2.4 Bose-Einstein condensation in an ideal gas. The role of the density of states

We first discuss an ideal Bose gas and introduce the phenomenon of Bose-Einstein condensation. Consider a three-dimensional (3D) Bose gas in free space at equilibrium at a finite temperature T. Then the Hamiltonian (2.35) contains only the kinetic energy term and reads:

$$\hat{H} = \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}}.$$

The equilibrium occupation numbers of the single-particle states with a given wavevector ${\bf k}$ are

$$N_k = \langle \hat{a}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}} \rangle = \frac{1}{\exp\left(\frac{E_k - \mu}{T}\right) - 1},$$
(2.46)

where the symbol $\langle \rangle$ means statistical average, $E_k = \hbar^2 k^2 / 2m$ is the kinetic energy of a particle with wavevector **k**, and $\mu \leq 0$ is the chemical potential.

Let us establish a relation between μ and the total number of particles, N, at a given T. We have:

$$N = \sum_{\mathbf{k}} N_k = \int \frac{V d^3 k}{(2\pi)^3} \frac{1}{\exp\left(\frac{E_k - \mu}{T}\right) - 1}.$$
 (2.47)

The chemical potential decreases with T and becomes zero at a critical temperature

$$T_c = \frac{3.31\hbar^2}{m} n^{2/3},\tag{2.48}$$

with n = N/V being the gas density (see Fig. 2.1). The critical temperature is obtained straightforwardly from Eq. (2.47) at $\mu = 0$:

$$n = \frac{N}{V} = \int_0^\infty \frac{4\pi k^2 dk}{(2\pi)^3} \frac{1}{\exp\left(\frac{E_k}{T_c}\right) - 1},$$

and equation (2.47) does not have a solution for $T < T_c$. Note that at $T = T_c$ the gas is already quantum degenerate, and the corresponding degeneracy parameter is

$$n\Lambda_{T_c}^3 = 2.62.$$
 (2.49)

The way to resolve the situation at $T < T_c$ has been revealed by Bose and Einstein in 1924. The idea is that at $T < T_c$ a macroscopic number of particles goes to a single quantum state. In free space this is the state with momentum $\hbar k = 0$. Accordingly, for the total number of particles we have:

$$N = N(k = 0) + N(k > 0),$$



Figure 2.1: The temperature dependence of the chemical potential for the uniform 3D ideal Bose gas (brown cureve). The brown point shows the critical temperature of Bose-Einstein condensation, T_c .

where particles with finite momenta obey the Bose distribution relation (2.46) at $\mu = 0$. The total number of such particles is

$$N(k>0) = \int_0^\infty \frac{V \, 4\pi k^2 dk}{(2\pi)^3} \frac{1}{\exp\left(\frac{E_k}{T}\right) - 1} = N\left(\frac{T}{T_c}\right)^{3/2}.$$
 (2.50)

The (macroscopic) number of particles in the state with k = 0 is then given by

$$N_0 \equiv N(k=0) = N \left[1 - \left(\frac{T}{T_c}\right)^{3/2} \right].$$
 (2.51)

These particles are usually called Bose-condensed, and the part of the gas formed by them is called *Bose-Einstein condensate*. In some sense, the phenomenon of Bose-Einstein condensation can be treated as "condensation in the momentum space". Note that in an ideal Bose gas at T = 0 all particles are in the condensate, which is clearly seen from Eq. (2.51).

Let us now consider a two-dimensional (2D) Bose gas in free space and show that in this case the phenomenon of Bose-Einstein condensation is absent. The relation between N and μ now reads:

$$N = \int_0^\infty \frac{A \, 2\pi k dk}{(2\pi)^2} \frac{1}{\exp\left(\frac{E_k - \mu}{T}\right) - 1},\tag{2.52}$$

where A is the surface area. Then, a straightforward calculation yields:

$$\mu = -T \ln \left[\frac{1}{1 - \exp(-n\Lambda_T^2)} \right], \qquad (2.53)$$

with n = N/A being the 2D density. Equation (2.53) is valid at any T and n. For $n\Lambda_T^2 \ll 1$ we recover the classical result

$$\mu = -T \ln \left[\frac{1}{n\Lambda_T^2} \right],$$

whereas in the deeply quantum degenerate regime $(n\Lambda_T^2 \gg 1)$ we have

$$\mu = -T \exp(-n\Lambda_T^2)$$

We thus see that the chemical potential continuously decreases with temperature and always remains finite (see Fig. 2.2), and there is no Bose-Einstein condensation.

In order to understand the difference between the 3D and 2D cases we introduce the (energy) density of states:

$$\nu(E) = \int \delta(E - E(k)) \frac{V d^d k}{(2\pi)^d},$$
(2.54)

where d is the dimension of the system, and $E(k) = \hbar^2 k^2/2m$. The quantity $\nu(E)$ represents the number of states per unit energy interval, and equation (2.47) can be represented in the form:

$$N = \int_0^\infty \frac{\nu(E)dE}{\exp\left(\frac{E-\mu}{T}\right) - 1}.$$
(2.55)

In the 3D case we have:

$$\nu(E) = \left(\frac{mV}{2\pi^2\hbar^2}\right) \left(\frac{2mE}{\hbar^2}\right)^{1/2} \propto \sqrt{E},$$
(2.56)

whereas in 2d the density of states is energy independent:

$$\nu(E) = \frac{mA}{2\pi\hbar^2}.\tag{2.57}$$

The key reason for the emergence of Bose-Einstein condensation is that for $\nu(E)$ decreasing with E, below a certain critical temperature one can not distribute a given number of particles according to the Bose distribution function. This is what is happening in the 3D ideal Bose gas in free space.



Figure 2.2: The temperature dependence of the chemical potential for the 2D ideal uniform Bose gas (blue curve).

Problems 2

2.1. Consider a 2D ideal Bose gas in a harmonic potential $V(r) = m\omega^2 r^2/2$. Use a quasiclassical approach and show that there is a phenomenon of Bose-Einstein condensation (BEC). Calculate the BEC transition temperature.

The (quasi)classical approach assumes that the particle energy can be written as

$$E = \frac{\hbar^2 k^2}{2m} + \frac{m\omega^2 r^2}{2}.$$
 (2.58)

Then for the energy density of states instead of Eq. (2.54) we have:

$$\nu(E) = \int \delta(E - E(k, r)) \frac{d^2k}{(2\pi)^2} d^2r,$$
(2.59)

where E(k, r) is given by Eq. (2.58). Turning to new variables

$$y = \frac{\hbar^2 k^2}{2m} - \frac{m\omega^2 r^2}{2}$$

and

$$\tilde{E} = E(k, r),$$

we have the limits of integration from $-\tilde{E}$ to \tilde{E} for y and from 0 to ∞ for \tilde{E} . Taking into account that

$$\frac{d^2rd^2k}{(2\pi)^2} = \frac{d\tilde{E}dy}{2\hbar^2\omega^2},$$

from Eq. (2.59) we obtain

$$\nu(E) = \frac{1}{2\hbar^2\omega^2} \int_0^\infty d\tilde{E}\,\delta(E-\tilde{E}) \int_{-\tilde{E}}^{\tilde{E}} dy = \frac{E}{\hbar^2\omega^2} \propto E.$$
(2.60)

Then, Eq. (2.55) takes the form:

$$N = \int_0^\infty \frac{E}{\hbar^2 \omega^2} \frac{dE}{\exp\left(\frac{E-\mu}{T}\right) - 1},$$
(2.61)

and we find that the chemical potential decreases with temperature and reaches zero at a certain critical temperature. The latter follows from Eq. (2.61) with $\mu = 0$:

$$N = \left(\frac{T_c}{\hbar\omega}\right)^2 \sum_{j=0}^{\infty} \frac{1}{(j+1)^2} \approx 1.23 \left(\frac{T_c}{\hbar\omega}\right)^2$$

and is given by

$$T_c \approx 0.9\sqrt{N}\hbar\omega.$$
 (2.62)

For $T < T_c$ equation (2.61) does not have a solution. So, we have the phenomenon of BEC, i.e at temperatures below T_c (2.62) a macroscopic number of particles goes to the ground state of the potential V(r). In order to calculate the number of non-condensed particles we put $\mu = 0$ in Eq. (2.61). This yields

$$N(E > 0) \equiv N' = N\left(\frac{T}{T_c}\right)^2, \qquad (2.63)$$

and for the number of particles in the condensate we have:

$$N_0 = N \left[1 - \left(\frac{T}{T_c}\right)^2 \right]. \tag{2.64}$$

2.2 Consider a 1D ideal Bose gas in an external potential $V(x) = \alpha |x|^q$ and use the quasiclassical approach. Find for which q, not necessirily integer, one has the phenomenon of BEC. Calculate the BEC transition temperature T_c and the condensed fraction of particles at T below T_c .

Lecture 3. Bose-Einstein condensation in a weakly interacting gas. Gross-Pitaevskii equation

3.1 Gross-Pitaevskii equation for the condensate wavefunction

We now discuss Bose-Einstein condensation (BEC) of interacting ultracold bosons. We will assume that the gas is in the weakly interacting regime and characteristic particle momenta satisfy the condition (1.26) so that the criterion of weak interactions is given by Eq. (1.25). Since in an ideal 3D Bose gas at T = 0all particles are in the condensate, for the weakly interacting Bose gas almost all particles will be Bose-condensed at T = 0. In free space these are particles with k = 0. In this *Lecture* we restrict ourselves to the case of T = 0, and the situation at finite temperatures will be discussed later. Let us introduce the field operator for Bose-condensed particles, $\hat{\psi}_0(\mathbf{r})$. As the condensate contains a macroscopic number of particles $(N_0 \to 0)$, the matrix element of $\hat{\psi}_0^{\dagger}$ corresponding to the creation of a condensed particle can be put equal to $\psi_0^*(\mathbf{r})$, where $|\psi_0(\mathbf{r})|^2 = n_0(\mathbf{r})$ with $n_0(\mathbf{r})$ being the condensate density. For example, in free space where we have $\hat{\psi}_0 = \hat{a}_0^{\dagger} / \sqrt{V}$. The matrix element of \hat{a}_0^{\dagger} is equal to $\sqrt{N_0+1}$ and we omit unity compared to N_0 . Since the matrix element of $\hat{\psi}_0$ corresponding to the annihilation of a condensed particle is $\psi_0(\mathbf{r})$, this is equivalent to regarding $\hat{\psi}_0(\mathbf{r})$ as a *c*-number. In other words, we assume that there is an average value of $\hat{\psi}_0(\mathbf{r})$, equal to $\psi_0(\mathbf{r})$:

$$\langle \hat{\psi}_0(\mathbf{r}) \rangle = \psi_0(\mathbf{r}).$$
 (3.1)

Let us now turn to the Heisenberg representation, where an operator $\hat{A}(\mathbf{r})$ of the Schroedinger representation is transformed to:

$$\hat{A}(\mathbf{r},t) = \exp(i\hat{H}t/\hbar)\hat{A}(\mathbf{r})\exp(-i\hat{H}t/\hbar), \qquad (3.2)$$

so that there is the Heisenberg equation of motion:

$$i\hbar \frac{\partial A(\mathbf{r},t)}{\partial t} = [\hat{A}\hat{H}] \equiv (\hat{A}\hat{H} - \hat{H}\hat{A}).$$
(3.3)

The operator \hat{A} in the Schroedinger picture does not explicitly depend on time t. The time dependence of average values of physical quantities arises only through the time dependence of the wavefunctions. The Heisenberg representation transfers the time dependence from the wavefunctions to the operators. Note that the Heisenberg and Schroedinger representations are identical for the operator of any conserved quantity, i.e. for an operator that commutes with the Hamiltonian. In partricular, this is the case for the Hamiltonian itself and for the particle number operator.

Consider now $\hat{A}(\mathbf{r},t) = \hat{\Psi}(\mathbf{r},t)$, where we use the notation $\hat{\Psi}$ for the field operator in the Heisenberg representation, while still keeping the notation $\hat{\psi}$ for

the Schroedinger-picture field operator. Then we rewrite Eq. (3.3) in the form of a non-linear equation for the field operator:

$$i\hbar\frac{\partial\hat{\Psi}}{\partial t} = \left(-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + V(\mathbf{r}) + g\hat{\Psi}^{\dagger}\hat{\Psi}\right)\hat{\Psi}.$$
(3.4)

Let us now represent the field operator $\hat{\Psi}$ as a sum of the condensate part, *c*-number $\Psi_0(\mathbf{r}, t)$, and a non-condensed part $\hat{\Psi}'(\mathbf{r}, t)$:

$$\hat{\Psi}(\mathbf{r},t) = \Psi_0(\mathbf{r},t) + \hat{\Psi}'(\mathbf{r},t).$$
(3.5)

To zero order we omit the (small) non-condensed part Ψ' and get an equation for the condensate wavefunction:

$$i\hbar\frac{\partial\Psi_0}{\partial t} = \left(-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + V(\mathbf{r}) + g|\Psi_0|^2\right)\Psi_0.$$
(3.6)

This is the Gross-Pitaevskii equation for the condensate wavefunction obtained by Gross and by Pitaevskii in 1961.

The stationary solution of Eq. (3.6) has the form:

$$\Psi_0(\mathbf{r},t) = \psi_0(\mathbf{r}) \exp(-i\mu t/\hbar), \qquad (3.7)$$

where

$$\mu = \frac{\partial E}{\partial N} \tag{3.8}$$

is the chemical potential, and the Schroedinger-picture condensate wavefunction $\psi_0(\mathbf{r})$ is governed by the time-independent Gross-Pitaevskii equation:

$$\left(-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + V(\mathbf{r}) + g|\psi_0|^2 - \mu\right)\psi_0 = 0.$$
(3.9)

The time dependence of the Heisenberg-picture condensate wavefunction $\Psi_0(\mathbf{r},t)$ given by Eq. (3.7) is easy to obtain. Let us recall that the relation $\langle \hat{\Psi}_0 \rangle = \Psi_0$, which is Eq. (3.1) rewritten in the Heisenberg representation (assuming that $\langle \hat{\Psi}' \rangle = 0$), is introduced only in the sense that the condensate with N_0 particles is equivalent to the condensate with $(N_0 - 1)$ particles, aside from corrections of the order of $1/N_0$ ($N_0 \gg 1$). Actually, acting with the operator $\hat{\Psi}_0$ on the state with N_0 particles we get the state with $(N_0 - 1)$ particles:

$$\tilde{\Psi}_0 |N_0\rangle = \Psi_0 |N_0 - 1\rangle.$$
 (3.10)

However, the time dependence of the wavefunctions of the stationary states with N_0 and $(N_0 - 1)$ particles is given by

$$\Psi(N_0) \propto \exp(-iE(N_0)t/\hbar) \tag{3.11}$$

$$\Psi(N_0 - 1) \propto \exp(-iE(N_0 - 1)t/\hbar).$$
(3.12)

This means that transferring the time dependence from the wavefunctions to the operators and writing $\langle \hat{\Psi}_0 \rangle = \Psi_0$, we have to write the time dependence of
Ψ_0 as $\Psi_0 \propto \exp(-\mu t/\hbar)$, with $\mu = E(N_0) - E(N_0 - 1) = \partial E/\partial N_0$ assuming $N_0 \to \infty$. We thus arrive at Eq. (3.7).

For a uniform condensate $(V(\mathbf{r}) = 0)$ the ground state solution is

$$\Psi_0 = \sqrt{n_0} \exp(-i\mu t/\hbar), \qquad (3.13)$$

where the chemical potential is given by the relation

$$\mu = n_0 g. \tag{3.14}$$

This is because the kinetic energy (Laplacian) term in Eq. (3.9) can be omitted, since $\psi_0 = \text{const.}$ Note that for the ground state BEC the Laplacian term is important only in the presence of an external potential $V(\mathbf{r})$. For $V(\mathbf{r}) = 0$, omitting the Laplacian term and putting $|\psi_0|^2 = n_0$ in the Gross-Pitaevskii equation (3.9) we get Eq. (3.14). Then, substituting $\psi_0 = \sqrt{n_0}$ into Eq. (3.7) we obtain Eq. (3.13).

3.2 Density-phase representation. Collapsing condensates

Formally, equations (3.13) and (3.14) are valid for both repulsive (g > 0) and attractive (g < 0) interaction between particles. However, in reality these results are correct only for g > 0. The reason is that for g < 0 the solution (3.13) is unstable and in 3D (also in 2D) one has the phenomenon of collapse. Let us put g < 0 and consider Eq. (3.6) in free space. Writing the condensate wavefunction in the form $\Psi_0(\mathbf{r}, t) \exp(-i\mu t/\hbar)$, where $\mu = n_0 g$ is the chemical potential of the stationary state at an unperturbed constant density n_0 , we have:

$$i\hbar\frac{\partial\Psi_0}{\partial t} = -\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}\Psi_0 + g|\Psi_0|^2\Psi_0 - \mu\Psi_0.$$
(3.15)

In the presence of perturbations, we turn to the density-phase representation and write

$$\Psi_0 = \sqrt{n} \exp(i\phi), \tag{3.16}$$

where the density n and phase ϕ are real. We now assume that $n = n_0 + \delta n$, where δn is a small perturbation in the density, and the derivatives of ϕ are also small. Keeping only the terms that are linear in δn and derivatives of ϕ we have

$$\begin{split} i\hbar\dot{\Psi}_0 &= \left(-\hbar\dot{\phi} + i\frac{\hbar\delta\dot{n}}{2n_0}\right)\Psi_0,\\ \Delta_{\mathbf{r}}\Psi_0 &= \left(\frac{\Delta_{\mathbf{r}}\delta n}{2n_0} + i\Delta_{\mathbf{r}}\phi\right)\Psi_0,\\ g|\Psi_0|^2\Psi_0 - \mu\Psi_0 &= g\delta n\Psi_0. \end{split}$$

Substituting these expressions into Eq. (3.15) and equalizing real parts and imaginary parts we obtain:

$$\hbar\delta\dot{n} = -\frac{\hbar^2 n_0}{m} \Delta_{\mathbf{r}}\phi \tag{3.17}$$

$$-\hbar\dot{\phi} = -\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}\left(\frac{\delta n}{2n_0}\right) + g\delta n.$$
(3.18)

Equations (3.17) and (3.18) represent the continuity and Euler equations of the hydrodynamic approach.

We then consider a perturbation of the density (and phase) that has a long length and time scale so that the Fourier component is

$$\delta n(k) \propto \cos(\mathbf{kr} - \omega t) \tag{3.19}$$

with very small k and ω . Accordingly, the term $(\hbar^2/2m)\Delta_{\mathbf{r}}(\delta n/2n_0)$ in the right hand side of the Euler equation (3.18) will be much smaller than $g\delta n$ and can be omitted. This transforms Eq. (3.18) to

$$-\hbar\dot{\phi} = g\delta n. \tag{3.20}$$

Taking the time derivative in this equation and substituting $\delta \dot{n}$ from Eq. (3.17) we obtain an equation for δn :

$$\delta \ddot{n} = \frac{n_0 g}{m} \Delta_{\mathbf{r}} \delta n. \tag{3.21}$$

This gives a relation between ω and k:

$$\omega^2 = \frac{n_0 g}{m} k^2. \tag{3.22}$$

For negative g, assuming real k we obtain negative ω^2 and, hence, imaginary frequencies:

$$\omega = \pm ik \left(\frac{n_0|g|}{m}\right)^{1/2}.$$
(3.23)

According to Eq. (3.19) this means that δn will grow exponentially:

$$\delta n \propto \exp\left(\sqrt{\frac{n_0|g|}{m}}kt\right).$$
 (3.24)

This is nothing else than collapse. In a given part of space where an extremely small perturbation of the density appears, its amplitude starts to grow exponentially (see Fig.3.1) and the condensate eventually collapses to a droplet.

3.3 Stable condensates. Healing length

We thus see that a stable BEC in free space exists only for repulsive interaction between particles (g > 0). Let us introduce a characteristic length scale for a weakly interacting BEC with g > 0. Consider a condensate in a potential V(x) that depends only on the coordinate x (not on y and z) and represents an infinite wall at x = 0 so that the condensate exists only in the half-space x > 0(see Fig.3.2). Being a continuous function of x, the condensate wavefunction ψ_0 vanishes at x = 0.

We now solve Eq. (3.9) and find the wavefunction ψ_0 of the ground state BEC. First of all, ψ_0 does not depend on y and z. We thus rewrite Eq. (3.9) as

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_0}{dx^2} + g|\psi_0|^2\psi_0 - \mu\psi_0 = 0$$
(3.25)



Figure 3.1: Spatial density profile of a collapsing condensate. A change of color from blue to red corresponds to growing peak density with increasing time.



Figure 3.2: External potential depending only on the coordinate x and representing an infinite wall at x = 0. The condensate exists at x > 0.

and put the boundary condition

$$\psi_0(0) = 0. \tag{3.26}$$

Setting ψ_0 to be real we multiply Eq. (3.25) by $d\psi_0/dx$ and integrate over dx. This yields

$$-\frac{\hbar^2}{4m} \left(\frac{d\psi_0(x)}{dx}\right)^2 + \frac{g}{4}\psi_0^4(x) - \frac{\mu}{2}\psi_0^2(x) = C,$$
(3.27)

where C is the integration constant. Since $d\psi_0/dx = 0$ at $x \to \infty$, we have

$$C = \frac{g}{4}n_0^2 - \frac{\mu}{2}n_0,$$

with n_0 being the condensate density at $x \to \infty$. On the other hand, for $x \to \infty$ we also have $d^2\psi_0/dx^2 = 0$ and, hence, Eq. (3.25) gives $\psi_0(\infty) = \sqrt{n_0} = \text{const}$ and $\mu = n_0 g$. This reduces the expression for the integration constant C to

$$C = -\frac{1}{4}n_0^2 g = -\frac{1}{4}\mu n_0.$$
(3.28)

From Eq. (3.27) we then obtain:

$$\frac{d\psi_0(x)}{dx} = \pm \sqrt{\frac{m}{\hbar^2}} \left(\frac{\mu}{\sqrt{g}} - \sqrt{g}\psi_0^2(x)\right) = \pm \sqrt{\frac{mg}{\hbar^2}} n_0 \left(1 - \frac{\psi_0^2(x)}{n_0}\right).$$
(3.29)

The solution of Eq. (3.29) is

$$\psi_0(x) = \pm \sqrt{n_0} \tanh\left(\frac{x}{\xi}\right),$$
(3.30)

where the quantity

$$\xi = \frac{\hbar}{\sqrt{mn_0g}} \tag{3.31}$$

is called the healing length. It is a characteristic distance from the wall at which the condensate wavefunction acquires its asymptotic value (see Fig.3.3).

3.4 Bose-Einstein condensation in an external harmonic potential

Let us now consider Bose-Einstein condensation of particles in a spherical harmonic potential given by

$$V(r) = \frac{m\omega^2 r^2}{2}.$$
 (3.32)

For finding the ground state condensate wavefunction we should solve Eq. $\left(3.9\right)$ which now takes the form:

$$-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}\psi_0 + \frac{m\omega^2 r^2}{2}\psi_0 + g|\psi_0|^2\psi_0 - \mu\psi_0 = 0.$$
(3.33)

For an ideal gas BEC (g = 0) the ground state solution is simply the ground state wavefunction of a harmonic oscillator:

$$\psi_0 = \frac{\sqrt{N_0}}{\pi^{3/4} l_h^{3/2}} \exp\left(-\frac{r^2}{2l_h^2}\right),\tag{3.34}$$

where

$$l_h = \left(\frac{\hbar}{m\omega}\right)^{1/2} \tag{3.35}$$



Figure 3.3: Ground state wavefunction ψ_0 versus x for the condensate in the potential V(x) representing an infinite wall at x = 0 in the y,z plane.

is the harmonic oscillator length. The solution (3.34) has orbital angular momentum l = 0, and the chemical potential is $\mu = 3\hbar\omega/2$. The energy per particle in the first excited state is higher by $\hbar\omega$. So, if there is a small interaction between particles and at the maximum density we have

$$n_{max}|g| \ll \hbar\omega, \tag{3.36}$$

then the condensate wavefunction is still given by Eq. (3.34) irrespective of the sign of g.

Consider now g > 0 and assume that in the central part of the sample, where the density is the largest, we have

$$n_{max}g \gg \hbar\omega. \tag{3.37}$$

This is the so-called Thomas-Fermi limit. It is then reasonable to assume that the kinetic energy term can be omitted in the central part of the gas. Equation (3.33) then becomes an algebraic equation:

$$g|\psi_0|^2 = \mu - \frac{m\omega^2 r^2}{2}.$$
(3.38)

Thus, the condensate wavefunction has the shape of an inverted parabola (see Fig.3.4):

$$\psi_0 = \sqrt{\frac{\mu}{g} \left(1 - \frac{r^2}{R_{TF}^2}\right)} \,\theta(R_{TF} - r), \qquad (3.39)$$

where the Thomas-Fermi radius of the condensate is given by

$$R_{TF} = \left(\frac{2\mu}{m\omega^2}\right)^{1/2}.$$
(3.40)

Equation (3.40) contains the theta function, which is equal to unity at positive values of the argument and to zero at a negative argument. This means that $\psi_0 = 0$ for any distance r from the origin larger than R_{TF} so that in the Thomas-Fermi approximation R_{TF} is really the radius of the BEC.



Figure 3.4: Thomas-Fermi ground state solution for the condensate wavefunction $\psi_0(r)$ in the spherical harmonic potential $V(r) = m\omega^2 r^2/2$

The normalization condition for ψ_0 is

$$\int_{0}^{R_{TF}} |\psi_0(r)|^2 d^3 r = N_0 \tag{3.41}$$

and it gives a relation between the chemical potential μ and the number of particles N_0 . Using ψ_0 (3.39) in Eq. (3.41) we obtain:

$$N_0 = \frac{8\pi}{15} \frac{\mu R_{TF}^3}{g},$$

and with R_{TF} from Eq. (3.40) this leads to

$$\mu = \left(N_0 g \frac{15}{16\sqrt{2\pi}}\right)^{2/5} (m\omega^2)^{3/5}.$$
(3.42)

So, due to the spatial inhomogeneity we have $\mu \propto N_0^{2/5}$, in contrast to $\mu \propto N_0$ for a uniform condensate.

The maximum density is at r = 0:

$$n_{max} = \psi_0^2(0) = \frac{\mu}{g} \tag{3.43}$$

so that $\mu = n_{max}g$. The healing length at maximum density is $\xi = \hbar/\sqrt{mn_{max}g}$ and owing to the Thomas-Fermi condition (3.37) it is much smaller than the harmonic oscillator length:

$$\frac{\xi}{l_h} = \left(\frac{\hbar\omega}{n_{max}g}\right)^{1/2} \ll 1.$$
(3.44)

The inequalities (3.37) and (3.44) indicate that the discrete structute of the energy levels of the harmonic potential (3.32) is smeared out by the interparticle interaction.

Let us now estimate the omitted kinetic energy term of Eq. (3.33). Using the obtained Thomas-Fermi solution (3.39) we have

$$\tilde{K} = -\frac{\hbar^2}{2m}\psi_0 \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)\psi_0 = n_{max}\frac{\hbar^2\omega^2}{\mu}\frac{(3 - 2r^2/R_{TF}^2)}{(1 - r^2/R_{TF}^2)}.$$
(3.45)

On the other hand, the term of the interparticle interaction is

$$\tilde{P} = \mu \psi_0^2 = \mu \left(1 - \frac{r^2}{R_{TF}^2} \right), \qquad (3.46)$$

and we obtain the ratio

$$\frac{\tilde{K}}{\tilde{P}} = \left(\frac{\hbar\omega}{2n_{max}g}\right)^2 \frac{(3 - 2r^2/R_{TF}^2)}{(1 - r^2/R_{TF}^2)^2}.$$
(3.47)

We see that under the condition of the Thomas-Fermi regime given by Eq. (3.37) the kinetic energy term is much smaller than the interaction term at any $r < R_{TF}$, except near the border of the trapped condensate. The Thomas-Fermi solution (3.39) is violated at distances from the border which are of the order of $\sim R_{TF}(\hbar\omega/4n_{max}g) \ll R_{TF}$. This is not a problem as in the major part of the sample this solution is valid. Therefore, it is widely used in the analysis of trapped Bose-Einstein condensates.

Problems 3

3.1 Consider a condensate with g < 0 in a spherical harmonic potential $V(r) = m\omega^2 r^2/2$. Estimate a critical value of |g| above which the condensate undergoes a collapse.

Let us write the energy functional:

$$E = \int d^3r \left\{ -\frac{\hbar^2}{2m} \psi_0^* \Delta_{\mathbf{r}} \psi_0 + \frac{m\omega^2}{2} |\psi_0|^2 + \frac{1}{2} g |\psi_0|^4 \right\}.$$
 (3.48)

Suppose that ψ_0 has a Gaussian shape with a size L which will be a variational parameter:

$$\psi_0 = \frac{\sqrt{N_0}}{\pi^{3/4} L^{3/2}} \exp\left(-\frac{r^2}{2L^2}\right). \tag{3.49}$$

The calculation of the integrals in Eq. (3.48) is straightforward:

$$\int d^3r - \frac{\hbar^2}{2m} \psi_0 \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) \psi_0 = \frac{3}{4}\frac{\hbar^2}{mL^2}N_0$$
$$\int d^3r \frac{m\omega^2 r^2}{2} \psi_0^2 = \frac{3}{4}m\omega^2 L^2 N_0$$
$$\int d^3r \frac{1}{2}g\psi_0^4 = -\frac{|g|N_0^2}{2(2\pi)^{3/2}L^3}.$$

We thus have:

$$E = \frac{3}{4} \frac{\hbar^2}{mL^2} N_0 + \frac{3}{4} m\omega^2 L^2 N_0 - \frac{|g|}{2(2\pi)^{3/2} L^3} N_0^2, \qquad (3.50)$$

where the first term in the right hand side of Eq. (3.50) originates from the kinetic energy of the condensate, the second term from the interaction of particles with the external harmonic potential, and the third term from the attractive interparticle interaction.

We now turn to a dimensionless energy $\varepsilon = E/N_0 \hbar \omega$ and dimensionless size $\kappa = L/l_h$, where $l_h = (\hbar/m\omega)^{1/2}$ is the harmonic oscillator length introduced in section 3.4. In terms of ε and κ equation (3.50) reads:

$$\varepsilon = \frac{3}{4\kappa^2} + \frac{3\kappa^2}{4} - \frac{\eta}{\sqrt{2\pi}\kappa^3}.$$
(3.51)

Here we also took into account that $|g| = 4\pi\hbar^2 |a|/m$ and introduced the parameter

$$\eta = \frac{N_0|a|}{l_h}.\tag{3.52}$$

The dependence $\varepsilon(\kappa)$ will be now analyzed at different values of η .

For $\eta \ll 1$ the interaction between particles described by the last term in Eq. (3.51) is not important at $\kappa \gtrsim 1$. It becomes crucial only for $\kappa \ll 1$, where the energy becomes more and more negative with decreasing size (see Fig.3.5). This indicates the presence of *collapse*. It is energetically favorable for the gas to get smaller and smaller size. However, the situation is more peculiar. At small κ the energy is increasing with the size and reaches maximum at $\kappa_{max} \sim \eta$. Then, for larger κ it decreases with increasing κ , reaches minimum at $\kappa = \kappa_{min}$

(at small η the dimensionless size κ_{min} is close to 1), and grows at larger κ (see Fig.3.5). This growth is provided by the interaction of particles with the external harmonic potential, described by the second term in Eq. (3.51). Let the system be initially prepared in the local minimum, i.e. with $\kappa = \kappa_{min}$ and, hence, with the size $L = \kappa_{min} l_h$. Then, in order to get to the region with $\kappa < \kappa_{max}$ and collapse, the system should undergo a macroscope quantum tunneling through the potential barrier. The height of the barrier is large ($\sim 1/\eta$) and its width is ~ 1 so that the tunneling probability is vanishingly small. We thus conclude that the trapped Bose-Einstein condensate with g < 0 is stable at $\eta \ll 1$.



Figure 3.5: Dimensionless energy ε versus dimensionless size κ for a trapped condensate with g < 0 and $\eta \ll 1$.

For $\eta \gg 1$ the kinetic energy term, i.e. the term proportional to κ^2 in Eq. (3.51), is not important and we have a monotonic dependence $\varepsilon(\kappa)$ depicted in Fig.3.6. The energy is decreasing with the size at any κ , and the system is absolutely unstable (collapsing).

For η approaching 1 from below we still have a non-monotonic curve $\varepsilon(\kappa)$ like in Fig3.5. The local minimum and the local maximum will be much more shallow, but the system can still be considered as stable similarly to the case of $\eta \ll 1$. Under a continuous increase in η the minimum and maximum become more shallow and eventually disappear. The non-monotonic curve $\varepsilon(\kappa)$ then changes to a monotonic one like in Fig.3.6, and the system becomes unstable.

Let us now find a critical value of η at which the minimum and maximum disappear, that is the value of η at the border of stability. The positions of the



Figure 3.6: The dependence $\varepsilon(\kappa)$ for $\eta \gg 1$.

minimum and maximum are determined by the condition:

$$\frac{d\varepsilon}{d\kappa} = -\frac{3}{2\kappa^3} + \frac{3\kappa}{2} + \frac{3\eta}{\sqrt{2\pi\kappa^4}} = 0.$$
(3.53)

For the minimum one has the second derivative $d^2\varepsilon/d\kappa^2 > 0$ and for the maximum $d^2\varepsilon/d\kappa^2 < 0$. Getting more shallow the local minimum and maximum approach each other with increasing η . They merge and become a saddle point (see Fig.3.7) when η is such that at their location one has

$$\frac{d^2\varepsilon}{d\kappa^2} = \frac{9}{2\kappa^4} + \frac{3}{2} - \frac{12\eta}{\sqrt{2\pi\kappa^5}} = 0.$$
(3.54)

Multiplying Eq. (3.54) by κ and substracting it from Eq. (3.53) we obtain a relation between κ and η at the critical point:

$$\kappa_c = \frac{5}{2} \frac{\eta_c}{\sqrt{2\pi}}.\tag{3.55}$$

From Eq. (3.53) we then get the critical value of η :

$$\eta_c = \frac{2}{5} \left(\frac{4\pi^2}{5}\right)^{1/4} \approx 0.68.$$
(3.56)



Figure 3.7: The dependence $\varepsilon(\kappa)$ at the border of stability, $\eta = \eta_c$.

Using Eq. (3.52) we then obtain the critical value of the interaction strength (scattering length):

$$|a_c| \approx 0.68 \frac{l_H}{N_0}.$$
 (3.57)

In other words, for a negative a such that $|a| < |a_c|$ the trapped condensate is stable.

We can also raise the problem differently and obtain a critical number of particles at a fixed negative scattering length. This yields

$$N_c \approx 0.68 \frac{l_h}{|a|}.\tag{3.58}$$

For $N_0 < N_c$ the BEC is stable, whereas for $N_0 > N_c$ it collapses. This has been observed in lithium experiments at Rice.

3.2 Consider a two-dimensional Bose-Einstein condensate in a circularly symmetrical potential $V(r) = m\omega^2 r^2/2$. For repulsive interaction between particles (g > 0) find the ground state solution for ψ_0 and the spatial density profile in the Thomas-Fermi regime. For g < 0 estimate a critical number of particles above which the condensate collapses.

Lecture 4. Dynamics of trapped Bose-Einstein condensates. Scaling approach

4.1 Exact scaling approach for a two-dimensional evolution of a trapped condensate

In this *Lecture* we will discuss dynamical properties of trapped Bose-Einstein condensates. Namely, we will analyze how the condensate responds to external perturbations, irrespective of whether they are large or small. Let us assume that initially the condensate is in a stationary state described by the stationary Gross-Pitaevskii equation (3.9) so that the Heisenberg-picture time-dependent condensate wavefunction is expressed through the Schroedinger-picture stationary wavefunction $\psi_0(\mathbf{r})$ by Eq. (3.7). Suppose that the external potential $V(\mathbf{r})$ is a harmonic potential in the x, y plane, $V(r) = m\omega^2 r^2/2$ where $r^2 = x^2 + y^2$. This corresponds to a purely two-dimensional problem, or to the three-dimensional problem in the geometry of an ideal cylinder where the motion in the z-direction is free (see Fig.4.1).



Figure 4.1: The geometry of an ideal cylinder for a trapped condensate.

In both cases the condensate wavefunction depends only on the coordinates x and y, not on z. Then, at a time t = 0 one starts to vary the frequency ω which becomes now a function of time, $\omega(t)$. The condensate starts to evolve although its wavefunction $\Psi_0(\mathbf{r}, t)$ remains independent of the coordinate z. The evolution is then described by the time-dependent Gross-Pitaevskii equation (3.6)

$$i\hbar \frac{\partial \Psi_0(\mathbf{r},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + \frac{m\omega(t)r^2}{2} + g|\Psi_0(\mathbf{r},t)|^2\right)\Psi_0(\mathbf{r},t),\qquad(4.1)$$

where $\mathbf{r} = \{x, y\}$, and $\Delta_{\mathbf{r}}$ is the two-dimensional Laplacian:

$$\Delta_{\mathbf{r}} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}.$$
(4.2)

Frequency variations change the time and distance scales, and we now turn to rescaled coordinates $\rho = \mathbf{r}/b(t)$ and rescaled time $\tau(t)$. The condensate wavefunction will be represented in the form:

$$\Psi_0(\mathbf{r},t) = \frac{\chi_0(\boldsymbol{\rho},\tau)}{b(t)} \exp\{i\Phi(\mathbf{r},t)\},\tag{4.3}$$

with the dynamical phase given by

$$\Phi(\mathbf{r},t) = \frac{mr^2}{2\hbar} \frac{\dot{b}(t)}{b(t)}.$$
(4.4)

The scaling parameter b(t) and the rescaled time $\tau(t)$ are certain functions of t and they will be determined later, as well as the function $\chi_0(\rho, \tau)$.

We now substitute Ψ_0 (4.3) into equation (4.1) and obtain:

$$\begin{split} &i\hbar\left\{-\frac{\dot{b}(t)}{b^{2}(t)}-\frac{\dot{b}(t)}{b^{3}(t)}(\mathbf{r}\nabla\boldsymbol{\rho})+\frac{1}{b(t)}\frac{d\tau}{dt}\frac{\partial}{\partial\tau}+i\frac{mr^{2}}{2\hbar}\left(\frac{\ddot{b}(t)}{b^{2}(t)}-\frac{\dot{b}^{2}(t)}{b^{3}(t)}\right)\right\}\chi_{0}(\boldsymbol{\rho},\tau)=\\ &-\frac{\hbar^{2}}{2m}\left\{\frac{1}{b^{3}(t)}\Delta\boldsymbol{\rho}+i\frac{2m}{\hbar}\frac{\dot{b}(t)}{b^{2}(t)}-\frac{mr^{2}}{\hbar^{2}}\frac{\dot{b}^{2}(t)}{b^{3}(t)}+i\frac{2m}{\hbar}\frac{\dot{b}(t)}{b^{3}(t)}(\mathbf{r}\nabla\boldsymbol{\rho})\right\}\chi_{0}(\boldsymbol{\rho},\tau)+\\ &\frac{m\omega^{2}(t)r^{2}}{2b(t)}\chi_{0}(\boldsymbol{\rho},\tau)+\frac{g}{b^{3}(t)}|\chi_{0}(\boldsymbol{\rho},\tau)|^{2}\chi_{0}(\boldsymbol{\rho},\tau). \end{split}$$

The first and second terms and the second part of the fourth term in the left hand side of this equation and the second, third, and fourth terms in the curly brackets in the right hand side cancel each other. We thus transform Eq. (4.1) to

$$\frac{i\hbar}{b(t)}\frac{d\tau}{dt}\frac{\partial\chi_0(\boldsymbol{\rho},\tau)}{\partial\tau} = \left\{-\frac{\hbar^2}{2m}\frac{1}{b^3(t)}\Delta\boldsymbol{\rho} + \frac{m}{2}[\ddot{b}(t) + \omega^2(t)b(t)]\boldsymbol{\rho}^2 + \frac{g|\chi_0(\boldsymbol{\rho},t)|^2}{b^3(t)}\right\}\chi_0(\boldsymbol{\rho},\tau). \tag{4.5}$$

The rescaled time $\tau(t)$ and the scaling parameter b(t) will be selected such that

$$\frac{d\tau}{dt} = \frac{1}{b^2(t)} \Rightarrow \quad \tau = \int^t \frac{dt'}{b^2(t')},\tag{4.6}$$

and b(t) satisfies the scaling equation

$$\ddot{b}(t) + \omega^2(t)b(t) = \frac{\omega_0^2}{b^3(t)},$$
(4.7)

with initial conditions

$$b(0) = 1; \ b(0) = 0$$
 (4.8)

and $\omega_0 = \omega(0)$ being the initial frequency. Equation (4.5) then becomes

$$i\hbar \frac{\partial \chi_0(\boldsymbol{\rho},\tau)}{\partial \tau} = \left(-\frac{\hbar^2}{2m}\Delta \boldsymbol{\rho} + \frac{m\omega_0^2 \rho^2}{2} + g|\chi_0(\boldsymbol{\rho},\tau)|^2\right)\chi_0(\boldsymbol{\rho},\tau).$$
(4.9)

We assume that the dependence of χ_0 on τ is given by

$$\chi_0(\boldsymbol{\rho},\tau) = \bar{\chi}_0(\boldsymbol{\rho}) \exp(-i\mu\tau/\hbar), \qquad (4.10)$$

where μ is the initial chemical potential. This transforms Eq. (4.9) into an equation for the stationary wavefunction $\bar{\chi}_0(\rho)$:

$$\left(-\frac{\hbar^2}{2m}\Delta\boldsymbol{\rho} + \frac{m\omega_0^2\rho^2}{2} + g|\bar{\chi}_0(\boldsymbol{\rho})|^2 - \mu\right)\bar{\chi}_0(\boldsymbol{\rho}) = 0.$$
(4.11)

This is the same equation as the one for the initial stationary condensate wavefunction $\psi_0(\mathbf{r})$, but in the rescaled coordinate variables $\boldsymbol{\rho} = \mathbf{r}/b(t)$. The normalization condition reads:

$$\int |\bar{\chi}_0(\boldsymbol{\rho})|^2 d^2 \rho = N_0.$$
(4.12)

Thus, we can say that

$$\bar{\chi}_0(\boldsymbol{\rho}) = \Psi_0(\mathbf{r} = \boldsymbol{\rho}; 0) = \psi_0(\boldsymbol{\rho})$$
(4.13)

and write Eq. (4.3) as

$$\Psi_0(\mathbf{r},t) = \frac{1}{b(t)}\psi_0\left(\frac{\mathbf{r}}{b(t)}\right) \exp\left\{i\frac{mr^2}{2\hbar}\frac{\dot{b}(t)}{b(t)} - i\frac{\mu\tau(t)}{\hbar}\right\}.$$
(4.14)

The evolving condensate acquires a dynamical phase, and the density profile is rescaled. Once we know the initial solution $\Psi_0(\mathbf{r}, 0)$, we obtain the solution at any time t. Note that the shape of $|\Psi_0|$ does not change whatever it is initially.

The discussed scaling approach has been introduced for a single particle in a time-dependent harmonic potential (A.M. Perelomov and V.S. Popov, Sov. Phys. JETP **30**, 910 (1970)) and then proposed for interacting Bose-Einstein condensates in the 2D and ideal cylinder geometries (Yu. Kagan, E.L. Surkov, and G.V. Shlyapnikov, Phys. Rev. A **54**, R1753 (1996); L.P. Pitaevskii and A. Rosch, Phys. Rev. A **55**, R853 (1997)).

We now return to the scaling equation (4.7) and consider the case where ω is put equal to zero at t = 0, i.e. the trapping potential V(r) is abruptly switched off. Then, for t > 0 the scaling equation takes the form:

$$\ddot{b} = \frac{\omega_0^2}{b^3}.\tag{4.15}$$

Multiplying both sides of equation (4.15) by \dot{b} and integrating we have;

$$\frac{\dot{b}^2}{2} = -\frac{\omega_0^2}{2b^2} + C, \tag{4.16}$$

where from the initial conditions (4.8) we obtain the integration constant $C = \omega_0^2/2$. The integration is then straightforward;

$$\frac{db}{dt} = \omega_0 \sqrt{1 - \frac{1}{b^2}}$$

$$b(t) = \sqrt{1 + \omega_0^2 t^2}.$$
(4.17)

and, hence,

Accordingly, Eq. (4.6) gives

$$\tau(t) = \frac{1}{\omega_0} \arctan \omega_0 t. \tag{4.18}$$

The condensate expands and the initial interaction energy is transferred to the kinetic energy of the expansion. The interaction between particles is important in the initial stages of the expansion. At $t \gg \omega_0^{-1}$ the density is already so small that the condensate enters the regime of free expansion. In this regime we have $b(t) = \omega_0 t$.

Suppose that the initial condensate is in the Thomas-Fermi regime in x, y directions, and $\psi_0(r) = \sqrt{n_m(1 - r^2/R_{TF}^2)}$, where n_m is the initial maximum density and $R_{TF} = \sqrt{2\mu/m\omega_0^2}$ the initial Thomas-Fermi radius. Then, according to Eq. (4.14) we have

$$|\Psi_0(\mathbf{r},t)|^2 = \frac{n_m}{b^2(t)} \left(1 - \frac{r^2}{b^2(t)R_{TF}^2}\right).$$
(4.19)

Equation (4.19) shows that the Thomas-Fermi size of the condensate increases as $R_{TF}(t) = R_{TF}b(t)$. At free expansion, where one has $b(t) = \omega_0 t$, the velocity of expansion is given by

$$v = \frac{d}{dt}R_{TF}(t) = R_{TF}\omega_0 = \sqrt{2\mu/m} = \sqrt{2}c_s$$

Within a numerical coefficient, the velocity of expansion coincides with the velocity of sound in the initial condensate, $c_s = \sqrt{\mu/m}$ (this quantity will be introduced in the next *Lecture*).

4.2 Scaling approach for evolving 3D trapped condensates

We now discuss the evolution of a 3D condensate under variations of the frequency of the confining spherically symmetrical harmonic potential. So, the initial condensate wavefunction obeys Eq. (3.9), and its evolution under variations of the frequency ω follows from Eq. (3.6). Instead of equation (4.3) we now write

$$\Psi_0(\mathbf{r},t) = \frac{1}{b^{3/2}(t)} \chi_0(\boldsymbol{\rho},\tau(t)) \exp\{i\Phi(\mathbf{r},t)\},$$
(4.20)

with the same expressions for ρ and $\Phi(\mathbf{r},t)$, so that the normalization condition $\int |\Psi_0(\mathbf{r},t)|^2 d^3r = N_0$ is transformed to $\int |\chi(\rho,\tau(t))|^2 d^3\rho = N_0$. Instead of Eq. (4.5) we then get:

$$\frac{i\hbar}{b(t)}\frac{d\tau}{dt}\frac{\partial\chi_0}{\partial\tau} = \left\{-\frac{\hbar^2}{2mb^3(t)}\Delta\boldsymbol{\rho} + \frac{m}{2}[\ddot{b}+\omega(t)b]\boldsymbol{\rho}^2 + \frac{g|\chi_0|^2}{b^4(t)}\right\}\chi_0.$$
(4.21)

Representing the function $\chi_0(\boldsymbol{\rho}, \tau(t))$ as

$$\chi_0(\boldsymbol{\rho}, \tau(t)) = \bar{\chi}_0(\boldsymbol{\rho}, \tau(t)) \exp(-i\mu\tau(t)), \qquad (4.22)$$

we transform Eq. (4.21) to

$$\frac{i\hbar}{b(t)}\frac{d\tau}{dt}\frac{\partial\bar{\chi}_0}{\partial\tau} = \left\{ -\frac{\hbar^2}{2mb^3(t)}\Delta\rho + \frac{m}{2}[\ddot{b}(t) + \omega^2(t)b(t)]\rho^2 + \frac{g|\bar{\chi}_0|^2}{b^4(t)} - \frac{\mu}{b(t)}\frac{d\tau}{dt} \right\} \bar{\chi}_0. \quad (4.23)$$

In the limit of $g \to 0$ we again set $\tau = \int^t dt'/b^2(t')$, assume that b(t) obeys the scaling equation (4.7), and put $\bar{\chi}_0$ independent of τ . Then Eq. (4.23) reduces to the initial equation for the stationary condensate wavefunction, but in terms of the rescaled coordinate variables ρ . This means that the scaling transformation for an ideal gas is the same as in the case of 2D BEC or BEC in the geometry of an ideal cylinder. The wavefunction of the evolving condensate is given by equation (4.20).

The situation is drastically different for 3D condensates in the Thomas-Fermi regime. In this limit the ratio of the Laplacian term related to the inhomogeneity in the density profile, to the interaction term is initially $(\hbar\omega_0/\mu)^2 \ll 1$ and it becomes $b(t)(\hbar\omega_0/\mu)^2$ in the course of the evolution. As long as

$$\left(\frac{\hbar\omega_0}{\mu}\right)^2 b(t) \ll 1 \tag{4.24}$$

one can drop the Laplacian term in Eq. (4.23). Then, putting $\bar{\chi}_0$ independent of τ we obtain:

$$\frac{m}{2}[\ddot{b}(t) + \omega^2(t)b(t)]\rho^2 + \frac{g|\bar{\chi}_0|^2}{b^4(t)} - \frac{\mu}{b(t)}\frac{d\tau}{dt} = 0.$$
(4.25)

We then have to set

$$\tau = \int^t \frac{dt'}{b^3(t')} \tag{4.26}$$

and write the scaling equation as

$$\ddot{b}(t) + \omega^2(t)b(t) = \frac{\omega_0^2}{b^4(t)}.$$
(4.27)

Equation (4.25) now becomes

$$\frac{m\omega_0^2\rho^2}{2} + g|\bar{\chi}_0|^2 - \mu = 0, \qquad (4.28)$$

i.e. is the same as the initial equation for the Thomas-Fermi condensate, but in terms of rescaled coordinates. Initially we have $\psi_0 = \sqrt{\mu/g(1 - r^2/R_{TF}^2)}$ and Eq. (4.28) gives

$$\bar{\chi}_0 = \sqrt{\frac{\mu}{g}} \left(1 - \frac{\rho^2}{R_{TF}^2} \right) = \psi_0(\boldsymbol{\rho}). \tag{4.29}$$

The time-dependent condensate wavefunction $\Psi_0(\mathbf{r}, t)$ then follows from Eqs. (4.22) and (4.20).

In the case of expansion ($\omega(t) = 0$), Eq. (4.27) reads:

$$\ddot{b} = \frac{\omega_0^2}{b^4}.\tag{4.30}$$

Multiplying both sides of this equation by $\dot{b}(t)$ and integrating we have:

$$\frac{\dot{b}^2(t)}{2} = -\frac{\omega_0^2}{3b^2(t)} + \frac{\omega_0^2}{3},\tag{4.31}$$

where we took into account the initial conditions (4.8). At large times where $b \gg 1$, one can drop the first term in the right hand side of Eq. (4.30). This gives

$$b(t) = \sqrt{\frac{2}{3}}\,\omega_0 t. \tag{4.32}$$

We thus see that the condition $b \gg 1$ is equivalent to $t \gg \omega_0^{-1}$ and Eq. (4.32) is valid in the regime of free expansion.

Note that for 3D Thomas-Fermi condensates the scaling solution is only an approximation. It has been proposed and used for the analysis of experiments with evolving 3D Bose-Einstein condensates (Yu. Kagan, E.L. Surkov, and G.V. Shlyapnikov, Phys. Rev. A 54, R1753 (1996); Y. Castin and R. Dum, Phys. Rev. Lett. **77**, 5315 (1996)).

4.3 Fundamental frequencies of oscillating condensates

When the trapping potential is not switched off completely, the condensate oscillates. Let us assume that $\omega(t) = \omega_0 - \delta\omega$, where $|\delta\omega| \ll \omega_0$. Then b(t) is close to unity and can be represented in the form b(t) = 1 + f(t), with $|f| \ll 1$. For a spherically symmetrical harmonic potential equation (4.27) now reads:

$$\ddot{f} + (\omega_0^2 - 2\delta\omega\omega_0 + \delta\omega^2)(1+f) = \omega_0^2(1 - 4f + 20f^2 + \dots),$$

where the symbol ... stands for higher powers of f. Keeping only terms that are linear in f or in $\delta\omega$ we obtain an equation:

$$\ddot{f} + 5\omega_0^2 f = 2\delta\omega\omega_0,\tag{4.33}$$

with initial conditions

$$f(0) = 0; \quad \dot{f}(0) = 0.$$
 (4.34)

The solution of Eq. (4.33) is

$$f(t) = \frac{2\delta\omega}{5\omega_0} \{1 - \cos(\sqrt{5}\omega_0 t)\}.$$
 (4.35)

We thus see that the condensate undergoes small oscillations with frequency

$$\Omega_{3D} = \sqrt{5}\omega_0. \tag{4.36}$$

These oscillations do not change the Thomas-Fermi shape of the density profile of the oscillating condensate. Therefore, the related oscillation mode is called 'breathing mode" and the frequency Ω_{3D} is often identified as fundamental frequency.

For 2D trapped condensates or condensates in the geometry of an ideal cylinder, where the scaling parameter obeys Eq. (4.7), substituting b = 1 + f and $\omega(t) = \omega_0 - \delta \omega$ into this equation and linearizing the resulting equation with respect to f and $\delta \omega$, we obtain:

$$\ddot{f} + 4\omega_0^2 f = 2\delta\omega\omega_0,\tag{4.37}$$

again with initial conditions (4.34). From the solution of Eq. (4.37), which reads

$$f(t) = \frac{\delta\omega}{2\omega_0} \{1 - \cos(2\omega_0 t)\},\tag{4.38}$$

we deduce the fundamental frequency of breathing oscillations:

$$\Omega_{2D} = 2\omega_0. \tag{4.39}$$

Problems 4

4.1 Consider a Bose-Einstein condensate in the Thomas-Fermi regime in a cylindrical harmonic trap ($\omega_x = \omega_y = \omega_\rho \neq \omega_z$):

$$V(z,\rho) = \frac{m}{2}(\omega_{\rho}^{2}\rho^{2} + \omega_{z}^{2}z^{2}); \quad \rho^{2} = x^{2} + y^{2}.$$
(4.40)

Obtain the Thomas-Fermi solution for the ground state and the scaling solution for $\Psi_0(\mathbf{r}, t)$ under arbitrary variations of ω_ρ and ω_z . For the case of free expansion obtain the aspect ratio of the expanding condensate at $t \to \infty$ for an initially sigar-shaped condensate where $\omega_\rho \gg \omega_z$ and, hence, the axial (z) size is much larger than the radial (ρ) size (Y. Castin and R. Dum, Phys. Rev. Lett. **77**, 5315 (1996)).

The solution for the ground state condensate wavefunction follows from the stationary Gross-Pitaevskii equation (3.9), and the corresponding time-dependent form of the wavefunction is given by Eq. (3.7). In the Thomas-Fermi regime we drop the kinetic energy terms in Eq. (3.9), which yields:

$$\frac{m}{2}(\omega_{\rho}^{2}\rho^{2} + \omega_{z}^{2}z^{2}) + g|\psi_{0}|^{2} - \mu = 0.$$
(4.41)

We then obtain the inverted-parabola solution:

$$\psi_0 = \sqrt{\frac{\mu}{g} \left(1 - \frac{\rho^2}{R_\rho^2} - \frac{z^2}{R_z^2} \right)}$$
(4.42)

for ρ and z at which the argument of the square root is positive, and zero otherwise. The radial (ρ) and axial (z) Thomas-Fermi radiai are given by

$$R_{\rho} = \sqrt{\frac{2\mu}{m\omega_{\rho}^2}},\tag{4.43}$$

$$R_z = \sqrt{\frac{2\mu}{m\omega_z^2}}, \qquad (4.44)$$

The presence of θ -functions in Eq. (4.42), which are equal to 1 at positive arguments and to zero at negative ones, indicates that the condensate wavefunction is exactly zero at $\rho \geq R_{\rho}$ and $|z| \geq R_z$. The chemical potential is $\mu = n_{max}g$, where n_{max} is the maximum density achieved at z = 0, $\rho = 0$. The relation between μ and the number of particles in the condensate, N_0 , is easily established from the normalization condition $\int |\psi_0|^2 d^2 \rho dz = N_0$.

The evolution of the condensate wavefunction $\Psi_0(\rho, z, t)$ under temporal variations of ω_{ρ} and ω_z is described by the Gross-Pitaevskii equation (3.6) which we rewrite here for the cylindrically symmetrical potential $V(z, \rho)$ (4.40):

$$i\hbar\frac{\partial\Psi_0}{\partial t} = \left\{-\frac{\hbar^2}{2m}(\Delta_{\rho} + \Delta_z) + \frac{m}{2}[\omega_{\rho}^2(t)\rho^2 + \omega_z^2(t)z^2] + g|\Psi_0|^2\right\}\Psi_0.$$
 (4.45)

We then search for the scaling solution in the form:

$$\Psi_0(\rho, z, t) = \frac{1}{\sqrt{\mathcal{V}(t)}} \chi_0(u_\rho, u_z, \tau) \exp\{i\Phi(\rho, z, t)\},$$
(4.46)

where $u_{\rho} = \rho/b_{\rho}(t)$, $u_z = z/b_z(t)$, and $\mathcal{V}(t) = b_{\rho}^2(t)b_z(t)$ is the dimensionless volume. The dynamical phase Φ is now taken to be

$$\Phi(\rho, z, t) = \frac{m}{2\hbar} \left(\frac{\dot{b}_{\rho}(t)}{b_{\rho}(t)} \rho^2 + \frac{\dot{b}_z(t)}{b_z(t)} z^2 \right),$$
(4.47)

and the scaling parameters $b_{\rho}(t)$, $b_{z}(t)$ are assumed to obey the scaling equations

$$\ddot{b}_{\rho}(t) + \omega_{\rho}^{2}(t)b_{\rho}(t) = \frac{\omega_{0\rho}^{2}}{b_{\rho}(t)\mathcal{V}(t)};$$
(4.48)

$$\ddot{b}_{z}(t) + \omega_{z}^{2}(t)b_{z}(t) = \frac{\omega_{0z}^{2}}{b_{z}(t)\mathcal{V}(t)},$$
(4.49)

with initial conditions

$$b_{\rho}(0) = b_z(0) = 1; \tag{4.50}$$

$$\dot{b}_{\rho}(0) = \dot{b}_{z}(0) = 0, \tag{4.51}$$

and with $\omega_{0\rho} = \omega_{\rho}(0)$, $\omega_{0z} = \omega_z(0)$ being the initial frequencies. Then, taking the rescaled time as

$$\tau = \int^t \frac{dt'}{\mathcal{V}(t')},\tag{4.52}$$

we transform Eq. (4.45) to

$$i\hbar\frac{\partial\chi_0}{\partial\tau} = \left\{-\frac{\hbar^2\mathcal{V}(t)}{2m} \left(\frac{1}{b_{\rho}^2(t)}\Delta_{u_{\rho}} + \frac{1}{b_{z}^2(t)}\Delta_{u_{z}}\right) + \frac{m}{2}(\omega_{0\rho}^2 u_{\rho}^2 + \omega_{0z}^2 u_{z}^2) + g|\chi_0|^2\right\}\chi_0.$$
(4.53)

In the Thomas-Fermi regime we omit the Laplacian terms in Eq. (4.53). Therefore, assuming that the dependence of χ_0 on τ is given by

$$\chi_0(u_\rho, u_z, \tau) = \bar{\chi}_0(u_\rho, u_z) \exp(-i\mu\tau/\hbar), \qquad (4.54)$$

with $\bar{\chi}_0$ independent of τ , we reduce Eq. (4.53) to the initial equation (4.41) for ground state BEC in which one should replace ψ_0 by $\bar{\chi}_0$, and ρ , z by u_ρ , u_z . This means that we may put $\bar{\chi}_0 = \psi_0(u_\rho, u_z)$ so that the scaling solution (4.46) reads:

$$\Psi_0(\rho, z, t) = \frac{1}{\mathcal{V}(t)} \psi_0\left(\frac{\rho}{b_\rho(t)}, \frac{z}{b_z(t)}\right) \exp\{i\Phi(\rho, z, t) - i\mu\tau(t)/\hbar\},\tag{4.55}$$

with the dynamical phase Φ following from Eq. (4.47) and condensate wavefunction given by

$$\psi_0\left(\frac{\rho}{b_{\rho}(t)}, \frac{z}{b_z(t)}\right) = \sqrt{\frac{\mu}{g}\left(1 - \frac{\rho^2}{b_{\rho}^2(t)R_{\rho}^2} - \frac{z^2}{b_z^2(t)R_z^2}\right)}$$
(4.56)

for positive arguments of the square root, and equal to zero otherwise.

Let us now consider the case of expansion where both frequencies are abruptly put equal to zero at t = 0 and the scaling equations (4.48) and (4.49) take the form

$$\ddot{b}_{\rho} = \frac{\omega_{0\rho}^2}{b_{\rho}^3 b_z};\tag{4.57}$$

$$\ddot{b}_z = \frac{\omega_{0z}^2}{b_z^2 b_\rho^2}.\tag{4.58}$$

For Eqs. (4.57) and (4.58) we see that the condensate initially elongated in the z-direction ($\omega_{0\rho} \gg \omega_{0z}$ and, hence $R_{\rho}(0) \ll R_z(0)$) expands much faster in the radial direction. This is a consequence of the fact that it is confined much tighter radially than axially, i.e because $\omega_{\rho} \gg \omega_z$. Therefore, not at very large times (let say at $t < t_0$ which is still much larger than $\omega_{0\rho}^{-1}$ and will be identified later) we may put $b_z = 1$ in Eq. (4.57). This immediately gives $b_{\rho}^2 = 1 + \omega_{0\rho}^2 t^2$ like in the case of two-dimensional expansion discussed in subsection 4.1. Then, substituting the obtained $b_{\rho}(t)$ and $b_z = 1$ into Eq. (4.58) and integrating we obtain

$$\dot{b}_z = \frac{\omega_{0z}^2}{\omega_{0\rho}} \arctan \omega_{0\rho} t.$$
(4.59)

Thus, at times in the range $\omega_{0\rho}^{-1} \ll t < t_0$ we have

$$\dot{b}_z = \frac{\pi \omega_{0z}^2}{2\omega_{0\rho}}.$$
(4.60)

This procedure is justified by the fact that b_z is still close to unity when the radial expansion speeds up and becomes free.

We now select the time t_0 such that $\omega_{\rho}^{-1} \ll t_0 \ll \omega_{0\rho} \omega_{0z}^{-2}$. One then clearly sees from Eq. (4.57) that the contribution of times $t > t_0$ to \dot{b}_{ρ} is small:

$$\dot{b}_{\rho}(\infty) - \dot{b}_{\rho}(t_0) < \int_{t_0}^{\infty} \frac{\omega_{0\rho}^2}{b_{\rho}^3(t)} dt \approx \frac{1}{2\omega_{0\rho}t_0^2} \ll \omega_{0\rho}.$$

In spite of the fact that b_z is close to unity at $t \sim t_0$, the axial expansion is also free at these times. The contribution of times $t > t_0$ to \dot{b}_z is much smaller than the result of Eq. (4.60):

$$\dot{b}_z(\infty) - \dot{b}_z(t_0) < \int_{t_0}^\infty \frac{\omega_{0z}^2}{b_\rho^2(t)} dt \approx \frac{\omega_{0z}^2}{\omega_{0\rho}^2 t_0} \ll \frac{\omega_{0z}^2}{\omega_{0\rho}}$$

We thus have:

$$b_{\rho} = \omega_{0\rho} t; \quad t \to \infty$$

$$\tag{4.61}$$

$$b_z = \frac{\pi \omega_{0z}^2}{2\omega_{0\rho}} t; \quad t \to \infty \tag{4.62}$$

The axial and radial sizes of the expanding Thomas-Fermi condensate follow from Eqs. (4.43), (4.44) and (4.56) and are given by

$$R_z(t) = \left(\frac{2\mu}{m\omega_{0z}^2}\right) b_z(t), \qquad (4.63)$$

$$R_{\rho}(t) = \left(\frac{2\mu}{m\omega_{0\rho}^2}\right) b_{\rho}(t).$$
(4.64)

The aspect ratio, i.e. the ratio of the axial to radial size is

$$A = \frac{R_z(t)}{R_\rho(t)} = \frac{\omega_{0\rho}b_z(t)}{\omega_{0z}b_\rho(t)}.$$
(4.65)

So, initially we have

$$A(0) = \frac{\omega_{0\rho}}{\omega_{0z}} \gg 1. \tag{4.66}$$

 $\widehat{\text{For}} t \to \infty$ equations (4.61) and (4.62) lead to

$$A(\infty) = \frac{\pi\omega_{0z}}{2\omega_{0\rho}} \ll 1.$$
(4.67)

We thus see that an initially sigar-shaped condensate expands much faster in the radial direction and eventually becomes a pancake. This is quite different from the expansion of a collisionless thermal gas. Being initially elongated in one direction, such a thermal gas eventually becomes a sphere. The asymmetry of free expansion was one of the key arguments on support of the existence of BEC in the first experiments at JILA and MIT.

4.2 Consider a spherical Thomas-Fermi condensate and find a scaling evolution of this condensate after an abrupt change of the coupling constant g, still keeping it positive (Yu. Kagan, E.L. Surkov, and G.V. Shlyapnikov, Phys. Rev. Lett. **79**, 2604 (1997)).

Lecture 5. Elementary excitations of a Bose-condensed gas. Quantum fluctuations and correlation properties

5.1 Bogoliubov transformation. Excitation spectrum of a uniform condensate

We now arrive at the discussion of elementary excitations. These are excited states of a Bose-condensed system, where only a small fraction of particles is excited out of the condensate. We will find the energies and eigenfunctions of these states, which will allow us to describe a response of the Bose-condensed system to any type of small external perturbations.

Let us consider a Bose-condensed weakly interacting gas in an external potential $V(\mathbf{r})$ and start with the non-linear Schroedinger equation (3.4) for the field operator $\hat{\Psi}$. Then, according to Eq. (3.5), we represent $\hat{\Psi}$ as a sum of the condensate wavefunction Ψ_0 and a (small) non-condensed part $\hat{\Psi}'$ and substitute this expression into equation (3.4). To zero order in $\hat{\Psi}'$, i.e. omitting the non-condensed part, we obtain the Gross-Pitaevskii equation (3.6). To linear order in $\hat{\Psi}'$ we find an equation:

$$i\hbar\frac{\partial\Psi'}{\partial t} = \left(-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + V(\mathbf{r}) + 2g|\Psi_0|^2 - \mu\right)\Psi' + g\psi_0^2\Psi'^{\dagger},\tag{5.1}$$

where we shifted the phase of the field operator by $-i\mu t/\hbar$ introducing a replacement $\Psi_0 \rightarrow \Psi_0 \exp(-i\mu t/\hbar)$, $\hat{\Psi}' \rightarrow \hat{\Psi}' \exp(-i\mu t/\hbar)$ so that the condensate wavefunction Ψ_0 for a stationary state is now time independent. Note that equation (5.1) can also be obtained as a Heisenberg equation of motion from the Hamiltonian

$$\hat{H}_{B} = \int d^{3}r \left\{ \hat{\Psi}^{\prime \dagger} \left[-\frac{\hbar^{2}}{2m} \Delta_{\mathbf{r}} + V(\mathbf{r}) + 2g |\Psi_{0}|^{2} - \mu \right] \hat{\Psi}^{\prime} + \frac{g}{2} (\Psi_{0}^{2} \hat{\Psi}^{\prime \dagger 2} + \Psi_{0}^{*2} \hat{\Psi}^{\prime 2}) \right\}.$$
(5.2)

The Hamiltonian \hat{H}_B follows directly from the initial Hamiltonian of the weakly interacting Bose gas, $\hat{H} - \mu \hat{N}$, where \hat{H} is given by Eq. (2.45). In order not to consider explicitly the fact that the number of particles is constant, we turn to the Hamiltonian $\hat{H} - \mu \hat{N}$, where $\hat{N} = \int \hat{\Psi}^{\dagger} \hat{\Psi} d^3 r$ is the operator of the number of particles. We thus substitute $\hat{\Psi} = \Psi_0 + \hat{\Psi}'$ into $\hat{H} - \mu \hat{N}$. Then, the terms that are linear in $\hat{\Psi}'$ and $\hat{\Psi}'^{\dagger}$ vanish due to the stationary Gross-Pitaevskii equation (3.9). Omitting terms that are cubic and fourth-order in Ψ' , $\hat{\Psi}'^{\dagger}$ we thus obtain $\hat{H} - \mu \hat{N} = H_0 + \hat{H}_B$, where H_0 contains only Ψ_0 and Ψ_0^* and is zero-order in $\hat{\Psi}'$ and $\hat{\Psi}'^{\dagger}$.

We now write $\tilde{\Psi}'$ in the form:

$$\Psi' = \sum_{\nu} u_{\nu}(\mathbf{r})\hat{b}_{\nu} \exp(-i\epsilon_{\nu}t/\hbar) - v_{\nu}^{*}(\mathbf{r})\hat{b}_{\nu}^{\dagger} \exp(i\epsilon_{\nu}t/\hbar), \qquad (5.3)$$

where the index ν labels quantum states of elementary excitations, \hat{b}_{ν} , \hat{b}_{ν}^{\dagger} are operators of the excitations, ϵ_{ν} are their eigenenergies, and u_{ν} , v_{ν} their eigenfunctions. The operators \hat{b}_{ν} , \hat{b}_{ν}^{\dagger} obey the usual commutation relations:

$$\hat{b}_{\nu}\hat{b}_{\nu'}^{\dagger} - \hat{b}_{\nu'}^{\dagger}\hat{b}_{\nu} = \delta_{\nu\nu'}; \qquad (5.4)$$

$$\hat{b}_{\nu}\hat{b}_{\nu'} - \hat{b}_{\nu'}\hat{b}_{\nu} = 0, \qquad (5.5)$$

and the functions u_{ν}, v_{ν} are normalized by the condition:

$$\int (u_{\nu}u_{\nu'}^{*} - v_{\nu}v_{\nu'}^{*})d^{3}r = \delta_{\nu\nu'}.$$
(5.6)

Taking a commutator of both sides of Eq. (5.1) with \hat{b}^{\dagger}_{ν} and repeating this procedure for the commutator with \hat{b}_{ν} we arrive at a set of coupled equations:

$$\left(-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + V(\mathbf{r}) + 2g|\Psi_0|^2 - \mu\right)u_\nu - g\Psi_0^2 v_\nu = \epsilon_\nu u_\nu \tag{5.7}$$

$$\left(-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + V(\mathbf{r}) + 2g|\Psi_0|^2 - \mu\right)v_\nu - g\Psi_0^{*2}u_\nu = -\epsilon_\nu v_\nu \qquad (5.8)$$

Equation (5.3) is called the Bogoliubov transformation, and equations (5.7) and (5.8) are usually called Bogoliubov-de Gennes equations for elementary excitations. These equations give the eigenfunctions and eigenenergies of the excitations. Using equations (5.3), (5.7), and (5.8) one reduces the bilinear Bogoliubov Hamiltonian \hat{H}_B to a diagonal form:

$$\hat{H}_B = \sum_{\nu} \epsilon_{\nu} \hat{b}^{\dagger}_{\nu} \hat{b}_{\nu}.$$
(5.9)

In the uniform case we may put $\psi_0 = \sqrt{n_0}$ and, taking into account that the index ν is now the excitation wavevector **k**, write the excitation wavefunctions in the form:

$$u_{\nu} = \frac{u_k}{\sqrt{\mathcal{V}}} \exp(i\mathbf{k}\mathbf{r}) \tag{5.10}$$

$$v_{\nu} = \frac{v_k}{\sqrt{\mathcal{V}}} \exp(i\mathbf{k}\mathbf{r}),\tag{5.11}$$

where \mathcal{V} is the system volume, and u_k , v_k are coordinate independent. The Bogoliubov-de Gennes equations (5.7) and (5.8) are then transformed to

$$\left(\frac{\hbar^2 k^2}{2m} + 2n_0 g - \mu\right) u_k - n_0 g v_k = \epsilon_k u_k;$$
(5.12)

$$\left(\frac{\hbar^2 k^2}{2m} + 2n_0 g - \mu\right) v_k - n_0 g u_k = -\epsilon_k v_k.$$
(5.13)

To zero order we may put $n_0 = n$ and $\mu = ng$, which reduces Eqs. (5.12) and (5.13) to

$$(E_k + ng)u_k - ngv_k = \epsilon_k u_k; \tag{5.14}$$

$$(E_k + ng)v_k - ngu_k = -\epsilon_k v_k, \tag{5.15}$$

with $E_k = \hbar^2 k^2 / 2m$. Equations (5.14) and (5.15) give the excitation spectrum

$$\epsilon_k = \sqrt{E_k^2 + 2ngE_k}.$$
(5.16)

Since the normalization condition (5.6) yields $|u_k|^2 - |v_k|^2 = 1$, we obtain

$$u_k = \frac{1}{2} \left(\sqrt{\frac{\epsilon_k}{E_k}} + \sqrt{\frac{E_k}{\epsilon_k}} \right), \tag{5.17}$$

$$v_k = \frac{1}{2} \left(\sqrt{\frac{\epsilon_k}{E_k}} - \sqrt{\frac{E_k}{\epsilon_k}} \right).$$
 (5.18)

(5.19)

Equations (5.14) and (5.15) also give negative energies $\epsilon_k = -\sqrt{E_k^2 + 2ngE_k}$. However, for such negative-energy excitations the norm $(|u_k|^2 - |v_k|^2)$ turns out to be negative, and hence they should be omitted.

We can also establish a relation between the excitation operators $\hat{b}_{\mathbf{k}}, \hat{b}_{\mathbf{k}}^{\dagger}$ and particle operators $\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{k}}^{\dagger}$. The Schroedinger operator of non-condensed particles $\hat{\psi}' = \sum_{\mathbf{k}} (1/\mathcal{V}) \hat{a}_{\mathbf{k}} \exp(i\mathbf{k}\mathbf{r})$, according to Eq. (5.3) can be rewritten as $\hat{\psi}' = \sum_{\mathbf{k}} (1/\mathcal{V}) [u_k \hat{b}_{\mathbf{k}} \exp(i\mathbf{k}\mathbf{r}) - v_k \hat{b}_{\mathbf{k}}^{\dagger} \exp(-i\mathbf{k}\mathbf{r})]$. We then find

$$\hat{a}_{\mathbf{k}} = u_k \hat{b}_{\mathbf{k}} - v_k \hat{b}_{-\mathbf{k}}^{\dagger}, \qquad (5.20)$$

$$\hat{a}^{\dagger}_{\mathbf{k}} = u_k \hat{b}^{\dagger}_{\mathbf{k}} - v_k \hat{b}_{-\mathbf{k}}.$$
(5.21)

The excitation spectrum ϵ_k (5.16) is displayed in Fig.5.1. Low-momentum excitations represent collective waves, i.e. particles moving back and forth. The collective nature of the excitations is due to the interactions. For $k \ll \xi^{-1} = \sqrt{mng}/\hbar$, which corresponds to energies $\epsilon_k \ll \mu$, the excitations are phonons or sound waves with the dispersion relation

$$\epsilon_k = \hbar c_s k, \tag{5.22}$$



Figure 5.1: Excitation spectrum of a uniform condensate.

where the quantity

$$c_s = \sqrt{\frac{ng}{m}} \tag{5.23}$$

is the velocity of sound. For $k \gg \xi^{-1}$, i.e. at energies $\epsilon_k \gg \mu$, excitations are single particles since their energy greatly exceeds the interaction per particle ng. In this case Eq. (5.16) gives

$$\epsilon_k = \frac{\hbar^2 k^2}{2m} + ng. \tag{5.24}$$

The presence of the term ng in Eq. (5.24) shows that high-energy particles interact with the condensate.

5.2 Non-condensed fraction. One-body density matrix and long-range order

We can now calculate the fraction of non-condensed particles and verify that it is small as has been assumed *apriori*. The density of non-condensed particles is given by

$$n' = \langle \hat{\Psi}^{\dagger}(\mathbf{r}, t) \hat{\Psi}^{\prime}(\mathbf{r}, t) \rangle.$$
(5.25)

In the uniform case, using Eqs. (5.3), (5.10), and (5.11) we have:

$$\hat{\Psi}'(\mathbf{r},t) = \left[\sum_{\mathbf{k}} \frac{u_k \hat{b}_{\mathbf{k}}}{\sqrt{\mathcal{V}}} \exp(i\mathbf{k}\mathbf{r} - i\epsilon_k t/\hbar) - \frac{v_k \hat{b}_{\mathbf{k}}^{\dagger}}{\sqrt{\mathcal{V}}} \exp(-i\mathbf{k}\mathbf{r} + i\epsilon_k t/\hbar)\right] \exp(-i\mu t/\hbar), \quad (5.26)$$

which leads to

$$\langle \hat{\Psi}'^{\dagger}(\mathbf{r},t)\hat{\Psi}'(\mathbf{r},t)\rangle = \frac{1}{\mathcal{V}} \sum_{\mathbf{k},\mathbf{k}'} \left[u_{k'}^{*}u_{k} \exp\{i(\mathbf{k}-\mathbf{k}')\mathbf{r}+i(\epsilon_{k'}-\epsilon_{k})t/\hbar\}\langle\hat{b}_{\mathbf{k}'}^{\dagger}\hat{b}_{\mathbf{k}}\rangle + v_{k'}^{*}v_{k} \exp\{i(\mathbf{k}'-\mathbf{k})\mathbf{r}+i(\epsilon_{k}-\epsilon_{k'})t/\hbar\}\langle\hat{b}_{\mathbf{k}'}\hat{b}_{\mathbf{k}}^{\dagger}\rangle - u_{k'}^{*}v_{k} \exp\{-i(\mathbf{k}'+\mathbf{k})\mathbf{r}+i(\epsilon_{k}+\epsilon_{k'})t/\hbar\}\langle\hat{b}_{\mathbf{k}'}^{\dagger}\hat{b}_{\mathbf{k}}^{\dagger}\rangle - v_{k'}^{*}u_{k} \exp\{i(\mathbf{k}'+\mathbf{k})\mathbf{r}-(\epsilon_{k}+\epsilon_{k'})t/\hbar\}\langle\hat{b}_{\mathbf{k}}\hat{b}_{\mathbf{k}}\rangle\right].$$

$$(5.27)$$

Using commutation relations (5.4) and (5.5) the expectation values of the excitation operators are

$$\langle \hat{b}_{\mathbf{k}'}^{\dagger} \hat{b}_{\mathbf{k}} \rangle = \delta_{\mathbf{k}'\mathbf{k}} N_k$$
(5.28)

$$\langle \hat{b}_{\mathbf{k}'} \hat{b}_{\mathbf{k}}^{\dagger} \rangle = \delta_{\mathbf{k}'\mathbf{k}} (1+N_k)$$

$$(5.29)$$

$$\langle \hat{b}_{\mathbf{k}} \hat{b}_{\mathbf{k}} \rangle = \langle \hat{b}_{\mathbf{k}'\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}}^{\dagger} \rangle = 0$$

$$(5.29)$$

$$\langle \hat{b}_{\mathbf{k}'} \hat{b}_{\mathbf{k}} \rangle = \langle \hat{b}_{\mathbf{k}'}^{\dagger} \hat{b}_{\mathbf{k}}^{\dagger} \rangle = 0, \qquad (5.30)$$

where N_k are the occupation numbers for the excitations given by the usual Bose distribution function

$$N_k = \frac{1}{\exp(\epsilon_k/T) - 1}.$$
(5.31)

At T = 0 we have $N_k = 0$ since we are in the ground state and excitations are not present. Then, setting $\langle \hat{b}_{\mathbf{k}'} \hat{b}_{\mathbf{k}}^{\dagger} \rangle = \delta_{\mathbf{k'k}}$ and putting the rest of the expectation values equal to zero, from Eqs. (5.25) and (5.27) we obtain:

$$n' = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} v_k^2. \tag{5.32}$$

Replacing the sum over \mathbf{k} by an integral:

$$\sum_{\mathbf{k}} \Rightarrow \int \frac{\mathcal{V}d^3k}{(2\pi)^3},$$

and using Eq. (5.18) we represent Eq. (5.32) in the form

$$n' = \int_0^\infty \frac{1}{4} \left(\sqrt{\frac{\epsilon_k}{E_k}} - \sqrt{\frac{E_k}{\epsilon_k}} \right)^2 \frac{4\pi k^2 dk}{(2\pi)^3}.$$
 (5.33)

We then substitute the Bogoliubov dispersion relation (5.16) for ϵ_k and obtain:

$$n' = \int_0^\infty \left(\frac{\epsilon_k}{E_k} + \frac{E_k}{\epsilon_k} - 2\right) \frac{k^2 dk}{8\pi^2} = \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty \left\{\sqrt{E + 2ng} - \sqrt{E} - \frac{ng}{\sqrt{E + 2ng}}\right\} \frac{dE}{8\pi^2}$$

so that the integration leads to the non-condensed fraction

$$\frac{n'}{n} = \frac{8}{3\sqrt{\pi}} (na^3)^{1/2}.$$
(5.34)

As we assumed *apriori* that the non-condensed fraction is small we now see that the small parameter of the Bogoliubov theory for a weakly interacting Bose-condensed gas at T = 0 is

$$(na^3)^{1/2} \ll 1. \tag{5.35}$$

We now calculate the one-body density matrix

$$g_1(\mathbf{r}, \mathbf{r}', t, t') = \langle \hat{\Psi}^{\dagger}(\mathbf{r}, t) \hat{\Psi}(\mathbf{r}', t') \rangle$$
(5.36)

at equal times, t = t', so that g_1 is independent of t and we may put t = t' = 0. In the uniform case g_1 depends only on the difference $|\mathbf{r} - \mathbf{r'}|$ and we may put $\mathbf{r'} = 0$. Representing the field operator as a sum of the condensate wavefunction and the non-condensed part as given by Eq. (3.5) and taking into account that $|\Psi_0(\mathbf{r},t)| = \sqrt{n_0}$ where n_0 is the condensate density, we thus have

$$g_1(\mathbf{r}) = n_0 + \langle \hat{\Psi}'^{\dagger}(\mathbf{r}, 0) \hat{\Psi}'(0, 0) \rangle.$$
(5.37)

For the second term in the right hand side of this equation, repeating the procedure that gave Eq. (5.32) we obtain:

$$\langle \hat{\Psi}'^{\dagger}(\mathbf{r},0)\hat{\Psi}'(0,0)\rangle = \int \frac{d^3k}{(2\pi)^3} v_k^2 \exp(i\mathbf{kr}).$$
 (5.38)

Using Eq. (5.18) and turning to the integration variable $x = k\xi$, where $\xi = \hbar/\sqrt{mng}$ is the healing length, we have:

$$g_1(r) = n_0 + \frac{1}{8\pi^2} \int_0^\infty \left(\frac{\epsilon_k}{E_k} + \frac{E_k}{\epsilon_k} - 2\right) \frac{\sin kr}{kr} k^2 dk$$

= $n_0 + \frac{1}{4\pi^2 \xi^2 r} \int_0^\infty \sin[x(r/\xi)] \left\{\sqrt{x^2 + 4} - x - \frac{2}{\sqrt{x^2 + 4}}\right\} dx.$

Integrating in parts we then get an expansion in powers of 1/r. For $r \to \infty$, keeping only the leading term of the expansion and substituting $g = 4\pi \hbar^2 a/m$ where a is the scattering length, we obtain

$$g_1(r) = n_0 + \frac{1}{4\pi^2 \xi^3} \left(\frac{\xi}{r}\right)^2 = n_0 + \frac{2}{\sqrt{\pi}} n(na^3)^{1/2} \left(\frac{\xi}{r}\right)^2; \quad r \to \infty.$$
(5.39)

The dependence $g_1(r)$ is shown in Fig.5.2. It is important that g_1 is tending to a constant value for $r \to \infty$. This type of behavior is called (off-diagonal) long-range order. It means that there will be a delta-functional term $n_0\delta(\mathbf{k})$ in the momentum distribution given by the formula $\int d^3r g_1(\mathbf{r}) \exp(-i\mathbf{kr})$, which reflects the fact that a macroscopic number of particles (with density n_0) is in the zero-momentum state.



Figure 5.2: One-body density matrix $g_1(r)$.

5.3 Quantum fluctuations of the density and phase

Let us now introduce the density-phase formalism in terms of field operators and discuss quantum (T = 0) fluctuations of the density and phase. In *Lecture* 3 we already introduced the density-phase representation, but this has been done for the condensate wavefunction Ψ_0 where the density (n_0) and phase are classical quantities. We then used this representation in the Gross-Pitaevskii equation for Ψ_0 , which is a classical-field equation. The term "classical" is used here in the sense that the related quantities are not operators. In quantum theory we start with physical quantities represented by operators. For example, discussing the density and phase fluctuations we introduce the field operators in the form:

$$\hat{\Psi}(\mathbf{r},t) = \exp\{i\hat{\phi}(\mathbf{r},t)\}\sqrt{\hat{n}(\mathbf{r},t)}$$
(5.40)

$$\hat{\Psi}^{\dagger}(\mathbf{r},t) = \sqrt{\hat{n}(\mathbf{r},t)} \exp\{-i\hat{\phi}(\mathbf{r},t)\},\tag{5.41}$$

where $\hat{n}(\mathbf{r}, t)$ and $\phi(\mathbf{r}, t)$ are the density and phase operators. Commutation relations for these operators are obtained straightforwardly from the commutation relations for $\hat{\Psi}$, $\hat{\Psi}^{\dagger}$ which at equal times are given by Eqs. (2.38) and (2.39). This leads to the commutation relation

$$[\hat{n}(\mathbf{r},t)\hat{\phi}(\mathbf{r}',t)] = i\delta(\mathbf{r}-\mathbf{r}').$$
(5.42)

Assuming small fluctuations of the density we may put $\hat{n} = n_0$ in the expres-

sion for the operator of the flux of particles. Then the flux operator becomes;

$$\hat{\mathbf{j}} = \frac{\hbar}{2mi} \left\{ \hat{\Psi}^{\dagger} \nabla \hat{\Psi} - \hat{\Psi} \nabla \hat{\Psi}^{\dagger} \right\} = \frac{\hbar n_0}{m} \nabla \hat{\phi}.$$
(5.43)

We can now write the continuity equation of the hydrodynamic approach, $\dot{n} + \text{div}\mathbf{j} = 0$, in terms of the density and phase operators. Writing $\hat{n} = n_0 + \delta \hat{n}$ where $\delta \hat{n}$ is the operator of the density fluctuations, for a stationary state (n_0 is time independent) we have:

$$\frac{\partial \delta \hat{n}}{\partial t} = -\text{div}\hat{\mathbf{j}} = -\frac{\hbar}{m}\nabla n_0\nabla\phi - \frac{\hbar n_0}{m}\Delta\hat{\phi}.$$
(5.44)

The formalism where one uses the field operators in the form given by Eqs. (5.40) and (5.41) is called the density-phase formalism. It is adequate if the density fluctuations are small and is often used in low-dimensional systems. Having in mind the use of this formalism later in the course we now show that the density fluctuations are really small in the 3D case. For brevity, we consider the uniform case.

The operator of the density fluctuations is given by

$$\delta \hat{n}(\mathbf{r},t) = \hat{n}(\mathbf{r},t) - \bar{n}(\mathbf{r},t) = \hat{\Psi}^{\dagger}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t) - \langle \hat{\Psi}^{\dagger}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\rangle.$$
(5.45)

Putting the mean density \bar{n} equal to the condensate density n_0 and writing $\hat{\Psi} = \Psi_0 + \hat{\Psi}'$, we divide the system of excitations in the non-condensed fraction $\hat{\Psi}'$ into two parts: the low-energy part with momenta $k < \xi^{-1} = \sqrt{mng}/\hbar$ and energies $\epsilon_k < ng$, and the high-energy part with $\epsilon_k > ng$. Considering the low-energy part we confine ourselves to the first order in $\hat{\Psi}'$ and obtain

$$\delta \hat{n}(\mathbf{r},t) = \Psi_0(\mathbf{r},t)\hat{\Psi}^{\dagger}(\mathbf{r},t) + \Psi_0^*(\mathbf{r},t)\hat{\Psi}^{\prime}(\mathbf{r},t).$$
(5.46)

For a uniform Bose-condensed gas, using Eqs. (5.3), (5.10), (5.11), (5.17), and (5.18), we have

$$\delta \hat{n}(\mathbf{r},t) = \sqrt{n_0} \sum_{\mathbf{k}} \left(\frac{E_k}{\epsilon_k}\right)^{1/2} \hat{b}_{\mathbf{k}} \exp(i\mathbf{k}\mathbf{r} - i\epsilon_k t/\hbar) + h.c.$$
(5.47)

Using Eq. (5.47) the mean square (relative) density fluctuations at T = 0 are given by

$$\frac{\langle \delta \hat{n}(\mathbf{r},t) \delta \hat{n}(\mathbf{r}',t) \rangle}{n_0^2} = \frac{1}{n_0 \mathcal{V}} \sum_{\mathbf{k}}^{|k| < \xi^{-1}} \frac{E_k}{\epsilon_k} \exp(i\mathbf{k}[\mathbf{r} - \mathbf{r}'])$$
$$= \frac{1}{n_0} \int_{|k| < \xi^{-1}} \frac{d^3k}{(2\pi)^3} \left(\frac{E_k}{\epsilon_k}\right) \exp(i\mathbf{k}[\mathbf{r} - \mathbf{r}']) = \frac{1}{n_0} \int_{\xi^{-1}}^{\infty} \frac{k^2 dk}{2\pi^2} \left(\frac{E_k}{\epsilon_k}\right) \frac{\sin k|\mathbf{r} - \mathbf{r}'|}{k|\mathbf{r} - \mathbf{r}'|}$$

The main contribution to the integral comes from momenta $k \sim \xi^{-1}$ and we find:

$$\frac{\langle \delta \hat{n}(\mathbf{r},t) \delta \hat{n}(\mathbf{r}',t) \rangle}{n_0^2} \lesssim (n\xi)^{-3} \sim (na^3)^{1/2}.$$
(5.48)

The high-energy part represents single particles with energies larger than ng, and the related contribution to the density fluctuations does not exceed the density of this part. The latter is smaller than $n_0(na^3)^{1/2}$ so that the contribution to $\langle \delta \hat{n}(\mathbf{r},t) \delta \hat{n}(\mathbf{r}',t) \rangle / n_0^2$ is small compared to $(na^3)^{1/2}$.

Relying on Eqs. (5.44) and (5.47) one can write the secondly quantized expression for the phase operator $\hat{\phi}$. It reads:

$$\hat{\phi}(\mathbf{r},t) = \frac{1}{2\sqrt{n_0 \mathcal{V}}} \sum_{\mathbf{k}} \left(\frac{\epsilon_k}{E_k}\right)^{1/2} \hat{b}_{\mathbf{k}} \exp(i\mathbf{k}\mathbf{r} - i\epsilon_k t/\hbar) + h.c.$$
(5.49)

It is then straightforward to show that the mean square fluctuations of the phase are small in 3D.

5.4 Quantum fluctuations and ground state energy

We now calculate the ground state energy of a Bose-condensed gas including corrections originating from quantum fluctuations. So, we again consider T =0 and recall that the Bogoliubov approach corresponds to diagonalizing the bilinear Hamiltonian \hat{H}_B (5.2). Let us now rewrite the total Hamiltonian $\hat{H} =$ $H_0 + \hat{H}_B$ (omitting the term associated with the chemical potential in \hat{H}_B) for the uniform case:

$$\hat{H} = \int d^3r \left\{ \frac{g}{2} |\Psi_0|^4 + \hat{\Psi}'^{\dagger} \left[-\frac{\hbar^2}{2m} \Delta_{\mathbf{r}} + 2g |\Psi_0|^2 \right] \hat{\Psi}' + \frac{g}{2} (\Psi_0^2 \hat{\Psi}'^{\dagger 2} + \Psi_0^{*2} \hat{\Psi}'^2) \right\}.$$
(5.50)

To zero order the ground state energy is given by the first term in the right hand side of Eq. (5.50) and is equal to $E = gn_0^2 \mathcal{V} = gN_0^2/2\mathcal{V}$. Dealing only with this order we usually replace the number of Bose-condensed particles N_0 by the total number of particles N.

The other terms in the right hand side of Eq. (5.50) provide corrections to the ground state energy, which is equal to their expectation value at zero occupation numbers of the excitations. This is the so-called correction due to quantum fluctuations. We should also take into account the difference between the condensate density n_0 and the total density n in the first term and write $|\Psi_0|^4 = n^2 - 2n\Psi'^{\dagger}\Psi'$. Then, in the largest term, $(g/2)n^2$, in the integrand of Eq. (5.50) we should renormalize the coupling constant g and include the second order correction to this quantity. This is equivalent to the replacement

$$g \Rightarrow g\left(1 + \frac{4\pi a}{\mathcal{V}}\right) \sum_{\mathbf{k}} \frac{1}{k^2}$$

In the uniform case the quantum numbers ν of the excitations are momenta **k**, and the functions u_{ν} , v_{ν} in the Bogoliubov transformation (5.3) are given by equations (5.10), (5.11), (5.17), and (5.18). Using Eq. (5.3) we reduce the

Hamiltonian (5.50) to

$$\hat{H} = \frac{g}{2}n^2\mathcal{V} + \int \frac{\mathcal{V}d^3k}{(2\pi)^3} \left\{ \epsilon_k \hat{b}^{\dagger}_{\mathbf{k}} \hat{b}_{\mathbf{k}} + \left[v_k^2(E_k + ng) - u_k v_k ng + \frac{mg^2 n^2}{2\hbar^2 k^2} \right] \right\}$$
$$= \frac{N^2g}{2\mathcal{V}} + \int \frac{d^3k}{(2\pi)^3} \left\{ \epsilon_k \hat{b}^{\dagger}_{\mathbf{k}} \hat{b}_{\mathbf{k}} + \left[\frac{\epsilon_k - E_k - ng}{2} + \frac{(ng)^2}{4E_k} \right] \right\}.$$
(5.51)

At T = 0 the expectation value $\langle \hat{b}^{\dagger}_{\mathbf{k}} \hat{b}_{\mathbf{k}} \rangle$ is equal to zero, and Eq. (5.51) leads to the ground state energy

$$E = \langle \hat{H} \rangle = \frac{N^2 g}{2\mathcal{V}} \left(1 + \frac{128}{15} \sqrt{\frac{Na^3}{\pi \mathcal{V}}} \right).$$
(5.52)

The chemical potential then is

$$\mu = \frac{\partial E}{\partial N} = ng\left(1 + \frac{32}{3}\sqrt{\frac{na^3}{\pi}}\right). \tag{5.53}$$

We thus see that at T = 0 all important quantities that should be small for the validity of the perturbative approach (non-condensed fraction, fluctuations of the density, correction to the ground state energy) are proportional to the small parameter

$$\sqrt{na^3} \ll 1. \tag{5.54}$$

This parameter is, therefore, crucial for the theory of a weakly interacting Bose gas. We will see later in the course how the situation can change at finite temperatures.

Problems 5

5.1 Find the spectrum of low-energy $(\epsilon_{\nu} \ll \mu)$ excitations with orbital angular momentum l = 0 for a Thomas-Fermi Bose-Einstein condensate in a spherical harmonic potential $V(r) = m\omega^2 r^2/2$ (S. Stringari, Phys. Rev. Lett. 77, 2360 (1996)).

We first rewrite the Bogoliubov-de Gennes equations (5.7) and (5.8) in terms of the functions $f_{\nu}^{\pm} = u_{\nu} \pm v_{\nu}$. Assuming that the (Schroedinger-picture) condensate wavefunction ψ_0 is real and taking into account that the orbital angular momentum of the excitations is zero, we have

$$-\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \frac{m\omega^2 r^2}{2} + g\psi_0^2(r) - \mu\right) f_\nu^+ = \epsilon_\nu f_\nu^-; \quad (5.55)$$

$$-\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \frac{m\omega^2 r^2}{2} + 3g\psi_0^2(r) - \mu\right) f_\nu^- = \epsilon_\nu f_\nu^+.$$
 (5.56)

Using the Gross-Pitaevskii equation

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)\psi_0(r) + \frac{m\omega^2 r^2}{2}\psi_0(r) + g\psi_0(r)^3 - \mu\psi_0(r) = 0$$

we rewrite Eq. (5.55) as

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)f_{\nu}^+ + \frac{\hbar^2}{2m}\frac{f_{\nu}^+}{\psi_0(r)}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)\psi_0(r) = \epsilon_{\nu}f_{\nu}^-.$$
 (5.57)

We then substitute f_{ν}^{-} following from Eq. (5.57) into Eq. (5.56) and recall that in the Thomas-Fermi regime one has a small parameter

$$\frac{\hbar\omega}{\mu} \ll 1. \tag{5.58}$$

Considering excitations with energies ϵ_{ν} that can be greater than $\hbar\omega$ but are still much smaller than μ , we may omit the term $(-\hbar^2/2m)\Delta f_{\nu}^-$ in the resulting equation, since this term is small at least as $(\epsilon_{\nu}/\mu)^2$ compared to other terms. Substituting the Thomas-Fermi expression for the condensate wavefunction: $\psi_0^2 = (\mu/g)(1 - r^2/R_{TF}^2)$ for $r \leq R_{TF}$ and zero otherwise, where $R_{TF} = (2\mu/m\omega^2)^{1/2}$ is the Thomas-Fermi radius, at $r \leq R_{TF}$ we eventually transform Eq. (5.56) to

$$\frac{\hbar^2 \mu}{m} \left(1 - \frac{r^2}{R_{TF}^2} \right) \left[- \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) f_{\nu}^+ + \frac{f_{\nu}^+}{\sqrt{1 - r^2/R_{TF}^2}} \right] \\ \times \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) \sqrt{1 - r^2/R_{TF}^2} = \epsilon_{\nu}^2 f_{\nu}^+.$$
(5.59)

Turning to a dimensionless coordinate $y = r/R_{TF}$ and dimensionless excitation energies $\tilde{\epsilon}_{\nu} = \epsilon_{\nu}/\hbar\omega$ we rewrite Eq. (5.59) as

$$(1-y^2)\left\{-\left(\frac{d^2}{dy^2}+\frac{2}{y}\frac{d}{dy}\right)f_{\nu}^++\frac{f_{\nu}^+}{\sqrt{1-y^2}}\left(\frac{d^2}{dy^2}+\frac{2}{y}\frac{d}{dy}\right)\sqrt{1-y^2}\right\}=\tilde{\epsilon}_{\nu}^2f_{\nu}^+$$

and introducing the function $W_{\nu} = f_{\nu}^+ / \sqrt{(1-y^2)}$ we transform this equation to

$$(1-y^2)\left(\frac{d^2}{dy^2} + \frac{2}{y}\frac{d}{dy}\right)W_{\nu} - 2y\frac{dW_{\nu}}{dy} + 2\tilde{\epsilon}_{\nu}^2W_{\nu} = 0.$$
(5.60)

In terms of the dimensionless coordinate $x = y^2$ equation (5.60) becomes

$$x(1-x)\frac{d^2W_{\nu}}{dx^2} + \left(\frac{3}{2} - \frac{5}{2}x\right)\frac{dW_{\nu}}{dx} + \frac{\tilde{\epsilon}_{\nu}^2}{2}W_{\nu} = 0.$$
 (5.61)

Let us also keep in mind that since Eq. (5.59) was written for $0 \le r \le R_{TF}$, equation (5.61) is valid for $0 \le x \le 1$. The function W_{ν} is proportional to the

fluctuations of the density and phase due to the excitation mode ν . So, it should be regular at x = 0 and finite at $x \to 1$.

Equation (5.61) is the well-known hypergeometrical equation which is usually written in the form:

$$x(1-x)W''_{xx} + [\gamma - (\alpha + \beta + 1)x]W'_x - \alpha\beta W = 0$$
(5.62)

and has two linearly independent solutions. The one which is regular at x = 0 reads

$$W = F(\alpha, \beta, \gamma, x) = 1 + \frac{\alpha\beta}{\gamma}x + \frac{\alpha(\alpha+1)\beta(\beta+1)}{\gamma(\gamma+1)}\frac{x^2}{2!} + \dots$$
$$= \sum_{n=0}^{\infty} \frac{\Gamma(\alpha+n)\Gamma(\beta+n)\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\beta)\Gamma(\gamma+n)}\frac{x^n}{n!},$$
(5.63)

assuming that γ is not a negative integer. The series of expansion in Eq. (5.63) is convergent at $x \to 1$ if $\alpha + \beta 1$ $\langle \gamma \rangle$ or for any relation between $(\alpha + \beta)$ and γ if either α or β is equal to -j where j is a positive integer. In the latter case the hypergeometrical function F is reduced to a polynomial.

In our case $\alpha + \beta = \gamma = 3/2$, and we have to have $\alpha = -j$ and $\beta = j + 3/2$ or vice versa $\beta = -j$ and $\alpha = j + 3/2$. Then the relation $\alpha\beta = -\tilde{\epsilon}_{\nu}^2/2$ becomes a quadratic equation

$$j^2 + \frac{3}{2}j - \frac{\tilde{\epsilon}_j^2}{2} = 0, \qquad (5.64)$$

where we put the excitation quantum number ν equal to the positive integer j. Equation (5.64) gives the values of the excitation energy $\tilde{\epsilon}_j = \sqrt{2j^2 + 3j}$, and restoring the dimensions we have the spectrum of low-energy excitations with orbital angular momentum l = 0:

$$\epsilon_j = \hbar\omega\sqrt{2j^2 + 3j}.\tag{5.65}$$

Since j is a positive integer, the excitation spectrum is discrete. This is a consequence of a finite size of the system. For j = 1 we have $\epsilon_j = \sqrt{5}\hbar\omega$, i.e. we recover the breathing mode obtained in *Lecture* 4 from the scaling approach. It is important that the spectrum of low-energy excitations does not explicitly depend on the interaction between particles. This is a consequence of the harmonicity of the confining potential in combination with the Thomas-Fermi density profile.

As we already said, if α or β is a negative integer, then the hypergeometrical function is reduced to a polynomial. In our case we have

$$W_j(x) = F\left(-j, j + \frac{3}{2}, \frac{3}{2}, x\right) = P_j^{(1/2,0)}(1 - 2y^2),$$
(5.66)

where $P_j^{(1/2,0)}$ are Jacobi polynomials. Omitting the small kinetic energy term in Eq. (5.56) we see that $f_{\nu}^- = [\epsilon_{\nu}/2\mu(1-y^2)]f_{\nu}^+$. Thus, the wavefunctions f_j^{\pm} of the excitations can be represented in the form:

$$f_j^{\pm} = C \left[\frac{2\mu(1-y^2)}{\epsilon_j} \right]^{\pm 1/2} P_j^{(1/2,0)} (1-2y^2).$$
 (5.67)

The absolute value of the coefficient C follows from the normalization condition (5.6).

5.2 Find the lowest excitations for a Thomas-Fermi condensate in a cylindrical harmonic potential $V = m(\omega_z^2 z^2 + \omega_\rho^2 \rho^2)/2$.

Lecture 6. Bose-condensed gas at a finite temperature. Superfluidity

6.1 Non-condensed fraction and the one-body density matrix at finite temperatures

In this *Lecture* we discuss the influence of finite temperatures on the properties of a Bose-condensed gas and introduce the phenomenon of superfluidity. Let us assume that the gas temperature T is well below the BEC transition temperature T_c and most of the particles are in the condensate. We then calculate the density of non-condensed particles, $n' = \langle \Psi'^{\dagger}(\mathbf{r}, t)\Psi'(\mathbf{r}, t)\rangle$, in a similar way as at T = 0. So, we consider a uniform Bose-condensed gas and use equations from (5.25) to (5.31). Then, at a finite T where $N_k \neq 0$, Eq. (5.27) gives

$$n' = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} [v_k^2 + (u_k^2 + v_k^2)N_k].$$
(6.1)

The first term in the right hand side of Eq. (6.1) is the zero-temperature noncondensed density n'(T = 0), i.e. the contribution to the non-condensed fraction from quantum fluctuations. It has been calculated in *Lecture 5* and is given by Eq. (5.34). The second term represents the contribution of the so-called thermal fluctuations and we denote it as n'_T . The total fraction of non-condensed particles is given by

$$\frac{n'}{n} = \frac{n'(T=0)}{n} + \frac{n'_T}{n}.$$
(6.2)

Using equations (5.17), (5.18), and (5.31) we have the following expression for the thermal contribution to the non-condensed density:

$$n_T' = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} (u_k^2 + v_k^2) N_k = \int_0^\infty \frac{4\pi k^2 dk}{(2\pi)^3} \left(\frac{\epsilon_k}{2E_k} + \frac{E_k}{2\epsilon_k}\right) \frac{1}{\exp(\epsilon_k/T) - 1}.$$
 (6.3)

At temperatures $T \ll \mu = ng$ the main contribution to the integral in Eq. (6.3) comes from excitations of the phonon branch where $\epsilon_k = \hbar c_s k$, and

from Eq. (6.3) we obtain:

$$n'_{T} = \int_{0}^{\infty} \frac{k^{2} dk}{4\pi^{2}} \left(\frac{2mc_{s}}{\hbar k} + \frac{\hbar k}{2c_{s}m}\right) \frac{1}{\exp(\hbar c_{s}k/T) - 1}.$$
 (6.4)

The second term in the round brackets is not important, and the contribution of the first one reads:

$$n_T' = \frac{mT^2}{2\pi^2\hbar^3 c_s} \int_0^\infty \frac{xdx}{\exp x - 1} = \frac{mT^2}{12\hbar^3 c_s}.$$
 (6.5)

Recalling that the sound velocity is $c_s = \sqrt{ng/m}$ and the coupling constant g is expressed through the scattering length and density as $g = 4\pi\hbar^2 na/m$, we find:

$$\frac{n'_T}{n} = \frac{2}{3\sqrt{\pi}} (na^3)^{1/2} \left(\frac{\pi T}{ng}\right)^2; \quad T \ll ng.$$
(6.6)

Comparing the result of Eq. (6.6) with the zero-temperature non-condensed density n'(T=0) following from Eq. (5.34) we see that at temperatures $T \ll ng$ the thermal contribution n'_T is small and can be omitted when calculating the total non-condensed fraction (6.2).

The situation is quite different at temperatures $T \gg ng$, where the main contribution to n'_T (6.3) comes from single-particle excitations which have energies $\epsilon_k \gg ng$. Then $(\epsilon_k/E_k + E_k/\epsilon_k) \approx 2$ and from Eq. (6.3) we obtain:

$$n_T' \approx \left(\frac{mT}{2\pi\hbar^2}\right)^{3/2} \zeta(3/2); \qquad T \gg ng, \tag{6.7}$$

where $\zeta(3/2)$ is the Riemann Zeta function given by

$$\zeta(3/2) = \sum_{j=1}^{\infty} \frac{1}{j^{3/2}} \approx 2.61.$$

The obtained n'_T is nothing else than the density of non-condensed particles in an ideal gas, which according to Eq. (2.50) can be expressed as $n' = n(T/T_c)^{3/2}$ with T_c being the temperature of Bose-Einstein condensation. One can easily check that n'_T of Eq. (6.7) greatly exceeds the zero-temperature contribution n'(T = 0) (5.34). So, for $T \gg ng$, but still $T \ll T_c$, we have the ideal-gas result for the density of non-condensed particles and, hence, for the total noncondensed fraction (6.2). This means that one can use the ideal gas model for finding n' at temperatures comparable with T_c .

In a similar way as at T = 0, we calculate the one-body density matrix $g_1(\mathbf{r})$ which is given by Eq. (5.37). At finite temperatures, repeating the procedure that gives n', for the uniform Bose-condensed gas we have

$$\langle \hat{\Psi}^{\prime \dagger}(\mathbf{r}, 0) \hat{\Psi}^{\prime}(0, 0) \rangle = \int \frac{d^3k}{(2\pi)^3} v_k^2 \exp(i\mathbf{kr}) + \int \frac{d^3k}{(2\pi)^3} (u_k^2 + v_k^2) N_k \exp(i\mathbf{kr}).$$
 (6.8)

The first term is the zero temperature contribution calculated in *Lecture 5* and given by Eq. (5.39), and the second term is the thermal contribution which we denote as $\langle \hat{\Psi}'^{\dagger}(\mathbf{r}, 0) \hat{\Psi}'(0, 0) \rangle_T$. Like in the calculation of n'_T , using Eqs. (5.17), (5.18), and (5.31) the thermal contribution to the density matrix is written as

$$\langle \hat{\Psi}^{\prime \dagger}(\mathbf{r},0)\hat{\Psi}^{\prime}(0,0)\rangle_{T} = \int_{0}^{\infty} \frac{k^{2}dk}{4\pi^{2}} \left(\frac{\epsilon_{k}}{E_{k}} + \frac{E_{k}}{\epsilon_{k}}\right) \frac{\exp(i\mathbf{k}\mathbf{r})}{\exp(\epsilon_{k}/T) - 1}.$$

For $r \to \infty$, momenta $k \sim 1/r$ which provide the main contribution to the integral are very small so that $\epsilon_k = \hbar c_s k \gg E_k = \hbar^2 k^2/2m$ and we can omit the second term in the round brackets. We also have $\epsilon_k \ll T$ and expand the exponent in powers of ϵ_k/T . This yields

$$\langle \hat{\Psi}'^{\dagger}(\mathbf{r},0)\hat{\Psi}'(0,0)\rangle_T = \frac{mT}{2\pi^2\hbar^2} \int_0^\infty \frac{\sin kr}{kr} dk = \frac{mT}{4\pi\hbar^2} \frac{1}{r}.$$
 (6.9)

The thermal contribution (6.9) decays as 1/r at $r \to \infty$ and it exceeds the zero temperature contribution which is represented by the first term in the right hand side of Eq. (6.8) and decays as $1/r^2$. Thus, for the one-body density matrix from Eqs. (5.37) and (6.9) we have:

$$g_1(r) = n_0 + \frac{\Lambda_T^2}{2r}; \qquad r \to \infty, \tag{6.10}$$

where $\Lambda_T = (2\pi\hbar^2/mT)^{1/2}$ is the thermal de Broglie wavelength. Qualitatively, the behavior of the finite-temperature density matrix (6.10) is the same as the one shown in Fig.5.2 for the case of T = 0, and one clearly sees the presence of the long-range order. However, at finite temperatures the density matrix approaches its asymptotic value n_0 much slower than at T = 0.

6.2 Landau criterion of superfluidity. Superfluid and normal density

We now turn to transport properties at finite temperatures. Let us first consider a Bose-condensed gas (Bose liquid) moving with velocity \mathbf{v} in a capillary at $T \to 0$. So, in the reference frame where the liquid is at rest, the walls of the capillary move with velocity $-\mathbf{v}$. Imagine that there appears an excitation with momentum \mathbf{p} and energy ϵ_p in the liquid (in this subsection \mathbf{p} is the true momentum, not the wavevector $\mathbf{k} = \mathbf{p}/\hbar$ used previously in the course and called momentum). Then, in the reference frame where the liquid is at rest, its energy becomes equal to ϵ_p and the momentum to \mathbf{p} . Let us now go back to the reference frame where the walls are at rest and the liquid moves with velocity \mathbf{v} . In this frame, the energy of the liquid will be

$$E = \epsilon_p + \mathbf{pv} + \frac{Mv^2}{2}.$$
(6.11)

The last term in Eq. (6.11) is the initial kinetic energy of the liquid. So, the term $\epsilon_p + \mathbf{pv}$ is the excitation energy in the reference frame where the liquid is
moving with velocity **v**. In order to have $\epsilon_p + \mathbf{pv} < 0$ and get a spontaneous creation of excitations, which will provide friction, one should at least have

$$\epsilon_p - pv < 0 \rightarrow v > \frac{\epsilon_p}{p}.$$
 (6.12)

Otherwise, the liquid moves without friction. In this case it is called *superfluid*.

The minimum value of ϵ_p/p is called the critical velocity v_c . So, according to Eq. (6.12) the Bose liquid (gas) is superfluid if its velocity satisfies the inequality

$$v < v_c = \min\left\{\frac{\epsilon_p}{p}\right\}.$$
 (6.13)

This condition is called the Landau criterion of superfluidity. For a weakly interacting Bose-condensed gas we have $\epsilon_p = \sqrt{(p^2/2m)^2 + ngp^2/m}$ as given by Eq. (5.16) and displayed in Fig5.1. We thus have $v_c = \min\{\epsilon_p/p\} = c_s = \sqrt{ng/m}$ so that the weakly interacting Bose-condensed gas is superfluid at velocities smaller than the velocity of sound.

For an ideal Bose gas one has $\epsilon_p = p^2/2m \to \epsilon_p/p = p/2m$ and the critical velocity v_c (6.13) is zero. Thus, the ideal Bose gas is not superfluid, and we see that interactions are crucial for the phenomenon of superfluidity.

Let us now consider low but finite temperatures. Then the liquid contains excitations which we will treat as a "gas of quasiparticles" not interacting with each other but interacting with the walls of the capillary. Imagine that the gas of these quasiparticles moves with velocity \mathbf{v} with respect to the liquid. The distribution function for the moving gas is obtained from the distribution function of the gas at rest by replacing the quasiparticle energy ϵ_p with ($\epsilon_p - \mathbf{pv}$), where \mathbf{p} is the quasiparticle momentum. Hence, the total momentum of the gas of quasiparticles per unit volume is given by

$$\mathbf{P} = \int \mathbf{p} N(\epsilon_p - \mathbf{p}\mathbf{v}) \frac{d^3 p}{(2\pi\hbar)^3}.$$
(6.14)

Assuming that the velocity \mathbf{v} is small we expand the distribution function $N(\epsilon_p - \mathbf{pv})$ in powers of \mathbf{v} . The integration of the zero order term gives zero, and the integration of the linear term yields

$$\mathbf{P} = -\int \mathbf{p}(\mathbf{p}\mathbf{v}) \frac{dN(\epsilon_p)}{d\epsilon_p} \frac{d^3p}{(2\pi\hbar)^3} = -\frac{\mathbf{v}}{3} \int \frac{dN(\epsilon_p)}{d\epsilon_p} p^2 \frac{d^3p}{(2\pi\hbar)^3}, \quad (6.15)$$

where we averaged over the directions of **p**. We thus see that the motion of the gas of quasiparticles is accompanied by a transfer of a mass. The transferred mass per unit volume is $\rho_n = P/v$ and is called *normal density*. This is because the gas of quasiparticles collides with the walls, exchanges energy with them, and eventually ceases to move. In this respect the situation is similar to that in an ordinary thermal gas.

So, the Bose-condensed gas (liquid) behaves itself at T > 0 as if it consists of two components: "normal" and "superfluid". The total mass density is $\rho =$ $\rho_n + \rho_s$, where ρ_s is called *superfluid density*. The expression for the normal density ρ_n follows from equation (6.15):

$$\rho_n = \frac{P}{v} = -\frac{1}{3} \int \frac{dN(\epsilon_p)}{d\epsilon_p} p^2 \frac{d^3p}{(2\pi\hbar)^3}.$$
 (6.16)

At T = 0 we have $N(\epsilon_p) = 0$ and $\rho_n = 0$ so that the whole liquid is superfluid and $\rho_s = \rho$. This shows that ρ_n does not coincide with the non-condensed density, and ρ_s does not coincide with the density of the condensate. This is clearly seen from the calculation of ρ_n at $T \ll \mu = ng$, where one can put $\epsilon_p = pc_s$. On the basis of Eq. (6.16), integrating in parts and using Eq. (5.31) for the distribution function $N(\epsilon_p)$ we find:

$$\rho_n = \frac{2}{3\pi^2 \hbar^3 c_s} \int_0^\infty N(\epsilon_p) p^3 dp = \frac{2\pi^2 \hbar}{45c_s} \left(\frac{T}{\hbar c_s}\right)^4.$$
(6.17)

The normal density behaves as $\rho_n \propto T^4$, whereas we found earlier that the noncondensed density at such temperatures contains a temperature-independent term $n'(T = 0) \propto n(na^3)^{1/2}$ originating from quantum fluctuations, and the term $n'_T \propto T^2$ related to thermal fluctuations.

At temperatures $T \gg \mu = ng$ one may put $\epsilon_p = p^2/2m$. Then, after integrating in parts, Eq. (6.16) gives

$$\rho_n = m \int N(\epsilon_p) \frac{d^3 p}{(2\pi\hbar)^3} = m \left(\frac{mT}{2\pi\hbar^2}\right)^{3/2} \zeta(3/2),$$
(6.18)

and ρ_n/m coincides with the non-condensed density n'_T (6.7). For obtaining the difference between n' and ρ_n/m at $T \gg ng$ one should calculate higher order corrections to both quantities.

6.3 Beyond Bogoliubov. Beliaev damping of elementary excitations

Let us now discuss how accurate is the picture of Bogoliubov elementary excitations that we obtained by diagonalizing a bilinear (in $\hat{\Psi}'$) Hamiltonian \hat{H}_B (5.2). So, we substituted $\hat{\Psi} = \Psi_0 + \hat{\Psi}'$ into the total Hamiltonian \hat{H} (2.45) and kept the terms independent of $\hat{\Psi}'$ and quadratic in $\hat{\Psi}'$ (linear terms vanish due to the Gross-Pitaevskii equation). After diagonalizing the resulting Hamiltonian \hat{H}_B , it takes the form (5.9). However, we omitted the terms that are qubic and fourth-power in $\hat{\Psi}'$. At temperatures $T \ll T_c$ where the non-condensed fraction is small, the fourth-power terms are much less important than the qubic terms and will also be omitted here. The qubic terms give the following contribution to the Hamiltonian:

$$\hat{H}^{(3)} = \int g\{\Psi_0^*(\mathbf{r},t)\hat{\Psi}^{\prime\dagger}(\mathbf{r},t)\hat{\Psi}^{\prime}(\mathbf{r},t)\hat{\Psi}^{\prime}(\mathbf{r},t) + \Psi_0(\mathbf{r},t)\hat{\Psi}^{\prime\dagger}(\mathbf{r},t)\hat{\Psi}^{\prime\dagger}(\mathbf{r},t)\hat{\Psi}^{\prime}(\mathbf{r},t)\}d^3r.$$
(6.19)

So, after making the Bogoliubov procedure we actually have the Hamiltonian

$$\hat{H} = E_0 + \sum_{\nu} \epsilon_{\nu} \hat{b}^{\dagger}_{\nu} \hat{b}_{\nu} + \hat{H}^{(3)}.$$
(6.20)

The Hamiltonian term $\hat{H}^{(3)}$ describes the interaction of elementary excitations with each other. Using the Bogoliubov transformation (5.3) and assuming that $\Psi_0 = \psi_0(\mathbf{r}) \exp(-i\mu t/\hbar)$ with $\psi_0(\mathbf{r})$ being real, it takes the form:

$$\hat{H}^{(3)} = g \int d^3 r \psi_0(\mathbf{r}) \sum_{\nu_1, \nu_2, \nu_3} \{ u_{\nu_1}^* \hat{b}_{\nu_1}^\dagger \exp(i\epsilon_{\nu_1} t/\hbar) - v_{\nu_1} \hat{b}_{\nu_1} \exp(-i\epsilon_{\nu_1} t/\hbar) \}$$

$$\times \{ (u_{\nu_2}^* - v_{\nu_2}^*) \hat{b}_{\nu_2}^\dagger \exp(i\epsilon_{\nu_2} t/\hbar) + (u_{\nu_2} - v_{\nu_2}) \hat{b}_{\nu_2} \exp(-i\epsilon_{\nu_2} t/\hbar) \}$$

$$\times \{ u_{\nu_3} \hat{b}_{\nu_3} \exp(-i\epsilon_{\nu_3} t/\hbar) - v_{\nu_3}^* \hat{b}_{\nu_3}^\dagger \exp(i\epsilon_{\nu_3} t/\hbar) \}.$$
(6.21)

The Hamiltonian $\hat{H}^{(3)}$ is qubic in the operators \hat{b}_{ν} , which leads to a shift of the eigenenergies of the excitations and to their damping. We will discuss the damping rates and, hence, omit the terms creating or annihilating three excitations as such processes do not satisfy the energy conservation law and do not contribute to these rates.

Let us discuss the uniform case, where $\psi_0(\mathbf{r}) = \sqrt{n_0}$, the index ν is the particle momentum **k**, and the functions u_{ν}, v_{ν} are given by Eqs. (5.10), (5.11), (5.17), and (5.18). Then, integrating over d^3r we rewrite equation (6.21) as

$$\hat{H}^{(3)} = \frac{g\sqrt{n_0}}{2\sqrt{\mathcal{V}}} \sum_{\mathbf{k},\mathbf{p}} \{3f_p^- f_{|\mathbf{p}-\mathbf{k}|}^- f_k^- + f_p^+ f_{|\mathbf{p}-\mathbf{k}|}^+ f_k^- + f_p^+ f_{|\mathbf{p}-\mathbf{k}|}^- f_k^+ - f_p^- f_{|\mathbf{p}-\mathbf{k}|}^+ f_k^+ \}$$
$$\times \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{p}-\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{p}} \exp[i(\epsilon_p - \epsilon_k - \epsilon_{|\mathbf{p}-\mathbf{k}|})t/\hbar] + h.c.$$
(6.22)

where the functions f_k^{\pm} are given by

$$f_k^{\pm} = u_k \pm v_k = \left(\frac{\epsilon_k}{E_k}\right)^{\pm 1/2}.$$
(6.23)

We now consider T = 0 and calculate the damping rate for a phonon with momentum **p** which was created "by hands" in the system. In the phonon branch of the Bogoliubov spectrum one has $\epsilon_p = \hbar c_s p$, and from the form of the Hamiltonian $\hat{H}^{(3)}$ (6.22) we conclude that the phonon can decay into two other phonons with lower energies and momenta (see Fig.6.1). Besides the momentum conservation, one has the energy conservation law:

$$\epsilon_p = \epsilon_{|\mathbf{p}-\mathbf{k}|} + \epsilon_k \tag{6.24}$$

and we see that in the phonon branch of the spectrum the vectors \mathbf{p} , \mathbf{k} , and $\mathbf{p}-\mathbf{k}$ are practically parallel to each other. Indeed, writing the phonon dispersion relation for each of the phonons shown in Fig.6.1 we obtain $p = k + |\mathbf{p} - \mathbf{k}|$ or

$$p^{2} + k^{2} - 2pk = p^{2} + k^{2} - 2pk\cos\theta, \qquad (6.25)$$



Figure 6.1: Diagram for the decay of a phonon with momentum \mathbf{p} into two other phonons. The red wiggle line indicates that the phonon-phonon interaction occurs through the condensate as is seen from the Hamiltonian (6.22).

where θ is the angle between the vectors **p** and **k**. Equation (6.25) shows that $\cos \theta = 1$, and writing the dispersion relation more exactly one finds that $\cos \theta$ is slightly smaller than unity.

The damping rate will be calculated assuming that $\hat{H}^{(3)}$ is small and using the Fermi golden rule. In the Heisenberg picture one should write the following expression for the damping rate:

$$\Gamma_p = \frac{1}{\hbar^2} \sum_f \int_{-\infty}^{+\infty} H_{if}(0) H_{if}(t) dt, \qquad (6.26)$$

where the indices *i* and *f* label initial and final states of the transition, and $H_{if}(t) = \langle i | \hat{H}^{(3)} | f \rangle$ are the transition matrix elements. In our case the initial state is the ground state BEC gas plus a phonon with momentum **p**, and in the final state instead of this phonon we have two phonons, with momenta **k** and **p** - **k**, respectively. Using Eq. (6.22) for $\hat{H}^{(3)}$ and integrating over dt in Eq. (6.26) we immediately get

$$\Gamma_p = \frac{2\pi}{\hbar} \sum_{\mathbf{k}} |\langle \mathbf{k}, \, \mathbf{p} - \mathbf{k} | \hat{H}^{(3)}(0) | \mathbf{p} \rangle|^2 \delta(\epsilon_p - \epsilon_k - \epsilon_{|\mathbf{p} - \mathbf{k}|}), \tag{6.27}$$

where $\hat{H}^{(3)}(0)$ is given by Eq. (6.22) with t = 0 so that Eq. (6.27) represents the Fermi golden rule in the Schroedinger picture. We also notice that due to the energy conservation law the contribution of three last terms in the curly brackets in Eq. (6.22) is equal to the contribution of the first term. This is easily established recalling that the free particle energy E_k is expressed through the Bogoliubov energy ϵ_k (5.16) as $E_k = \sqrt{\epsilon_k^2 + ng} - ng$, and in the phonon branch where $\epsilon_k \ll ng$ we have $E_k = \epsilon_k^2/2ng - \epsilon_k^4/8n^3g^3$. Then, taking into account that occupation numbers for excitations with momenta **k** and **p** - **k** are zero at T = 0 (the phonon with momentum **p** was created "by hands"), we obtain:

$$\Gamma_p = \frac{2\pi}{\hbar} \times 9ng^2 \int_0^\infty \frac{2\pi k^2 dk}{(2\pi)^3} \int_{-1}^1 d\cos\theta \, \frac{E_p E_k E_{|\mathbf{p}-\mathbf{k}|}}{\epsilon_p \epsilon_k \epsilon_{|\mathbf{p}-\mathbf{k}|}} \delta(\epsilon_p - \epsilon_k - \epsilon_{|\mathbf{p}-\mathbf{k}|}). \tag{6.28}$$

Taking into account that one may put $E_k = \epsilon_k^2/2ng$ for any momentum in the integrand of Eq. (6.28) and substituting $|\mathbf{p} - \mathbf{k}| = \sqrt{p^2 + k^2 - 2pk\cos\theta}$, after integrating over $d\cos\theta$ we find:

$$\Gamma_p = \frac{9}{16\pi} \frac{g}{\hbar} \left(\frac{\hbar c_s}{ng}\right)^2 \int_0^p k^2 (p-k)^2 dk.$$
(6.29)

We now have to divide the final result by a factor of 2 in order to avoid double counting of phonon pairs with momenta \mathbf{k} and $\mathbf{p} - \mathbf{k}$. The final result reads:

$$\Gamma_p = \frac{3g}{320\pi\hbar} \left(\frac{\hbar c_s}{ng}\right)^2 p^5 = \frac{3}{320\pi} \frac{\hbar}{mn} p^5.$$
(6.30)

Since we consider the phonon branch of the spectrum where $\epsilon_p = \hbar c_s p \ll \mu = ng$, recalling that $g = 4\pi \hbar^2 a/m$, we can rewrite Eq. (6.30) in the form

$$G_p = \frac{3\sqrt{\pi}}{40} (na^3)^{1/2} \left(\frac{\epsilon_p}{ng}\right)^4 \frac{\epsilon_p}{\hbar}.$$
(6.31)

The discussed damping mechanism is called Beliaev damping. It is rather slow at $T \to 0$. Even close to the border of the phonon branch, i.e. for ϵ_p approaching ng, a characteristic damping time Γ_p^{-1} is of the order of seconds at densities $n \approx 2 \times 10^{14} \text{ cm}^{-3}$ typical for experiments with ⁸⁷Rb where $a \approx 50$ Å.

6.4 Landau damping. Small parameter of the theory at finite temperatures

At finite temperatures one has a more important damping mechanism, the socalled Landau damping which we will discuss for phonons in the uniform case. According to this mechanism, a phonon (created "by hands") interacts with a thermal excitation, both get annihilated, and an excitation with a higher energy is created (see Fig.6.2). Using again the Fermi golden rule we assume that the number of phonons (created "by hands") with momentum \mathbf{p} is N_p and that the occupation numbers of thermal excitations are given by the Bose distribution relation (5.31). Then, in a similar way as in the derivation of Eq. (6.27), we obtain

$$\frac{dN_p}{dt} = -\frac{2\pi N_p}{\hbar} \int \frac{d^3k}{(2\pi)^3} \{ |\langle \mathbf{p} + \mathbf{k} | \hat{H}^{(3)} | \mathbf{p}, \mathbf{k} \rangle|^2 - |\langle \mathbf{p}, \mathbf{k} | \hat{H}^{(3)} | \mathbf{p} + \mathbf{k} \rangle|^2 \}$$

$$\delta(\epsilon_{|\mathbf{p}+\mathbf{k}|} - \epsilon_p - \epsilon_k).$$
(6.32)

We consider for simplicity temperatures $T \gg \mu = ng$ and present the result without derivation which is transferred to the section of Problems. The damping rate Γ_p is obtained from Eq. (6.32) as

$$\Gamma_p = -\frac{1}{N_p} \frac{dN_p}{dt},\tag{6.33}$$

and the expression for this quantity reads:

$$\Gamma_p = \frac{\epsilon_p}{\hbar} \frac{3\pi^{3/2}}{4} \frac{T}{ng} (na^3)^{1/2}.$$
(6.34)



Figure 6.2: Diagram for the Landau dampuing of a phonon with momentum **p**. The red wiggle line indicates that the phonon-phonon interaction occurs through the condensate.

The perturbation theory for a Bose-condensed gas assumes that Bogoliubov quasiparticles are good elementary excitations and the qubic Hamiltonian term $\hat{H}^{(3)}$ leads to small energy shifts and damping rates. So, we should have the inequality $\hbar\Gamma_p \ll \epsilon_p$. According to Eq. (6.33), at $T \gg ng$ this requires the condition

$$\frac{T}{ng} (na^3)^{1/2} \ll 1, \tag{6.35}$$

which is much stronger than the inequality $(na^3)^{1/2} \ll 1$ obtained in *Lecture 5* for $T \to 0$.

We should also make here an important remark. The treatment of damping that we have done requires the relaxation time τ_{rel} of thermal excitations to be slow. One should at least have

$$\frac{\epsilon_p}{\hbar} \gg \frac{1}{\tau_{\rm rel}}.$$
 (6.36)

In this case we may assume that the phonons (created "by hands") do not disturb the thermal distribution in the cloud. This is usually identified as the collisionless regime. For the Landau damping the most important are thermal excitations with energies $\sim \mu$. Their relaxation rate according to Eq. (6.34) is

$$\Gamma_{\mu} = \tau_{\rm rel}^{-1} \sim \frac{T}{\hbar} (na^3)^{1/2}.$$
(6.37)

So, the collisionless regime that we actually consider here is realized for excitations with energies

$$\epsilon_p \gg T(na^3)^{1/2}.\tag{6.38}$$

Problems 6

6.1 Calculate the rate of Landau damping for a phonon with momentum p in a uniform finite-temperature Bose-condensed gas. Assume that $T \gg \mu$ and the thermal cloud is in the collisionless regime.

According to equations (6.32) and (6.33), the rate of Landau damping is given by

$$\Gamma_p = \frac{2\pi}{\hbar} \int \frac{d^3k}{(2\pi)^3} \{ |\langle \mathbf{p} + \mathbf{k} | \hat{H}^{(3)} | \mathbf{p}, \mathbf{k} \rangle|^2 - |\langle \mathbf{p}, \mathbf{k} | \hat{H}^{(3)} | \mathbf{p} + \mathbf{k} \rangle|^2 \} \delta(\epsilon_{|\mathbf{p}+\mathbf{k}|} - \epsilon_p - \epsilon_k).$$
(6.39)

The transition matrix elements can be expressed as

$$\langle \mathbf{p} + \mathbf{k} | \hat{H}^{(3)} | \mathbf{p}, \mathbf{k} \rangle = \sqrt{(N_k (N_{|\mathbf{p}+\mathbf{k}|} + 1))} H_{\text{int}}, \qquad (6.40)$$

$$\langle \mathbf{p}, \mathbf{k} | \hat{H}^{(3)} | \mathbf{p} + \mathbf{k} \rangle = \sqrt{(N_k + 1)N_{|\mathbf{p}+\mathbf{k}|}} H_{\text{int}},$$
 (6.41)

where

$$H_{\rm int} = \frac{g\sqrt{n}}{2\sqrt{\mathcal{V}}} \{3f_p^- f_{|\mathbf{p}+\mathbf{k}|}^- f_k^- + f_p^+ f_{|\mathbf{p}+\mathbf{k}|}^+ f_k^- + f_p^- f_{|\mathbf{p}+\mathbf{k}|}^+ f_k^+ - f_p^+ f_{|\mathbf{p}+\mathbf{k}|}^- f_k^+ \}.$$
(6.42)

Thus, Eq. (6.39) is transformed to

$$\Gamma_p = \frac{2\pi}{\hbar} \int \frac{\mathcal{V}d^3k}{(2\pi)^3} |H_{\rm int}|^2 (N_k - N_{|\mathbf{p}+\mathbf{k}|}) \delta(\epsilon_{|\mathbf{p}+\mathbf{k}|} - \epsilon_p - \epsilon_k).$$
(6.43)

The energy conservation law reads:

$$\epsilon_{|\mathbf{p}+\mathbf{k}|} = \epsilon_p + \epsilon_k. \tag{6.44}$$

Taking into account Eq. (6.44) the calculation of $H_{\rm int}$ yields

$$H_{\rm int} = \frac{g\sqrt{n}}{2\sqrt{\mathcal{V}}} \left\{ 3 \left(\frac{E_{|\mathbf{p}+\mathbf{k}|} E_p E_k}{\epsilon_{|\mathbf{p}+\mathbf{k}|} \epsilon_p \epsilon_k} \right)^{1/2} \left(\frac{\epsilon_{|\mathbf{p}+\mathbf{k}|} \epsilon_p E_k}{E_{|\mathbf{p}+\mathbf{k}|} E_p \epsilon_k} \right)^{1/2} \left(\frac{\epsilon_{|\mathbf{p}+\mathbf{k}|} E_k E_p}{E_p E_k \epsilon_{|\mathbf{p}+\mathbf{k}|}} \right)^{1/2} \left(\frac{\epsilon_p \epsilon_k E_{|\mathbf{p}+\mathbf{k}|}}{E_p E_k \epsilon_{|\mathbf{p}+\mathbf{k}|}} \right)^{1/2} \right\}$$
$$= \frac{g\sqrt{n}}{2\sqrt{\mathcal{V}}} \left\{ \left(\frac{3E_k}{\epsilon_k} + \frac{\epsilon_k}{E_k} \right) \left(\frac{E_p}{\epsilon_p} \right)^{1/2} + \frac{\epsilon_p E_k - \epsilon_p \epsilon_k \partial E_k / \partial \epsilon_k}{E_k \epsilon_k} \left(\frac{\epsilon_p}{E_p} \right)^{1/2} \right\}. \quad (6.45)$$

Here, assuming that $p \ll k$ we put $E_{|\mathbf{p}+\mathbf{k}|} = E_k$ and $\epsilon_{|\mathbf{p}+\mathbf{k}|} = \epsilon_k$ in the terms proportional to $(E_p/\epsilon_p)^{1/2}$. In the terms proportional to $(\epsilon_p/E_p)^{1/2}$ we use Eq. (6.44) for $\epsilon_{|\mathbf{p}+\mathbf{k}|}$ and put

$$E_{|\mathbf{p}+\mathbf{k}|} = E_k + \epsilon_p \frac{\partial E_k}{\partial \epsilon_k}$$

Since $E_k = \sqrt{\epsilon_k^2 + \mu^2} - \mu$ with $\mu = ng$, we have

$$\frac{\partial E_k}{\partial \epsilon_k} = \frac{\epsilon_k}{\sqrt{\epsilon_k^2 + \mu^2}} = \frac{\epsilon_k}{E_k + \mu}.$$

Then, taking into account that $\epsilon_p, E_p \ll \mu$, Eq. (6.45) is reduced to

$$H_{\rm int} = \frac{g\sqrt{n}}{2\sqrt{\mathcal{V}}} \left(\frac{E_p}{\epsilon_p}\right)^{1/2} \left\{ \left(\frac{3E_k}{\epsilon_k} + \frac{\epsilon_k}{E_k}\right) - \frac{2\mu^2}{\epsilon_k(E_k + \mu)} \right\} = g\sqrt{\frac{n}{\mathcal{V}}} \left(\frac{E_p}{\epsilon_p}\right)^{1/2} \frac{E_k}{\epsilon_k} \left(2 + \frac{\mu}{E_k + \mu}\right). \quad (6.46)$$

The equilibrium occupation numbers depend only on the energies of the excitations. Hence, for $p \ll k$ we can write

$$N_{|\mathbf{p}+\mathbf{k}|} = N_k + \frac{\partial N_k}{\partial \epsilon_k} \epsilon_p. \tag{6.47}$$

Substituting H_{int} (6.46) and $N_{|\mathbf{p}+\mathbf{k}|}$ (6.47) into Eq. (6.43) and integrating over the angle between \mathbf{k} and \mathbf{p} we obtain

$$\Gamma_p = \frac{ng^2}{2\pi\hbar} \frac{E_p}{p} \int_0^\infty k^2 dk \, \frac{m\epsilon_k}{\hbar^2 k(E_k+\mu)} \frac{E_k^2}{\epsilon_k^2} \left(2 + \frac{\mu}{E_k+\mu}\right)^2 \left(-\frac{\partial N_k}{\partial \epsilon_k}\right). \quad (6.48)$$

The main contribution to the integral in Eq. (6.48) comes from excitations with energies $\epsilon_k \sim \mu$. Thus, considering temperatures $T \gg \mu$ we can write $N_k = T/\epsilon_k$ and, hence, $\partial N_k/\partial \epsilon_k = -T/\epsilon_k^2$. Then, turning to a dimensionless variable $x = \mu/\epsilon_k$ Eq. (6.48) is transformed to

$$\Gamma_p = \frac{mg^2 nT}{4\pi\mu\hbar^3 c_s} \frac{\epsilon_p}{\hbar} \int_0^\infty \frac{dx}{1+x^2} \left(\sqrt{1+x^2} - x\right)^2 \left(2 + \frac{x}{\sqrt{1+x^2}}\right)^2, \quad (6.49)$$

and with $g = 4\pi \hbar^2 a/m$ and $\mu = ng$ we eventually obtain:

$$\Gamma_p = \frac{3\pi^{3/2}}{4} \frac{\epsilon_p}{\hbar} \frac{T}{ng} (na^3)^{1/2}.$$
(6.50)

This is equation (6.34) given in *Lecture* 6 without derivation. So, in order to have the inequality $\hbar\Gamma_p \ll \epsilon_p$, which is necessary for the applicability of the perturbation theory, at $T \gg ng$ we should have a small parameter $(T/ng)(na^3)^{1/2} \ll 1$ as given by Eq. (6.35).

6.2 An impurity particle is moving in a weakly interacting Bose-condensed gas with an initial velocity v. The gas is at T = 0. The impurity can create excitations and loose its energy. Calculate how the kinetic energy of the impurity decreases with time.

7.1 Vortices in rotating and non-rotating superfluids. Circulation

In this *Lecture* we discuss macroscopically excited Bose-condensed states - vortices, that is the states with an orbital angular momentum. First, we give several qualitative arguments. Let us consider a vessel with a Bose liquid and rotate it with an angular velocity (frequency) Ω (see Fig.7.1). Only the normal component starts to rotate with the vessel due to friction. The superfluid component stays at rest. So, at T = 0 where the whole liquid is superfluid, nothing happens and the liquid does not move.



Figure 7.1: Rotating vessel with a superfluid.

However, at sufficiently large Ω this state becomes energetically unfavorable. The condition of equilibrium is that the energy in the rotating frame,

$$E_{\rm rot} = E - L_z \Omega, \tag{7.1}$$

is minimum, where E and L_z are the energy and orbital angular momentum in the lab frame. It is the term $-L_z\Omega < 0$ that can induce a superfluid motion at large Ω . This looks as a violation of the irrotational character of the superfluid motion expressed by

$$\operatorname{curl} \mathbf{v}_s = 0. \tag{7.2}$$

Excitations are density waves and there can be nothing else than Eq. (7.2). One should have in mind that the condition (7.2) is violated only at (microscopically) narrow lines which have measure zero and are called "vortex lines". Around these lines a superfluid undergoes a "potential rotation".

Let us calculate the circulation of the superfluid velocity around a vortex line:

$$\oint \mathbf{v}_s d\mathbf{l} = \oint \frac{\hbar}{m} \nabla S \, d\mathbf{l} = \frac{2\pi\hbar}{m} s. \tag{7.3}$$

The quantity S is given by

$$S(\mathbf{r},t) = \frac{1}{\hbar} \left[m\mathbf{v}\mathbf{r} - \left(\frac{1}{2}mv^2 + \mu\right)t \right], \qquad (7.4)$$

where one may put $\mathbf{v} = \mathbf{v}_s$. Note that the expression

$$\Psi(\mathbf{r} - \mathbf{v}t, t) \exp\{iS(\mathbf{r}, t)\}$$

gives a Galilean transformation for the field operator (and Ψ_0). So, in the reference frame where the fluid moves with velocity \mathbf{v} , the condensate wavefunction becomes

$$\Psi_0 = \sqrt{n_0} \exp(iS).$$

Hence, the superfluid velocity is

$$\mathbf{v}_s = \frac{\hbar}{m} \nabla S,$$

and in order to have Ψ_0 single valued one should have integer s. Thus, the circulation is quantized in units of \hbar/m .

Consider now a straight vortex line along the symmetry axis z of the vessel in Fig.7.1. The streamlines of \mathbf{v}_s are circles in planes perpendicular to z. From Eq. (7.3) we have

$$v_s = s \frac{\hbar}{mr},\tag{7.5}$$

where r is the distance from the line. Note that v_s (7.5) is quite different from the velocity $v = \Omega r$ associated with a rapid rotation.

The angular momentum of the fluid is easily calculated:

$$L_z = \int \rho_s v_s r d^3 r = \pi s \mathcal{R}^2 \mathcal{L} \frac{\hbar \rho_s}{m}, \qquad (7.6)$$

with \mathcal{R} and \mathcal{L} being the radius and length of the vessel. The energy associated with the vortex line is dominated by the kinetic energy and is given by

$$E_v = \int \frac{1}{2} \rho_s v_s^2 d^3 r = \pi \rho_s s^2 \mathcal{L} \left(\frac{\hbar}{m}\right)^2 \ln\left(\frac{\mathcal{R}}{r_c}\right), \qquad (7.7)$$

where r_c is the size of the vortex core representing the low-distance cut-off for the integration over dr in Eq. (7.7).

The critical value Ω_c above which the vortex state becomes energetically favorable follows from the condition

$$E_{\rm rot} = E_v - \Omega_c L_z = 0. \tag{7.8}$$

Using Eqs. (7.6) and (7.7) this gives

$$\Omega_c = \frac{E_v}{L_z} = \frac{\hbar}{m\mathcal{R}^2} \ln\left(\frac{\mathcal{R}}{r_c}\right) \tag{7.9}$$

for |s| = 1. Note that the states with |s| > 1 are unstable. For the same Ω the state with two single-charged vortices (|s| = 1) has lower energy than the state with one double-charged vortex (vortex with |s| = 2).

For a large rotation frequency, $\Omega \gg \Omega_c$, one can estimate the equilibrium number of vortices per unit area minimizing the energy. According to Eq. (7.3) we have

$$\oint \mathbf{v}_s d\mathbf{l} = 2\pi N_v \frac{\hbar}{m},\tag{7.10}$$

where N_v is the number of vortices inside a contour around the surface area A. On the other hand, for a large N_v we may use the relations for a rotating rigid body. The rotation of a rigid body leads to $v_s = \Omega r$ and $|\text{curl}\mathbf{v}_s| = 2\Omega$. So, one has $\oint \mathbf{v}_s d\mathbf{l} = 2\Omega A$, which gives the number of vortices per unit area

$$n_v = \frac{N_v}{A} = \frac{m\Omega}{\pi\hbar}.$$
(7.11)

7.2 Gross-Pitaevskii equation for the vortex state

We now turn to the description of the vortex state on the basis of the Gross-Pitaevskii equation and consider a single vortex with |s| = 1 in free space, assuming that the vortex line is a straight line along the z-axis. Since we search for the solution with orbital angular momentum l = 1, the condensate wavefunction has the form

$$\psi_0 = \sqrt{n_0} f(r) \exp(i\phi), \qquad (7.12)$$

with the function f depending only on the distance $r = \sqrt{x^2 + y^2}$ from the vortex line, and ϕ being the angle around it. In our case the Laplacian takes the form

$$\Delta_{\mathbf{r}} = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2},$$

and using Eq. (7.12) the stationary Gross-Pitaevskii equation (3.9) is transformed to the following equation for the function f:

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{1}{r^2}\right)f + n_0g|f|^2f - \mu f = 0.$$
(7.13)

Putting $\mu = n_0 g$ and introducing a dimensionless coordinate $\tilde{r} = r/\sqrt{2}\xi$, with $\xi = \hbar/\sqrt{m\mu}$ being the healing length, we have:

$$\frac{d^2f}{d\tilde{r}^2} + \frac{1}{\tilde{r}}\frac{df}{d\tilde{r}} - \frac{f}{\tilde{r}^2} - f^3 + f = 0,$$
(7.14)

where we assume that f is real. For $\tilde{r} \to 0$ and $\tilde{r} \to \infty$ we obtain

$$f \propto \tilde{r}, \quad \tilde{r} \to 0;$$
 (7.15)

$$f \propto \left(1 - \frac{1}{2\tilde{r}^2}\right), \quad \tilde{r} \to \infty.$$
 (7.16)

The numerically calculated function $f(\tilde{r})$ is displayed in Fig.7.2. One clearly sees that the radius of the vortex core is $r_c \sim \xi$ so that substituting $\mu = n_0 g$ and $g = 4\pi\hbar^2 a/m$ we have $r_c \sim 1/\sqrt{n_0 a}$. Recalling that $n_0 a^3 \ll 1$ we find $r_c \gg n_0^{-1/3}$, i.e. there are many particles inside the vortex core. This is the condition that is necessary for the validity of the Gross-Pitaevskii equation at $r \lesssim r_c$.



Figure 7.2: The function $f(\tilde{r})$.

The vortex state is a macroscopically excited BEC state, i.e. all particles are in the same excited quantum state. It has a topological quantum number, circulation, so that it can not decay in the bulk. The vortex can only decay when going to the border of the system.

7.3 Excitations of the vortex state. Fundamental modes

Let us now discuss elementary excitations around the vortex state. The Bogoliubovde Gennes equations for the vortex in free space are given by Eqs. (5.7) and (5.8) with $V(\mathbf{r}) = 0$ and they read:

$$\left(-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + 2g|\psi_0|^2 - \mu\right)u_{\nu} - g\psi_0^2 v_{\nu} = \epsilon_{\nu}u_{\nu}$$
(7.17)

$$\left(-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + 2g|\psi_0|^2 - \mu\right)v_{\nu} - g\psi_0^{*2}u_{\nu} = -\epsilon_{\nu}v_{\nu}$$
(7.18)

Far from the vortex line we may put $\psi_0 = \sqrt{n_0} \exp(i\phi)$ and omit all centrifugal terms (the terms proportional to $1/r^2$). Then, setting

$$u_{\nu} = \tilde{u}_{\nu} \exp(i\phi) \tag{7.19}$$

$$v_{\nu} = \tilde{v}_{\nu} \exp(-i\phi), \qquad (7.20)$$

where \tilde{u}_{ν} , \tilde{v}_{ν} can also depend on ϕ , we get equations for the excitation modes \tilde{u}_{ν} , \tilde{v}_{ν} rotationg together with the superfluid. The excitation energies and wave-functions will be the same as without a vortex.

However, on approach to the vortex line the situation changes. Due to the absence of translational invariance the momentum \mathbf{k} is no longer a good quantum number. The excitation incident on the vortex with momentum \mathbf{k} can be scattered with a different momentum \mathbf{k}' . We will discuss this issue in the problem section.

Let us now consider the behavior of excitations near the vortex line and, moreover, analyze excitations related to the motion of the vortex line. In order to gain insight into the problem it is convinient to find first the so-called fundamental modes, that is the modes with $\epsilon_{\nu} = 0$. Assuming that the functions u, v are independent of the coordinate z along the straight vortex line we write the Bogoliubov-de Gennes equations (7.17) and (7.18) for these modes as

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2} \right) u_{\nu} + 2g|\psi_0||^2 u_{\nu} - g\psi_0^2 v_{\nu} - \mu u_{\nu} = 0;(7.21)$$
$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2} \right) v_{\nu} + 2g|\psi_0|^2 v_{\nu} - g\psi_0^{*2} u_{\nu} - \mu v_{\nu} = 0.(7.22)$$

An obvious fundamental mode is the one with $u = \sqrt{n_0} \exp(i\phi) = \psi_0$ and $v = \sqrt{n_0} \exp(-i\phi) = \psi_0 \exp(-2i\phi)$, and it trivially reproduces ψ_0 . The fundamental mode that will be of interest for us is the mode with

$$u = \frac{1}{\sqrt{4\pi\mathcal{L}}} \left(\frac{f}{r} + \frac{\partial f}{\partial r}\right),\tag{7.23}$$

$$v = \frac{1}{\sqrt{4\pi\mathcal{L}}} \left(\frac{f}{r} - \frac{\partial f}{\partial r}\right) \exp(-2i\phi), \qquad (7.24)$$

where the function f is expressed through the condensate wavefunction by Eq. (7.12) and obeys the Gross-Pitaevskii equation (7.13), and \mathcal{L} is the length of the vortex line in the z-direction. One can easily check that the u, v-functions of Eqs. (7.23) and (7.24) satisfy the normalization condition (5.6) and the Bogoliubov-de Gennes equations (7.21) and (7.22). Indeed, substituting u (7.23)

and v (7.24) into equations (7.21) and (7.22) we represent them in the form

$$\begin{bmatrix} -\frac{\hbar^2}{2m} \left(\frac{d^3f}{dr^3} + \frac{1}{r} \frac{d^2f}{dr^2} - 2\frac{df}{dr} + 2\frac{f}{r^3} \right) + 3n_0gf^2\frac{df}{dr} - \mu\frac{df}{dr} \end{bmatrix} + \begin{bmatrix} -\frac{\hbar^2}{2m} \left(\frac{1}{r} \frac{d^2f}{dr^2} + \frac{1}{r^2} \frac{df}{dr} - \frac{f}{r^3} \right) + n_0g\frac{f^3}{r} - \mu\frac{f}{r} \end{bmatrix} = 0.$$
(7.25)
$$\begin{bmatrix} \frac{\hbar^2}{2m} \left(\frac{d^3f}{dr^3} + \frac{1}{r} \frac{d^2f}{dr^2} - 2\frac{df}{dr} + 2\frac{f}{r^3} \right) - 3n_0gf^2\frac{df}{dr} + \mu\frac{df}{dr} \end{bmatrix} + \begin{bmatrix} -\frac{\hbar^2}{2m} \left(\frac{1}{r} \frac{d^2f}{dr^2} + \frac{1}{r^2} \frac{df}{dr} - \frac{f}{r^3} \right) + n_0g\frac{f^3}{r} - \mu\frac{f}{r} \end{bmatrix} = 0.$$
(7.26)

The first term in square brackets in each of the obtained equations is nothing else than equation (7.13) differentiated with respect to r, and the second term is the same Eq. (7.13) divided by r. Thus, equalities (7.25) and (7.26) are automatically satisfied.

Going back to Eqs. (7.19) and (7.20) we see that the Bogoliubov functions (7.23) and (7.24) of the fundamental mode under consideration, in the reference frame rotating with the superfluid are $\{\tilde{u}, \tilde{v}\} \propto \exp(-i\phi)$. Thus, this mode describes a rotation in the direction opposite to the rotation direction of the superfluid.

It is worth noting that there is another fundamental mode:

$$u = C\left(\frac{f}{r} - \frac{\partial f}{\partial r}\right) \exp(2i\phi),$$
$$v = C\left(\frac{f}{r} + \frac{\partial f}{\partial r}\right),$$

with C being a normalization constant. This mode describes a rotation in the same direction in which the superfluid rotates. However, the norm $\int (|u|^2 - |v|^2) d^3r$ for this mode is negative and it has to be omitted.

7.4 Kelvin modes and vortex contrast

We now try to understand the physical meaning of the obtained fundamental mode. Let us assume that the motion in the z-direction is also excited and

$$u_{\nu} = \bar{u}_q \exp(iqz) \tag{7.27}$$

$$v_{\nu} = \bar{v}_q \exp(iqz - 2i\phi). \tag{7.28}$$

Then, instead of Eqs. (7.21) and (7.22) we have

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}\right)\bar{u}_q + 2n_0gf^2\bar{u}_q - gn_0f^2\bar{v}_q - \mu\bar{u}_q = \left(\epsilon_q - \frac{\hbar^2q^2}{2m}\right)\bar{u}_q; (7.29)$$
$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}\right)\bar{v}_q + 2n_0gf^2\bar{v}_q - n_0gf^2\bar{u}_q - \mu\bar{v}_q = \left(-\epsilon_q - \frac{\hbar^2q^2}{2m}\right)\bar{v}_q. (7.30)$$

We will consider low wavevectors q satisfying the inequality $q\xi \ll 1$. Then, at distances $r \ll q^{-1}$ we can omit the terms proportional to $(\pm \epsilon_q - \hbar^2 q^2/2m)$. We then return to Eqs. (7.21) and (7.22), and the solution is given by Eqs. (7.23) and (7.24).

At distances where $r \gg \xi$, we may use the asymptotoc expression $f = (1 - \xi^2/4r^2)$ given by Eq. (7.16). Then, putting $\mu = n_0 g$ and $\xi = \hbar \sqrt{mn_0 g}$, and turning to the functions $f_q^{\pm} = \bar{u}_q \pm \bar{v}_q$, equations (7.29) and 7.30) are transformed to

$$-\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{1}{r^2} - q^2\right) f_q^+ = \left(\epsilon_q + \frac{\hbar^2}{mr^2}\right) f_q^-;$$
(7.31)

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} + \frac{1}{r^2} - q^2 + 2n_0g\right)f_q^- = \left(\epsilon_q + \frac{\hbar^2}{mr^2}\right)f_q^+.$$
 (7.32)

Equations (7.31) and (7.32) are valid at any distance $r \gg \xi$, including distances where $q^{-1} \gg r \gg \xi$ and the functions f^+ , f^- follow from Eqs. (7.23) and (7.24). Using $f = (1 - \xi^2/4r^2)$ of Eq. (7.16), equations (7.23) and (7.24) give $|f^-| \ll |f^+|$ and this relation is also expected to be valid at larger r. Then, omitting the terms proportional to f_q^- in Eq. (7.31) we reduce it to the Bessel equation and obtain

$$f_q^+ = \frac{1}{\sqrt{\pi\mathcal{L}}} qK_1(qr), \qquad (7.33)$$

where K_1 is the decaying Bessel function. The normalization coefficient in Eq. (7.33) is chosen such that in the interval of distances $q^{-1} \gg r \gg \xi$ equation (7.33) yields $f_q^+ = 1/\sqrt{\pi \mathcal{L}}r$, which coincides with the result following from Eqs. (7.23) and (7.24).

We then notice that the leading terms in Eq. (7.32) are $2n_0gf_q^-$, ϵf_q^+ , and $(\hbar^2/mr^2)f_q^+$. We thus find

$$f_q^- = \frac{1}{2} \left(\frac{\epsilon_q}{n_0 g} + \frac{\xi^2}{r^2} \right) f_q^+.$$
(7.34)

One can easily check that the main contribution to the normalization integral

$$\int (|\bar{u}_q|^2 - |\bar{v}_q|^2) d^3r = \int f_q^+ f_q^- d^3r = 1$$

comes from distances $r \ll q^{-1}$ and the (small) q-dependent contribution of larger distances practically does not change the normalization coefficient obtained for the fundamental mode.

Note that $K_1(qr) \propto \exp(-qr)$ at $r \to \infty$. So, the modes that we are studying decay exponentially at large distances from the vortex core. These modes describe oscillations of the vortex line, which takes the form of a spiral rotating in the direction opposite to the rotation of the superfluid (see Fig.7.3). Such oscillations are called Kelvin modes or kelvons. They have been discovered by Kelvin (W. Thompson) for classical vortices. The fundamental mode discussed



Figure 7.3: Vortex line (black curve) undergoing Kelvin oscillations and rotating with frequency ϵ/\hbar in the direction opposite to the rotation of the superfluid.

in the previous subsection represents an extreme case of $q \to 0$ and undergoes a power law decay at $r \to \infty$.

For obtaining the dispersion relation for kelvons we return to Eqs. (7.27), (7.28), (7.29) and (7.30) and, putting $\mu = n_0 g$, consider them at distances $r \ll q^{-1}$ where the functions \bar{u}_q and \bar{v}_q follow from Eqs. (7.23) and (7.24) and are given by

$$\bar{u}_q = \frac{1}{4\pi\mathcal{L}}\left(\frac{f}{r} + \frac{df}{dr}\right); \quad \bar{v}_q = \frac{1}{4\pi\mathcal{L}}\left(\frac{f}{r} - \frac{df}{dr}\right).$$

We then multiply Eq. (7.29) by \bar{u}_q , and Eq. (7.30) by \bar{v}_q . Integrating the resulting equations over d^3r we add them to each other. With above written \bar{u}_q and \bar{v}_q , the left hand sides of Eqs. (7.29) and (7.30) give zero, and we obtain:

$$\epsilon_q \int (\bar{u}_q^2 - \bar{v}_q^2) d^3 r = \frac{\hbar^2 q^2}{2m} \int (\bar{u}_q^2 + \bar{v}_q^2) d^3 r.$$
(7.35)

Considering distances $r \ll q^{-1}$ we have to put the limits of integration 0 and $\sim q^{-1}$. Then the integral in the left hand side of Eq. (7.35) is practically equal to the normalization integral and, hence, equals unity. For the integral in the right hand side, we may replace the lower limit of integration by $\sim \xi$ and then

take $\bar{u}_q = \bar{v}_q = (\sqrt{4\pi \mathcal{L}}r)^{-1}$. This gives with logarithmic accuracy:

$$\epsilon_q = \frac{\hbar^2 q^2}{2m} \ln\left(\frac{1}{q\xi}\right). \tag{7.36}$$

The average density profile near the vortex line is influenced by quantum and thermal fluctuations due to kelvons. The density averaged over the z-direction is given by

$$\langle n \rangle = |\psi_0|^2 + \langle \hat{\psi}'^{\dagger} \hat{\psi}' \rangle, \qquad (7.37)$$

where

$$\hat{\psi}' = \sum_{q} [\bar{u}_q(r) \exp(iqz)\hat{b}_q - \bar{v}_q(r) \exp(-iqz + 2i\phi)\hat{b}_q^{\dagger}],$$
(7.38)

with \hat{b}_q , \hat{b}_q^{\dagger} being the creation and annihilation operators of kelvons. We thus obtain:

$$\langle n \rangle = |\psi_0|^2 + \int_{-\infty}^{\infty} \frac{dq}{2\pi} [(\bar{u}_q^2 + \bar{v}_q^2)N_q + \bar{v}_q^2], \qquad (7.39)$$

where $N_q = [\exp(\epsilon_q/T) - 1]^{-1}$ are equilibrium occupation numbers for the kelvons. We thus see that the average density at the vortex core $\langle n(0) \rangle \neq 0$, and the vortex contrast

$$C_v = \frac{\langle n(0) \rangle}{n_0} \tag{7.40}$$

has a non-zero value. The calculation of the vortex contrast due to kelvons is transferred to the problem section.

Problems 7

7.1 Consider a streaight vortex line in a BEC in the trapping geometry of an ideal cylinder (see Fig.7.1). The z-direction is free, and in the x, y-plane one has a harmonic confining potential $V(r) = m\omega^2 r^2/2$, where $r^2 = x^2 + y^2$. Write the condensate wavefunction in the Thomas-Fermi regime assuming that the trap is not rotating. Find an eigenfrequency and wavefunction of an excitation corresponding to the rotation of the vortex line around the z-axis.

As we are looking for the solution of the stationary Gross-Pitaevskii equation with orbital angular momentum 1, we write this equation in the form:

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{1}{r^2}\right)\psi_0 + \frac{m\omega^2 r^2}{2}\psi_0 + g|\psi_0|^2\psi_0 - \mu\psi_0 = 0.$$
(7.41)

In the Thomas-Fermi regime the radius of the trapped BEC in the x, y-plane is $R_{TF} = \sqrt{2\mu/m\omega^2}$. The chemical potential is $\mu \approx n_{max}g$, with n_{max} being the maximum density, and the Thomas-Fermi radius is $R_{TF} \gg \xi$ where $\xi =$ $\sqrt{\hbar^2/m\mu}$ is the size of the vortex core. In this case one can write an approximate solution of Eq. (7.41) as

$$\psi_0 = \sqrt{\frac{\mu}{g}} \psi_{TF}(r) f(r/\xi) \exp(i\phi), \qquad (7.42)$$

where the function $f(r/\xi)$ is determined by Eq. (7.14) and

$$\psi_{TF} = \sqrt{1 - \frac{r^2}{R_{TF}^2}} \tag{7.43}$$

for $r < R_{TF}$ and zero otherwise. The density profile corresponding to the solution (7.42) is displayed in Fig.7.4.



Figure 7.4: Density profile for the vortex state in a trapped condensate.

The mode that we have to find is analogous to the fundamental mode discussed in this *Lecture*. In this mode the vortex line rotates countercklockwise with respect to the BEC (which itself rotates clockwise). So, we have

$$u(r) = \overline{u}; \quad v(r) = \overline{v} \exp(-2i\phi),$$

and the Bogoliubov-de Gennes equations for the functions \bar{u}, \bar{v} read:

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr}\right)\bar{u} + 2g|\psi_0|^2\bar{u} - g|\psi_0|^2\bar{v} + \frac{m\omega^2 r^2}{2}\bar{u} - \mu\bar{u} = \epsilon\bar{u},$$
(7.44)

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{4}{r^2}\right)\bar{v} + 2g|\psi_0|^2\bar{v} - g|\psi_0^2\bar{u} + \frac{m\omega^2 r^2}{2}\bar{v} - \mu\bar{v} = -\epsilon\bar{v}.$$
 (7.45)

We now use a perturbative approach. First of all, in the absence of trapping the solutions of Eqs. (7.44) and (7.45) are given by equations (7.23) and (7.24)

and we assume that to zero order they locally remain the same for a trapped condensate. So, they should be simply multiplied by ψ_{TF} , and we thus have

$$\bar{u} = \frac{1}{\sqrt{4\pi\mathcal{L}}} \left(\frac{f}{r} + \frac{\partial f}{\partial r}\right) \psi_{TF},\tag{7.46}$$

$$\bar{v} = \frac{1}{\sqrt{4\pi\mathcal{L}}} \left(\frac{f}{r} - \frac{\partial f}{\partial r}\right) \psi_{TF}.$$
(7.47)

Using the Gross-Pitaevskii equation (7.41) we rewrite equations (7.44) and (7.45) in the form:

$$\frac{\hbar^2}{2m} \left[\frac{1}{\psi_0} \left(\frac{d^2 \psi_0}{dr^2} + \frac{1}{r} \frac{d\psi_0}{dr} \right) + \frac{1}{r^2} \right] \bar{u} + g \psi_0^2 (\bar{u} - \bar{v}) = \epsilon \bar{u}, \quad (7.48)$$

$$\frac{\hbar^2}{2m} \left[\frac{1}{\psi_0} \left(\frac{d^2 \psi_0}{dr^2} + \frac{1}{r} \frac{d\psi_0}{dr} \right) + \frac{4}{r^2} \right] \bar{v} - g \psi_0^2 (\bar{u} - \bar{v}) = -\epsilon \bar{v}.$$
(7.49)

Substituting the zero order solutions (7.46) and (7.47) and the condensate wavefunction (7.42) into Eqs. (7.48) and (7.49), we multiply the sum of the two equations by $(\bar{u} + \bar{v})$ and integrate over d^3r . This yields

$$\frac{2\hbar^2}{m} \int_0^\infty \frac{f^2}{r^2} \left\{ \frac{d^2 \psi_{TF}}{dr^2} + \frac{1}{r} \frac{d\psi_{TF}}{dr} + \frac{2}{f} \frac{d\psi_{TF}}{dr} \frac{df}{dr} \right\} \frac{d^3 r}{4\pi \mathcal{L}} = \epsilon.$$
(7.50)

The main contribution to the integral in the left hand side of Eq. (7.50) comes from distances where $\xi \ll r \ll R$. We then put $f \approx 1$ and $\psi''_{TF} = (1/r)\psi'_{TF} = (1/R_{TF}^2)$ and find

$$\epsilon = -\frac{4\hbar^2}{mR_{TF}^2} \int \frac{2\pi r dr}{4\pi r^2},\tag{7.51}$$

where the lower limit of integration should be put equal to ξ , and the upper limit to R_{TF} . This gives with logarithmic accuracy:

$$\epsilon = -\frac{2\hbar^2}{mR_{TF}^2} \ln\left(\frac{R_{TF}}{\xi}\right) = -\frac{\hbar^2\omega^2}{\mu} \ln\left(\frac{R_{TF}}{\xi}\right). \tag{7.52}$$

Thus, the obtained eigenfrequency is negative. This indicates the presence of thermodynamic (energetic) instability, as one may expect in a non-rotating trap where the vortex state is not the ground state.

7.2 Consider a straight vortex line in an ideal cylinder of length \mathcal{L} . Assume that the line is fixed at the edges. Find a quantization rule for kelvons and calculate the density profile taking into account quantum and thermal fluctuations due to kelvons.

Lecture 8. True and phase-fluctuating condensates in 2D Bose gases

8.1 Coupling constant for the interaction between particles

In this *Lecture* we discuss BEC in weakly interacting two-dimensional (2D) Bose gases and introduce the notion of phase-fluctuating condensates, or quasicondensdates. As well as in the 3D case, we have the Hamiltonian (2.45) and the non-linear Heisenberg equation of motion for the field operator, (3.4). We will consider later the criterion of the weakly interacting regime, which contains the coupling constant g. Let us first discuss what is g in the 2D case.

This question is, in general, beyond the scope of this lecturing course. We consider the situation where a 3D gas is strongly confined by a harmonic potential $V_0(z) = m\omega_0^2 z^2/2$ in one direction (z). Then, if it is confined to zero point oscillations, and the wavefunction of the particle motion in the z-direction is

$$\psi_z = \frac{1}{\pi^{1/4} l_0^{1/2}} \exp\left(-\frac{z^2}{2l_0^2}\right),\tag{8.1}$$

with $l_0 = (\hbar/m\omega_0)^{1/2}$ being the harmonic oscillator length for the tight confinement. Since only one mode of the motion in the z-direction is occupied, the field operator can be represented as

$$\hat{\psi}(z,\mathbf{r}) = \hat{\psi}(\mathbf{r})\psi_z(z), \qquad (8.2)$$

where $\mathbf{r} = \{x, y\}$. Substituting $\hat{\psi}$ (8.2) into the three-dimensional Hamiltonian (2.45) and integrating over dz we obtain an effective 2D Hamiltonian

$$\begin{aligned} \hat{H} &= \int_{-\infty}^{\infty} dz \Big\{ \psi_z^2 \int d^2 r \left(-\frac{\hbar^2}{2m} \hat{\psi}^{\dagger}(\mathbf{r}) \Delta_{\mathbf{r}} \hat{\psi}(\mathbf{r}) + \hat{\psi}^{\dagger}(\mathbf{r}) V(\mathbf{r}) \hat{\psi}(\mathbf{r}) \right) \quad (8.3) \\ &+ \frac{g_{3D}}{2} \psi_z^4 \int d^2 r \hat{\psi}^{\dagger}(\mathbf{r}) \hat{\psi}^{\dagger}(\mathbf{r}) \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r}) \Big\} \\ &= \int d^2 r \hat{\psi}^{\dagger}(\mathbf{r}) \left\{ -\frac{\hbar^2}{2m} \Delta_{\mathbf{r}} + V(\mathbf{r}) + \frac{g}{2} \hat{\psi}^{\dagger}(\mathbf{r}) \hat{\psi}(\mathbf{r}) \right\} \hat{\psi}(\mathbf{r}), \end{aligned}$$

where $g_{3D} = 4\pi \hbar^2 a/m$ and the coupling constant g is given by

$$g = \frac{g_{3D}}{\sqrt{2\pi}l_0} = \frac{2\sqrt{2\pi}\hbar^2 a}{ml_0}.$$
 (8.5)

The quantity $V(\mathbf{r})$ in Eq. (8.4) is an external shallow potential in the **r**-plane. So, the 2D Hamiltonian has the form (2.45) with the coupling constant determined by Eq. (8.5). Including the term

$$\hat{\psi}^{\dagger}(\mathbf{r})\psi_{z}\left(-\frac{\hbar^{2}}{2m}\frac{d^{2}}{dz^{2}}+\frac{1}{2}m\omega_{0}^{2}z^{2}\right)\hat{\psi}(\mathbf{r})\psi_{z}$$

in the 3D Hamiltonian in Eq. (8.3) simply shifts the chemical potential by $\hbar\omega_0/2$.

Note that since we used a 3D Hamiltonian for deriving the effective twodimensional Hamiltonian (8.4), the validity of this result requires the condition $|a| \ll l_0$.

8.2 Bose-Einstein condensation at zero temperature. Small parameter of the theory

Let us now consider a 2D weakly interacting gas of bosons repulsively interacting with each other and described by the Hamiltonian (8.4), at T = 0. Assuming that most of the particles are in the condensate we act in the same way as in the 3D case. We write $\hat{\Psi} = \Psi_0 + \hat{\Psi}'$ and obtain the Gross-Pitaevskii equation (3.6) for the Heisenberg-picture condensate wavefunction Ψ_0 and the stationary Gross-Pitaevskii equation (3.9) for the Schroedinger-picture wavefunction ψ_0 . Then, using the Bogoliubov transformation (5.3) we arrive at the Bogoliubovde Gennes equations (5.7) and (5.8) for the excitations. In the uniform case we have $\psi_0 = \sqrt{n_0}$, and the u, v functions of the excitations are given by Eqs. (5.10), (5.11), (5.17), and (5.18) with the excitation eigenenergy ϵ_k (5.16). Accordingly, the density of non-condensed particles at T = 0 is given by equation (5.32). The only difference is that now **k** is the two-dimensional vector. So, for the noncondensed density we obtain:

$$n' = \langle \hat{\psi}'^{\dagger}(\mathbf{r})\hat{\psi}'(\mathbf{r})\rangle = \sum_{\mathbf{k}} v_k^2 = \int \frac{1}{4} \left(\frac{\epsilon_k}{E_k} + \frac{E_k}{\epsilon_k} - 2\right) \frac{d^2k}{(2\pi)^2} = \frac{mg}{4\pi\hbar^2}n.$$
 (8.6)

We thus see two important consequences. First of all, equation (8.6) is consistent with the *apriori* assumption that there is a true BEC in the 2D Bose gas at zero temperature. Second, the requirement of the weakly interacting regime, $n' \ll n$, shows that the small parameter of the theory for this regime is

$$\frac{mg}{4\pi\hbar^2} \ll 1. \tag{8.7}$$

Using the coupling constant g from Eq. (8.5) we find that in the 2D regime obtained by tightly confining the motion of particles in one direction the small parameter (8.7) takes the form

$$\frac{a}{l_0} \ll 1. \tag{8.8}$$

The calculation of the one-body density matrix in the uniform case shows qualitatively the same picture as displayed in Fig.5.3 for the 3D case. It is tending to n_0 at $r \to \infty$, i.e. there is a long-range order. Rewriting equations (5.37) and (5.38) in terms of Schroedinger-picture field operators and bearing in mind that **k** is now a two-dimensional vector, we obtain

$$g_1(r) = n_0 + \langle \hat{\psi}'^{\dagger}(\mathbf{r}) \hat{\psi}'(0) \rangle = n_0 + \int \frac{d^2k}{(2\pi)^2} v_k^2 \exp(i\mathbf{kr})$$
$$= n_0 \left[1 + \frac{mg}{2\pi\hbar^2} I_1\left(\frac{r}{\xi}\right) K_1\left(\frac{r}{\xi}\right) \right], \qquad (8.9)$$

where I_1 and K_1 are the growing and decaying Bessel functions. At distances $r \gg \xi$ equation (8.9) gives

$$g_1(r) = n_0 \left(1 + \frac{mg}{4\pi\hbar^2} \frac{\xi}{r} \right), \quad r \gg \xi.$$
 (8.10)

Comparing Eq. (8.10) with Eq. (5.39) one sees that in 2D at zero temperature $g_1(r)$ approaches its asymptotic value n_0 much slower than in 3D.

8.3 Phase-fluctuating condensates at finite temperatures

We now turn to the case of finite temperatures. Then the non-condensed density is given by Eq. (6.1), where the vacuum (zero-temperature) contribution $\mathcal{V}^{-1}\sum_{\mathbf{k}} v_k^2$ is the one of Eq. (8.6) and for the thermal contribution we have a 2D analog of Eq. (6.3):

$$n'_{T} = \int \frac{d^{2}k}{(2\pi)^{2}} (v_{k}^{2} + u_{k}^{2}) N_{k} = \int_{0}^{\infty} \frac{kdk}{2\pi} \left(\frac{\epsilon_{k}}{2E_{k}} + \frac{E_{k}}{2\epsilon_{k}}\right).$$
(8.11)

For $k \to 0$ the excitation energy $\epsilon_k \propto k$, and since the single particle energy $E_k \propto k^2$ we have kdk/k^2 in the integrand of Eq. (8.11). The integral is divergent, which rules out the assumption of the presence of a true Bose-Einstein condensate.

The origin of this infrared divergence is related to long-wave fluctuations of the phase, which can be understood turning to the density-phase representation and writing the field operators in the form given by equations (5.40) and (5.41), with the commutation relation (5.42). Substituting $\hat{\Psi}(\mathbf{r}, t)$ (5.40) and $\hat{\Psi}^{\dagger}(\mathbf{r}, t)$ (5.41) into the non-linear Schroedinger equation (3.4) and equalizing real and imaginary parts, we get coupled continuity and Euler hydrodynamic equations for the density and phase operators:

$$-\hbar \frac{\partial \sqrt{\hat{n}}}{\partial t} = \frac{\hbar^2}{2m} \nabla (\nabla \hat{\phi} \sqrt{\hat{n}}), \qquad (8.12)$$

$$-\hbar\frac{\partial\hat{\phi}}{\partial t}\sqrt{\hat{n}} = \frac{\hbar^2}{2m}(\nabla\hat{\phi})^2\sqrt{\hat{n}} - \frac{\hbar^2}{2m}\Delta\sqrt{\hat{n}} + V(\mathbf{r})\sqrt{\hat{n}} + g\hat{n}^{3/2}.$$
 (8.13)

We now assume that fluctuations of the density are small on any distance scale. Eq. (8.12) then shows that fluctuations of the phase gradient are also small. Writing the density operator as $\hat{n} = n(\mathbf{r}) + \delta \hat{n}$ and shifting the phase by $-\mu t/\hbar$, we linearize Eqs. (8.12) and (8.13) with respect to $\delta \hat{n}$ and $\nabla \hat{\phi}$ around the stationary solution $\hat{n} = n$, $\nabla \hat{\phi} = 0$. The zero order terms give the Gross-Pitaevskii equation for the mean density n:

$$-\frac{\hbar^2}{2m}\frac{\Delta\sqrt{n}}{\sqrt{n}} + V(\mathbf{r}) + gn - \mu = 0.$$
(8.14)

The first order terms provide equations for the density and phase fluctuations:

$$\hbar \frac{\partial \delta \hat{n}}{\sqrt{n}\partial t} = \left[-\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}) + gn - \mu \right] 2\sqrt{n}\hat{\phi}, \qquad (8.15)$$

$$-\hbar \frac{2\partial\sqrt{n}\hat{\phi}}{\partial t} = \left[-\frac{\hbar^2}{2m}\Delta + V(\mathbf{r}) + 3gn - \mu\right]\frac{\delta\hat{n}}{\sqrt{n}}.$$
(8.16)

Solutions of Eqs. (8.15) and (8.16) are obtained in terms of elementary excitations:

$$\delta \hat{n} = \sqrt{n(\mathbf{r})} \sum_{\nu} f_{\nu}^{-}(\mathbf{r}) \exp(-i\epsilon_{\nu} t/\hbar) \hat{b}_{\nu} + h.c.$$
(8.17)

$$\hat{\phi} = \frac{-i}{2\sqrt{n(\mathbf{r})}} \sum_{\nu} f_{\nu}^{+}(\mathbf{r}) \exp(-i\epsilon_{\nu}t/\hbar)\hat{b}_{\nu} + h.c., \qquad (8.18)$$

where $f_{\nu}^{\pm}(\mathbf{r}) = u_{\nu}(\mathbf{r}) \pm v_{\nu}(\mathbf{r})$ and the functions u_{ν} , v_{ν} satisfy the Bogoliubov-de Gennes equations (5.7) and (5.8), with $|\Psi_0|^2$ replaced by n. We thus see that the assumption of small density fluctuations is sufficient for having the Bogoliubov wavefunctions of the excitations and the Bogoliubov excitation spectrum, irrespective of the presence or absence of a true Bose-Einstein condensate.

Let us now return to the uniform case and check that the density fluctuations are really small in 2D. Like in 3D in *Lecture 5*, we divide the system of excitations into two parts: the high-energy free-particle part with $\epsilon_k > ng$, and the lowenergy phonon part with $\epsilon_k < ng$, so that

$$\delta \hat{n} = \delta \hat{n}_p + \delta \hat{n}_f, \qquad (8.19)$$

$$\hat{\phi} = \hat{\phi}_p + \hat{\phi}_f, \qquad (8.20)$$

where the subscript p stands for the phonon part, and f for the free-particle part. For the free-particle branch of the spectrum we have $v_k \to 0$ and $u_k \to 1$. Denoting the field operator of this part as $\hat{\Psi}_f(\mathbf{r}, t)$, for the density of "free particles" we have:

$$\langle \hat{\Psi}_f^{\dagger}(0,0)\hat{\Psi}_f(0,0)\rangle \approx \int_{\epsilon_k > ng} \frac{d^2k}{(2\pi)^2} N_k < n\frac{T}{T_d} \ln\left(\frac{T}{T_d}\right),$$

with $T_d = 2\pi\hbar^2 n/m$ being the temperature of quantum degeneracy. At temperatures $T \ll T_d$ we then have $\langle \hat{\Psi}_f^{\dagger}(0,0)\hat{\Psi}_f(0,0)\rangle \ll n$. As the density fluctuations related to the free particle part of the spectrum are of the order of $\langle \hat{\Psi}_f^{\dagger}(0,0)\hat{\Psi}_f(0,0)\rangle$ or smaller, we conclude that they are small. The inequality $\langle \hat{\Psi}_f^{\dagger}\hat{\Psi}_f\rangle \ll n$ shows that the high-energy fluctuations of the phase are also small.

In order to estimate the low-energy fluctuations of the density we calculate the density-density correlation function $\langle \delta \hat{n}(0) \delta \hat{n}(\mathbf{r}) \rangle$ at equal times. A straightforward calculation using Eq. (8.17) yields

$$\frac{\langle \delta \hat{n}(0)\delta \hat{n}(\mathbf{r})\rangle}{n^2} = \frac{1}{n} \int_{\epsilon_k < ng} \frac{d^2k \ E_k}{(2\pi)^2 \epsilon_k} (1+2N_k) \cos \mathbf{kr} < \max\left\{\frac{T}{T_d}, \frac{mg}{4\pi\hbar^2}\right\}, \quad (8.21)$$

and at temperatures $T \ll T_d$ these density fluctuations are also small.

We thus see that omitting small fluctuations of the density the one-body density matrix can be found by using the field operators given by Eqs. (5.40) and (5.41), with $\sqrt{\hat{n}}$ replaced by the square root of the mean density, \sqrt{n} . Since at $T \ll T_d$ the high-energy part of the phase fluctuations is also small, we may confine ourselves to the low-energy part $\hat{\phi}_p$ in the phase operator and use the field operator in the form

$$\hat{\Psi} = \sqrt{n} \exp(i\hat{\phi}_p). \tag{8.22}$$

For the one-body density matrix at equal times we then have:

$$g_1(\mathbf{r}) = \langle \hat{\Psi}^{\dagger}(\mathbf{r}, 0) \hat{\Psi}(0, 0) \rangle = n \langle \exp i[\hat{\phi}_p(\mathbf{r}, 0) - \hat{\phi}_p(0, 0)] \rangle.$$
(8.23)

Relying on the Taylor expansion of the exponent one proves directly that

$$\langle \exp i[\hat{\phi}_p(\mathbf{r},0) - \hat{\phi}_p(0,0)] \rangle = \exp\{-\frac{1}{2}\langle [\hat{\phi}_p(\mathbf{r},0) - \hat{\phi}(0,0)]^2 \rangle\}$$

Vacuum low-energy fluctuations of the phase are small as $mg/2\pi\hbar^2$. However, thermal phase fluctuations grow logarithmically for $r \to \infty$. Using Eq. (8.18) we obtain:

$$\langle [\hat{\phi}_p(\mathbf{r},0) - \hat{\phi}_p(0,0)]^2 \rangle = \int_{k < \xi^{-1}} \frac{d^2k}{(2\pi)^2} \frac{(1 - \cos \mathbf{kr})}{n} \frac{\epsilon_k}{E_k} N_k = \frac{2T}{T_d} \ln\left(\frac{r}{\lambda_T}\right), \quad (8.24)$$

where $\lambda_T = \xi = \hbar/\sqrt{mng}$ for $T \gg ng = \mu$. In the limit of very low temperatures, $T \ll ng$, we have λ_T equal to the thermal de Broglie wavelength of the excitations, i.e. $\lambda_T = \hbar c_s/T$. Accordingly, the correlation function $g_1(r)$ undergoes a slow power law decay at large r:

$$g_1(r) = n \left(\frac{\lambda_T}{r}\right)^{T/T_d}; \quad r \gg \lambda_T.$$
 (8.25)

This is drastically different from the 3D case. In 2D long-wave fluctuations of the phase destroy the long-range order and true BEC.

What kind of state we get? Let us first introduce the distance l_{ϕ} at which the correlation function $g_1(r)$ significantly decreases, the so-called phase coherence length. From Eq. (8.25) we obtain

$$l_{\phi} \approx \lambda_T \exp\left(\frac{T_d}{T}\right) \gg \xi.$$
 (8.26)

Using this quantity the dependence $g_1(r)$ given by Eq. (8.25) is displayed in Fig.8.1. Since $l_{\phi} \gg \xi$, the system can be divided into blocks of size L such that $\xi \ll L \ll l_{\phi}$. Then, inside each block one has a true condensate, but the phases of different blocks are not correlated to each other (see Fig.8.2). This state is called phase-fluctuating Bose-Einstein condensate, or quasicondensate.



Figure 8.1: One-body density matrix $g_1(r)$ for a 2D Bose gas at $T \ll T_d$.

8.4 Kosterlitz-Thouless phase transition

Equation (8.25) shows that the correlation function $g_1(r)$ obtained at $T \ll T_d$ is strongly different from that in a thermal 2D Bose gas. Thus, one expects that there is a phase transition. How does it occur? It is called *Kosterlitz-Thouless* transition and it occurs through the formation of bound vortex-antivortex pairs. That is, vortices with an opposite circulation (s = 1 and s = -1) form bound pairs.

A detailed scenario of this phase transition is beyond the scope of this lecturing course. Nevertheless, we will consider "supporting arguments". Let us calculate the free energy

$$F = E - TS, \tag{8.27}$$

with S being the entropy. In Lecture 7 we have found that the energy of a single vortex is given by Eq. (7.7) and is proportional to the length of the vortex line. In 2D there are no vortex lines, but one has vortex points. The energy of a single-charged vortex in 2D is obtained from Eq. (7.7) by replacing the product of the 3D superfluid density ρ_s/m and the length of the vortex line \mathcal{L} by the 2D (superfluid) density n_s :

$$E = \frac{\pi \hbar^2}{2m} n_s \ln\left(\frac{\mathcal{R}^2}{r_c^2}\right),\tag{8.28}$$

where \mathcal{R} is the size of the 2D gas. The entropy is given by

$$S = \ln\left(\frac{\mathcal{R}^2}{r_c^2}\right),\tag{8.29}$$



Figure 8.2: Picture of the phase-fluctuating condensate. The phases of blocks that are separated by a distance $\sim l_{\phi}$ or larger are not correlated with each other.

since there are approximately \mathcal{R}^2/r_c^2 possible positions for the vortex core. So, for the free energy we have

$$F = \left\{\frac{\pi\hbar^2}{2m}n_s - T\right\} \ln\left(\frac{\mathcal{R}^2}{r_c^2}\right).$$
(8.30)

We thus see that for $T < T_c = \pi \hbar^2 n_s/2m$ the appearance of single vortices increases the free energy. Therefore, the probability of having single vortices will be vanishingly small. On the other hand, for $T > T_c$ the appearance of single vortices decreases the free energy and they spontaneously appear in the system. So, the temperature

$$T_c = \frac{\pi \hbar^2}{2m} n_s \tag{8.31}$$

is expected to correspond to a phase transition. Note that the superfluid density n_s depends itself on temperature. A detailed analysis of the Kosterlitz-Thouless phase transition shows that n_s entering Eq. (8.31) is the superfluid density just below the transition temperature T_c .

We now briefly discuss BEC in 2D trapped Bose gases. If a harmonically trapped gas is in the Thomas-Fermi regime, it has a size $R_{TF} = (2ng/m\omega^2)^{1/2}$, where ω is the trap frequency. Then, one should compare R_{TF} with the phase

coherence length l_{ϕ} (8.26). For $l_{\phi} \ll R_{TF}$ the situation is similar to that in an infinite system. There is a *quasicondensate*. However, if $l_{\phi} \gtrsim R_{TF}$, then one has a *true BEC*. This is a finite size effect. The finite size of the system introduced by the trapping potential provides a low-momentum cut-off for the phase fluctuations and thus reduces them.

Note that correlation properties of a quasicondensate on a distance scale smaller than l_{ϕ} are the same as those of a true condensate. Only the properties on a distance scale larger than l_{ϕ} are different.

Problems 8

8.1 Consider a 2D finite-temperature Bose-condensed gas in a harmonic potential $V(r) = m\omega^2 r^2/2$. Assume the Thomas-Fermi regime and express the condition of having a quasicondensate in terms of the number of particles Nand temperature T.

Using the Gross-Pitaevskii equation for the mean density (8.14) and omitting the Laplacian term, the Thomas-Fermi density profile is given by

$$n(r) = \frac{\mu}{g} \left(1 - \frac{r^2}{R_{TF}^2} \right), \qquad (8.32)$$

where the chemical potential is $\mu = n_{max}g$, with $n_{max} = n(0)$ being the maximum density, and $R_{TF} = \sqrt{2\mu/m\omega^2}$ is the Thomas-Fermi radius. The one-body density matrix at equal times and at a distance **r** from the origin is

$$g_1(\mathbf{r}) = \langle \hat{\Psi}^{\dagger}(\mathbf{r}, 0) \hat{\Psi}(0, 0) \rangle = \sqrt{n(r)n(0)} \exp\left\{-\frac{1}{2} \langle [\hat{\phi}(\mathbf{r}, 0) - \hat{\phi}(0, 0)]^2 \rangle\right\},\$$

and the BEC state is a quasicondensate if the mean square fluctuations of the phase, $\langle [\hat{\phi}(\mathbf{r}, 0) - \hat{\phi}(0, 0)]^2 \rangle$, are of the order of unity or larger on a distance scale $\sim R_{TF}$. At temperatures $T \gg \mu$ the main contribution to these fluctuations comes from excitations with energies much larger than $\hbar\omega$. These excitations are quasiclassical, and we have

$$\langle [\hat{\phi}(R_{TF},0) - \hat{\phi}(0,0)]^2 \rangle \approx \left(\frac{mg}{2\pi\hbar^2}\right) \frac{T}{\mu} \ln\left(\frac{R_{TF}}{\xi(0)}\right).$$
(8.33)

The ratio $R_{TF}/\xi(0)$ is

$$\frac{R_{TF}}{\xi(0)} = \left(\frac{2\mu}{m\omega^2}\right)^{1/2} \frac{(mn_{max}g)^{1/2}}{\hbar} = \frac{\sqrt{2}\mu}{\hbar\omega}.$$
(8.34)

From the normalization condition and Eq. (8.32) we obtain the chemical piotential in terms of the number of particles and the trap frequency:

$$N = \int_0^{R_{TF}} n(r) 2\pi r dr = \frac{\pi\mu}{2g} R_{TF}^2$$

and, hence,

$$\mu = \hbar \omega \left(\frac{Nmg}{\pi\hbar^2}\right)^{1/2}.$$
(8.35)

Accordingly, Eq. (8.34) is transformed to

$$\frac{R_{TF}}{\xi(0)} = \left(\frac{2Nmg}{\pi\hbar^2}\right)^{1/2}.$$
(8.36)

Substituting this ratio and μ (8.35) into Eq. (8.33) we obtain with logarithmic accuracy:

$$\langle [\hat{\phi}(R_{TF},0) - \hat{\phi}(0,0)]^2 \rangle \approx \frac{T}{2\sqrt{N}\hbar\omega} \left(\frac{mg}{\pi\hbar^2}\right)^{1/2} \ln N.$$
(8.37)

Assuming a Kosterlitz-Thouless type of phase transition we should have the transition temperature to the BEC regime

$$T_c \sim \frac{\hbar^2}{2m} n_{max}.$$

At the transition the trapped sample has a thermal size $\sim R_T \sim (T/m\omega^2)^{1/2}$. Hence, $n_{max} \sim N/R_T^2 \sim m\omega^2 N/T_c$. This gives $T_c \sim \sqrt{N}\hbar\omega$. So, the first two multiples in Eq. (8.37) are small, just because $T < T_c$ and $mg/4\pi\hbar^2$ is a small parameter of the theory. Therefore, in order to to have a quasicondensate one should have a very large number of particles satisfying the condition

$$\frac{T}{\sqrt{N}\hbar\omega} \left(\frac{mg}{4\pi\hbar^2}\right)^{1/2} \ln N \gtrsim 1.$$

8.2 Calculate the one-body density matrix for a 2D Bose-condensed gas at T = 0in a harmonic potential $V(r) = m\omega^2 r^2/2$ assuming the Thomas-Fermi regime.

Lecture 9. Regimes of quantum degeneracy in a weakly interacting 1D Bose gas

9.1 Coupling constant and criterion of weak interactions in 1D

In this *Lecture* we consider weakly interacting one-dimensional (1D) Bose gases and discuss the emerging regimes of quantum degeneracy. The first question is related to the value of the coupling constant g. Let us assume that there is a 3D gas tightly confined by a harmonic potential $V_0(\rho) = m\omega_0^2 r^2/2$ to zero point oscillations in the x, y-directions ($x^2 + y^2 = r^2$, see Fig.9.1). Then the motion of particles in these directions is governed by the wavefunction

$$\psi_r = \frac{1}{\sqrt{\pi}l_0} \exp\left(-\frac{r^2}{2l_0^2}\right),$$
(9.1)

where $l_0 = (\hbar/m\omega_0)^{1/2}$ is the harmonic oscillator length for the tight confinement. The field operator can be written in the form:

$$\hat{\psi}(\mathbf{r}, z) = \hat{\psi}(z)\psi_r. \tag{9.2}$$

We then act in a similar way as in the 2D case in *Lecture 8*. Substituting $\hat{\psi}$ (9.2) into the three-dimensional Hamiltonian (2.45) with the 3D coupling constant $g_{3D} = 4\pi\hbar^2 a/m$, and integrating over d^2r we obtain an effective 1D Hamiltonian

$$\begin{aligned} \hat{H} &= \int_0^\infty 2\pi r dr \Big\{ \psi_r^2 \int dz \left(-\frac{\hbar^2}{2m} \hat{\psi}^\dagger(z) \Delta_z \hat{\psi}(z) + \hat{\psi}^\dagger(z) V(z) \hat{\psi}(z) \right) (9.3) \\ &+ \frac{g_{3D}}{2} \psi_r^4 \int dz \hat{\psi}^\dagger(z) \hat{\psi}^\dagger(z) \hat{\psi}(z) \hat{\psi}(z) \Big\} \\ &= \int dz \hat{\psi}^\dagger(z) \left\{ -\frac{\hbar^2}{2m} \Delta_z + V(z) + \frac{g}{2} \hat{\psi}^\dagger(z) \hat{\psi}(z) \right\} \hat{\psi}(z), \end{aligned}$$
(9.4)

where V(z) is a shallow external potential in the z-direction, and the coupling constant g is expressed through l_0 and the 3D scattering length a as

$$g = \frac{2\hbar^2 a}{ml_0^2}.\tag{9.5}$$

Adding the term

$$\hat{\psi}^{\dagger}(z)\psi_r\left(-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}+\frac{1}{2}m\omega_0^2r^2\right)\hat{\psi}(z)\psi_r$$

in the 3D Hamiltonian in Eq. (9.3) shifts the chemical potential by $\hbar\omega_0$. Stricktly speaking, since we started with the 3D Hamiltonian (2.45), the validity of Eq. (9.5) requires the inequality $|a| \ll l_0$.



Figure 9.1: One-dimensional quantum gas obtained by tightly confining the motion of particles in two directions

We now obtain the criterion of the weakly interacting regime in 1D in a similar way as we did in *Lecture 1* for the 3D case. Consider particles in a segment with a length of the order of the mean interparticle separation $\bar{r} \sim 1/n$. On average there is only one particle in such a segment, and at T = 0 its characteristic kinetic energy is $K \approx \hbar^2/m\bar{r}^2 \approx \hbar^2 n^2/m$. This is because in the

weakly interacting regime the wavefunction of particles is not influenced by the interaction at interparticle disatances $\sim \bar{r}$. For the same reason one should have $K \gg I$ where I = n|g| is the energy of interaction per particle. So, we have

$$\frac{\hbar^2 n^2}{m} \gg ng$$

which gives a small parameter of the weakly interacting regime

$$\gamma = \frac{m|g|}{\hbar^2 n} \ll 1. \tag{9.6}$$

Note that the criterion of the weakly interacting regime given by Eq. (9.6) shows that the 1D gas becomes more non-ideal (strongly interacting) with decreasing density.

9.2 QuasiBEC regime

We first consider a 1D Bose gas at T = 0 in a large segment of length L. Assume that there is a true condensate and calculate the density of non-condensed particles $n' = \langle \hat{\Psi}'^{\dagger} \hat{\Psi}' \rangle$. Writing the Bogoliubov transformation as

$$\hat{\Psi} = \sum_{k < \pi/L} [u_k \hat{b}_k \exp(ikz - i\epsilon_k t/\hbar) - v_k \hat{b}_k^{\dagger} \exp(ikz + i\epsilon_k t/\hbar)],$$

like in 3D we obtain equations (5.16), (5.17), and (5.18) for the energy spectrum of elementary excitations and for the functions u_k , v_k . We thus find the following result for the non-condensed fraction:

$$\frac{n'}{n} = \int_{\pi/L}^{\infty} \frac{dk}{\pi} \frac{v_k^2}{n} = \frac{\sqrt{\gamma}}{\pi} \ln\left(\frac{2L}{e\pi\xi}\right),\tag{9.7}$$

where $\xi = \hbar / \sqrt{mng}$ is the healing length.

From Eq. (9.7) we see two important circumstances. First of all, for $L \to \infty$ one does not satisfy the condition $n' \ll n$. So, there is no true BEC in an infinite 1D system even at T = 0. Second, since $\gamma \ll 1$, the true BEC can be present in a finite size system where equation (9.7) gives $n' \ll n$.

Let us now discuss a large 1D Bose gas and use the same hydrodynamic approach as in the 2D case at $T \neq 0$. Writing again the field operators in the density-phase representation according to Eqs. (5.40) and (5.41), substituting them into the non-linear Schroedinger equation (3.4), and thus obtaining equations (8.12) and (8.13), we then assume small fluctuations of the density and write $\hat{n} = n + \delta \hat{n}$. Shifting the phase by $-\mu t/\hbar$ and linearizing Eqs. (8.12) and (8.13) with respect to $\delta \hat{n}$ and $\nabla \hat{\phi}$ around the stationary solution $\hat{n} = n$, $\nabla \hat{\phi} = 0$ leads to Eq. (8.14) for the mean density n and to Eqs. (8.17) and (8.18) for $\delta \hat{n}$ and $\hat{\phi}$. We then consider a uniform infinite 1D Bose gas and obtain the conditions under which the density fluctuations are small. Dividing the fluctuations into the low-energy (phonon) and high-energy (free-particle) parts we calculate the density-density correlation function at equal times due to low-energy fluctuations of the density,

$$\langle \delta \hat{n}(z) \delta \hat{n}(0) \rangle_p = n \int_{\epsilon_k < \mu} \frac{dk}{2\pi} (1 + 2N_k) \frac{E_k}{\epsilon_k} \cos kz \approx \left(\frac{\mu}{T_d^{1D}}\right)^{1/2} \max\left\{\frac{T}{\mu}, 1\right\}, \quad (9.8)$$

where the chemical potential is $\mu = ng$, and the temperature of quantum degeneracy is defined as

$$T_d^{1D} = \frac{\hbar^2 n^2}{m}.$$
 (9.9)

Like in the 2D case at $T \neq 0$, for the high-energy part we again estimate the density of "free particles":

$$\langle \hat{\Psi}_f(0,0)\hat{\Psi}_f(0,0)\rangle \approx \int_{\epsilon_k > \mu} \frac{dk}{2\pi} N_k \sim n \frac{T}{\sqrt{\mu T_d^{1D}}},\tag{9.10}$$

and note that the contribution of vacuum fluctuations to this quantity is negligible. So, from equations (9.8) and (9.10) we see that in order to have small fluctuations of the density we should satisfy the inequality

$$T \ll (T_d^{1D} ng)^{1/2} \approx \sqrt{\gamma} T_d^{1D}.$$
(9.11)

Note that the condition $\mu = ng \ll T_d^{1D}$ is automatically satisfied at $\gamma \ll 1$. We have $ng/T_d^{1D} = \gamma \ll 1$.

We thus obtain that in 1D it is not sufficient to have $T \ll T_d^{1D}$ in order to get small density fluctuations. One should have the inequality (9.11) which is much stronger. Let us understand what this means and calculate the one-body density matrix at equal times, $g_1(z) = \langle \hat{\Psi}^{\dagger}(z,0)\hat{\Psi}(0,0) \rangle$, using the field operator in the form (8.22). As well as in the 2D case, we then get

$$g_1(z) = n \exp\left\{-\frac{1}{2} \langle [\hat{\phi}_p(z) - \hat{\phi}_p(0)]^2 \rangle\right\},$$
(9.12)

and the mean square fluctuations of the phase are now given by

$$\langle [\hat{\phi}_p(z) - \hat{\phi}_p(0)]^2 \rangle = \frac{1}{2n} \int_{\epsilon_k < \mu} \frac{dk}{2\pi} \frac{\epsilon_k}{E_k} (1 + 2N_k) (1 - \cos kz)$$
$$= \frac{mT}{\hbar^2 n} |z| + \frac{\sqrt{\gamma}}{\pi} \ln\left(\frac{|z|}{\xi}\right); \quad |z| \gg \xi.$$
(9.13)

At T = 0 the one-body density matrix undergoes a power law decay at large z:

$$g_1(z) = n \exp\left\{-\frac{\sqrt{\gamma}}{2\pi} \ln\left(\frac{|z|}{\xi}\right)\right\} = n \left(\frac{\xi}{|z|}\right)^{\sqrt{\gamma}/2\pi}.$$
(9.14)

In this respect the situation is similar to that in 2D at finite temperatures, and the phase coherence length is exponentially large compared to the healing length;

$$l_{\phi} \approx \xi \exp\left(\frac{2\pi}{\sqrt{\gamma}}\right).$$
 (9.15)

We can, therefore, divide the system into segments of size L such that $\xi \ll L \ll l_{\phi}$, and there is a true BEC inside each segment but the phases of different segments are not correlated to each other. So, one has the regime of a quasicondensate in 1D at T = 0.

At a finite and sufficiently large temperature, but still satisfying the criterion (9.11), omitting the contribution of vacuum fluctuations given by the second term in the right hand side of Eq. (9.13) we obtain:

$$g_1(z) = n \exp\left(-\frac{mT}{2\hbar^2 n}|z|\right) \tag{9.16}$$

and see that the one-body density matrix decays exponentially at large distances. The phase coherence length in this case is

$$l_{\phi} \approx \frac{\hbar^2 n}{mT}.\tag{9.17}$$

The inequality (9.11) is equivalent to $l_{\phi} \gg \xi$. Repeating the same arguments as in the previous paragraph we then conclude that there is a quasicondensate at finite temperatures satisfying the condition (9.11). Note that this condition is required for the validity of Eqs. (9.13) and (9.16).

9.3 Quantum decoherent regime

At temperatures in the range $T_d^{1D} \gg T > \sqrt{\gamma} T_d^{1D}$ the gas is still quantum degenerate, but fluctuations of the density are strong and there is no quasiBEC. This regime is called *quantum decoherent*. Since for $T \gg \sqrt{\gamma} T_d^{1D}$ we automatically have $T \gg ng$, the quantum decoherent Bose gas can be treated as almost ideal. Then, assuming that the chemical potential $\mu < 0$, we have the following expression for the one-body density matrix at equal times:

$$g_{1}(z) = \langle \hat{\Psi}^{\dagger}(z,0)\hat{\Psi}(0,0)\rangle = \sum_{k} N_{k} \exp(ikz) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{\exp(ikz)}{\exp\{(E_{k}-\mu)/T\} - 1}$$
$$= \sqrt{\frac{mT^{2}}{2\hbar^{2}|\mu|}} \exp\left(-\sqrt{\frac{2m|\mu|}{\hbar^{2}}}|z|\right).$$
(9.18)

For z = 0 we have

$$g_1(0) = n = \sqrt{\frac{mT^2}{2\hbar^2|\mu|}}.$$

This gives

$$|\mu| = \frac{mT^2}{2\hbar^2 n^2} = \frac{T^2}{2T_d^{1D}} \ll T,$$
(9.19)

and the inequality $|\mu| \ll T$ was used in the calculation of the integral in Eq. (9.18). Using Eq. (9.19) equation (9.18) can be rewritten as

$$g_1(z) = n \exp\left(-\frac{mT}{\hbar^2 n}\right),\tag{9.20}$$

and we see that the correlation function $g_1(z)$ qualitatively does not change compared to that in the quasiBEC regime. Only the exponential factor acquires an extra factor 2.

A qualitative difference between the quantum decoherent and quasiBEC regimes is seen in the behavior of two-body correlation functions. Let us calculate the local density correlation $g_2 = \langle \hat{\Psi}^{\dagger} \hat{\Psi}^{\dagger} \hat{\Psi} \hat{\Psi} \rangle$, where all field operators are taken at equal times and equal coordinates. In the quantum decoherent regime, using the ideal gas approach we have

$$g_2 = \sum_{k_1, k_2, k_3} \frac{1}{L^2} \langle \hat{a}_{k_1}^{\dagger} \hat{a}_{k_2}^{\dagger} \hat{a}_{k_3} \hat{a}_{k_1 + k_2 - k_3} \rangle = \frac{2}{L^2} \sum_{k_1, k_2} \langle \hat{a}_{k_1}^{\dagger} \hat{a}_{k_1} \rangle \langle \hat{a}_{k_2}^{\dagger} \hat{a}_{k_2} \rangle = 2n^2.$$
(9.21)

On the other hand, in the quasiBEC regime where the density fluctuations are suppressed, we can use the field operators in the form $\hat{\Psi} = \sqrt{n} \exp(i\hat{\phi})$, $\hat{\Psi}^{\dagger} = \sqrt{n} \exp(-i\hat{\phi})$. This immediately gives $g_2 = n^2$, the result inherent for a Bose-condensed gas.

The phase diagram for a finite-temperature weakly interacting 1D Bose gas is displayed in Fig.9.2. The quasiBEC regime where the density fluctuations are suppressed but the phase fluctuates on a long distance scale l_{ϕ} , is realized at low temperatures $T \ll \sqrt{\gamma} T_d^{1D}$. At $T \sim \sqrt{\gamma} T_d^{1D}$ the phase coherence length l_{ϕ} (9.17) becomes of the order of ξ , the density fluctuations become large, and the gas continuously transforms into the quantum decoherent regime. This is a crossover, not a phase transition. At temperatures $T \gtrsim T_d^{1D}$ the decoherent regime transforms from quantum into classical, with $|\mu| \gg T$ ($\mu < 0$).

9.4 Trapped 1D weakly interacting Bose gas

As we already saw in the previous subsection, in a finite geometry one can have both true and quasi condensates. We now analyze the weakly interacting 1D Bose gas in an external harmonic potential $V(z) = m\omega^2 z^2/2$ at zero temperature and transfer the discussion of the finite-temperature case to the problem section. For a harmonically trapped gas, in addition to the parameter γ (9.6), one introduces a complementary dimensionless parameter

$$\alpha = \frac{mgl}{\hbar^2},\tag{9.22}$$

where $l = (\hbar/m\omega)^{1/2}$ is the harmonic oscillator length. The parameter α is the ratio of l to the characteristic interaction length $r_g = \hbar^2/mg$ (g > 0), i.e. the length at which the contact interaction can appreciably change the wavefunction of the relative motion of two particles in 1D.



Figure 9.2: Phase diagram for a finite-temperature weakly interacting 1D Bose gas.

Since the smallest possible size of the cloud is l, for a large number of particles N the maximum density $n_{max} \gg l^{-1}$. Therefore, writing $\alpha = mgl/\hbar^2 = \gamma nl$ we see that for $\alpha \ll 1$ we always have $\gamma \ll 1$. As the maximum density is $n_{max} \sim N/L$, where L is the size of the cloud, for $N\alpha \ll 1$ we have

$$N \sim n_{max} L \ll \frac{\hbar^2}{mgl},\tag{9.23}$$

which is equivalent to the inequality

$$n_{max}g \ll \frac{\hbar^2}{ml^2} \frac{l}{L} \lesssim \hbar\omega.$$
(9.24)

So, the mean field interaction is much smaller than that the level spacing in the trapping potential, and we have a Gaussian density profile. This is a true BEC.

For $N\alpha \gg 1$ we have the Thomas-Fermi regime with the density profile

$$n(z) = n_{max} \left(1 - \frac{z^2}{L_{TF}^2} \right)^{1/2},$$

at $|z| \leq L_{TF}$ and zero otherwise. The Thomas-Fermi size is $L_{TF} = (2\mu/m\omega^2)^{1/2}$, with the chemical potential $\mu = n_{max}g$. The normalization condition $\int_{-\infty}^{\infty} n(z)dz = N$ gives a relation between μ and the number of particles:

$$\mu = \hbar \omega \left(\frac{3N\alpha}{4\sqrt{2}}\right)^{1/2},\tag{9.25}$$

which justifies that for $N\alpha \gg 1$ we have the condition of the Thomas-Fermi regime, $n_{max}g \gg \hbar\omega$.

We estimate the phase coherence length in this case by using ξ and γ at the maximum density. This gives

$$l_{\phi} \sim \xi \exp\left\{\frac{2\pi}{\sqrt{\gamma}}\right\} \sim l\left(\frac{1}{N\alpha}\right)^{1/3} \exp\left\{\frac{2\pi N^{1/3}}{\alpha^{2/3}}\right\}.$$
(9.26)

Using Eq. (9.25) the Thomas-Fermi size can be written as $L_{TF} \sim l(N\alpha)^{1/3}$. We then clearly see that for α in the range $1 \gg \alpha \gg N^{-1}$ the phase coherence length is much smaller than the size of the system, L_{TF} . We thus have a true Thomas-Fermi condensate. For large α we first have to check whether the criterion of the weakly interacting regime, $\gamma \ll 1$, is satisfied, at least at the maximum density. We have

$$\gamma(n_{max}) = \frac{mg}{\hbar^2 n_{max}} \sim \frac{\alpha}{n_{max}l} \sim \frac{\alpha^{4/3}}{N^{2/3}}$$

Thus, the gas is weakly interacting only if the inequality

$$N \gg N_* = \alpha^2 \tag{9.27}$$

is satisfied. Then, rewriting the expressions for the Thomas-Fermi size and phase coherence length as

$$L_{TF} \approx l\alpha \left(\frac{N}{N_*}\right)^{1/2}$$

and

$$l_{\phi} \approx \frac{l}{\alpha} \left(\frac{N}{N_{*}}\right)^{1/3} \exp\left\{2\pi \left(\frac{N}{N_{*}}\right)^{1/3}\right\},\,$$

we obtain the ratio

$$\frac{l_{\phi}}{L_{TF}} \approx \frac{1}{\alpha^2} \left(\frac{N}{N_*}\right)^{5/6} \exp\left\{2\pi \left(\frac{N}{N_*}\right)^{1/3}\right\}.$$
(9.28)

In principle, one can think of having very large α and N, while maintaining the ratio $N/N_* \sim 10$. Then, according to Eq. (9.28), the phase coherence length can be smaller than L_{TF} , which corresponds to the zero-temperature regime of quasiBEC in 1D. However, for all N and α achieved so far in experiments with weakly interacting bosonic clouds the ratio (9.28) is large, and one expects a true BEC at $T \to 0$. The phase diagram for the trapped 1D weakly interacting Bose gas at T = 0 is shown in Fig.9.3.

Problems 9

9.1 Calculate the one-body density matrix for a finite-temperature 1D Bosecondensed gas in a harmonic potential $V(r) = m\omega^2 z^2/2$ in the Thomas-Fermi regime. Find conditionms under which it is a true condensate.



Figure 9.3: Phase diagram for a trapped weakly interacting 1D Bose gas at T = 0.

The Thomas-Fermi density profile of the trapped gas at sufficiently low temperatures is $(2)^{1/2}$

$$n(z) = n_{max} \left(1 - \frac{z^2}{L_{TF}^2}\right)^{1/2}$$

at $|z| \leq L_{TF}$ and zero otherwise, with the Thomas-Fermi size $L_{TF} = (2\mu/m\omega^2)^{1/2}$ and the chemical potential $\mu = n_{max}g$.Irrespective of whether one has a true or quasiBEC, the wavefunctions and energies of elementary excitations follow from the Bogoliubov-de Gennes equations (5.7) and (5.8). In the case of quasiBEC we should only replace $|\psi_0|^2$ by $\sqrt{n(z)}$. Writing Eqs. (5.7) and (5.8) in terms of the functions $f_{\nu}^{\pm} = u_{\nu} \pm v_{\nu}$ we will have a one-dimensional version of equations (5.55) and (5.56):

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + V(z) + n(z)g - \mu\right)f_{\nu}^+ = \epsilon_{\nu}f_{\nu}^-,\tag{9.29}$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + V(z) + 3n(z)g - \mu\right)f_{\nu}^- = \epsilon_{\nu}f_{\nu}^+.$$
 (9.30)
Using the Gross-Pitaevskii equation (8.14) for the mean density n(z) we rewrite Eqs. (5.55) and (5.56) in the form:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + \frac{\hbar^2}{2m\sqrt{n(z)}}\frac{d^2\sqrt{n(z)}}{dz^2}\right)f_{\nu}^+ = \epsilon_{\nu}f_{\nu}^-,\tag{9.31}$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + \frac{\hbar^2}{2m\sqrt{n(z)}}\frac{d^2\sqrt{n(z)}}{dz^2} + 2n(z)g\right)f_{\nu}^- = \epsilon_{\nu}f_{\nu}^+.$$
 (9.32)

Considering low-energy excitations ($\epsilon_{\nu} \ll \mu$) we can omit two first terms in the left hand side of Eq. (9.32) since away from the Thomas-Fermi boarder of the cloud they are small as $(\hbar\omega/\mu)^2$ compared to the third term. Then, substituting f_{ν}^- from Eq. (9.31) into Eq. (9.32) we obtain an equation for the function f_{ν}^+ which is responsible for the phase fluctuations:

$$\frac{\hbar^2 \mu}{m} \left\{ \left(1 - \frac{z^2}{L_{TF}^2} \right) \frac{d^2 f_{\nu}^+}{dz^2} - \sqrt{1 - \frac{z^2}{L_{TF}^2}} f_{\nu}^+ \frac{d^2}{dz^2} \sqrt{1 - \frac{z^2}{L_{TF}^2}} \right\} + \epsilon_{\nu}^2 f_{\nu}^+ = 0.$$
(9.33)

The solution reads:

$$f_j^+ = \left[\frac{(2j+1)\mu}{\epsilon_j L_{TF}} \left(1 - \frac{z^2}{L_{TF}^2}\right)\right]^{1/2} P_j\left(\frac{z}{L_{TF}}\right),$$
(9.34)

where the quantum number j is an integer, and P_j are Legendre polynomials. This solution is obtained by turning to the variable $y = z^2/L_{TF}^2$ and introducing the function $W_{\nu} = f_{\nu}^+/\sqrt{1-y}$. Then Eq. (9.33) is reduced to a hypergeometrical equation

$$y(1-y)\frac{d^2W_{\nu}}{dz^2} + \left(\frac{1}{2} - \frac{3}{2}y\right)\frac{dW_{\nu}}{dz} + \frac{1}{2}\frac{\epsilon_{\nu}^2}{\hbar^2\omega^2}W_{\nu} = 0$$
(9.35)

which has two linearly independent solutions that are analytical in \sqrt{y} at y = 0. The first one is

$$W_{\nu} = F(\alpha, \beta, \gamma, y), \qquad (9.36)$$

where F is the hypergeometrical function, and

$$\alpha + \beta = \gamma = 1/2, \tag{9.37}$$

$$\alpha\beta = -\frac{1}{2} \left(\frac{\epsilon_{\nu}}{\hbar\omega}\right)^2. \tag{9.38}$$

The hypergeometrical series for the function (9.36) is convergent at y = 1 ($|z| = L_{TF}$) only if either α or β is a negative integer (see arguments in the problem 5.1). So, we have $\alpha = -q$ and $\beta = 1/2 + q$ or vice versa, with q being a positive integer. This leads to

$$W_{\nu} = F\left(-q, \frac{1}{2} + q, \frac{1}{2}, y\right) \propto P_{2q}(\sqrt{y}).$$
 (9.39)

The other solution of Eq. (9.35) is

$$W_{\nu} = F(\alpha - \gamma + 1, \beta - \gamma + 1, 2 - \gamma, y), \qquad (9.40)$$

with the same relations (9.37) and (9.38) for α, β, γ . Since the hypergeometrical series for the function (9.40) is convergent at y = 1 if $\alpha + 1/2$ or $\beta + 1/2$ is a negative integer, this function becomes

$$W_{\nu} = F\left(-q, q + \frac{3}{2}, \frac{3}{2}, y\right) \propto P_{2q+1}(\sqrt{y}).$$
(9.41)

So, equations (9.39) and (9.41) together yield $W_{\nu} \propto P_j(\sqrt{y})$, with *j* being a positive integer. Including the normalization factor this leads to Eq. (9.34), where we changed the subscript ν to *j*. Equation (9.38) leads to the spectrum

$$\epsilon_j = \hbar\omega \sqrt{j(j+1)/2}.\tag{9.42}$$

Let us now calculate the one-body density matrix at equal times. According to Eq. (9.12) we have

$$g_1(z) = \langle \hat{\Psi}^{\dagger}(z,0)\hat{\Psi}(0,0)\rangle = n \exp\left\{-\frac{1}{2}\langle [\hat{\phi}(z) - \hat{\phi}(0)]^2\rangle\right\}.$$

For the mean square fluctuations, using Eqs. (8.18) and (9.34) we obtain

$$\langle [\hat{\phi}(z) - \hat{\phi}(0)]^2 \rangle = \sum_j \frac{(j+1/2)}{L_{TF}} \frac{\mu N_j}{n_{max}\epsilon_j} \left[P_j \left(\frac{z}{L_{TF}} \right) - P_j(0) \right]^2.$$
(9.43)

There is an upper bound for the summation over j in Eq. (9.43), equal to $\sim \mu$. For $|z| \gg \xi$, excitations with energies much smaller than μ are just the ones that give the main contribution to the sum and are described by equations (9.34) and (9.42). The summation gives

$$\langle [\hat{\phi}(z) - \hat{\phi}(0)]^2 \rangle = \frac{4T\mu}{3T_d^{1D}\hbar\omega} \ln\left[\frac{1 + |z|/L_{TF}}{1 - |z|/L_{TF}}\right],\tag{9.44}$$

where the temperature of quantum degeneracy for the trapped 1D Bose gas is $T_d^{1D} = N\hbar\omega$. We thus see that there is a characteristic temperature

$$T_{\phi} = T_d^{1D} \frac{\hbar\omega}{\mu} \ll T_d^{1D} \tag{9.45}$$

which separates the true and quasiBEC states. For $T \gg T_{\phi}$ the phase fluctuations on a distance scale $\sim L_{TF}$ are large and one has quasiBEC. For $T \ll T_{\phi}$ these fluctuations are small and the state is a true BEC.

9.2 Do the same as in the problem 9.1 for a 1D Bose gas in a rectangular box (see Fig.9.4).



Figure 9.4: 1D Bose gas in a rectangular box.

Lecture 10. Solitons in Bose-condensed gases

10.1 Bright solitons

We now continue to discuss one-dimensional Bose gases and turn to Bosecondensed states called *solitons*. Our discussion will rely on the Gross-Pitaevskii equation for the considensate wavefunction. In view of the conclusions made in *Lecture 9* we thus consider a weakly interacting 1D Bose-condensed gas on a length scale smaller than the phase coherence length. This is relevant at very low temperatures, in particular at T = 0 where the phase coherence length is exponentially large compared to the healing length. We will not deal with phase coherence phenomena and omit the discussion of quantum fluctuations etc.

As we already saw, in 3D an infinite Bose-Einstein condensate of attractively interacting particles (the coupling constant g < 0) collapses. What is the situation in 1D? Let us consider a stationary Gross-Pitaevskii equation for g < 0 in free 1D space and assume that the condensate wavefunction ψ is real:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} - |g|\psi^2 - \mu\right)\psi = 0.$$
(10.1)

Multiplying Eq. (10.1) by $d\psi/dz$ and integrating over dz we have:

$$-\frac{\hbar^2}{4m} \left(\frac{d\psi}{dz}\right)^2 - \frac{|g|}{4}\psi^4 - \frac{\mu}{2}\psi^2 = C,$$
 (10.2)

with C being the integration constant. Assuming that at a certain point, let

say z = 0, we have $d\psi/dz = 0$, equation (10.2) gives

$$\frac{\hbar^2}{4m}\frac{d\psi}{dz} = \left(-\frac{|g|}{4}\psi^2 - \frac{\mu}{2}\psi^2 + \frac{|g|}{4}\psi^4(0) + \frac{\mu}{2}\psi^2(0)\right)^{1/2}.$$

Placing the boundary condition $\psi(\infty) = 0$ and integrating this equation we find:

$$\psi = \frac{\sqrt{n_0}}{\cosh(z/\xi)},\tag{10.3}$$

where

$$\xi = \frac{\hbar}{\sqrt{m|g|n_0}},\tag{10.4}$$

with $n_0 = \psi^2(0)$ being the central density.

The solution (10.3) is called *bright soliton*. The number of particles N in this state and the central density n_0 are related to each other by the normalization condition

$$N = \int_{-\infty}^{\infty} \psi^2(z) dz$$

Using Eq. (10.3) it gives $N = 2n_0\xi$, or

$$n_0 = \frac{m|g|}{4\hbar^2} N^2; (10.5)$$

$$\xi = \frac{2\hbar^2}{m|g|N}.\tag{10.6}$$

So, a given number of attractively interacting bosons forms the bright soliton state with a maximum density n_0 and width ξ given by Eqs. (10.5) and (10.6). With increasing the number of particles, the maximum density increases, whereas the width decreases (see Fig.10.1).

Note that equation (10.5) can be rewritten as

$$\gamma_0 = \frac{m|g|}{\hbar^2 n_0} = \frac{4}{N^2} \ll 1. \tag{10.7}$$

Equation (10.7) clearly shows that the bright soliton state satisfies the criterion of the weakly interacting regime for a large number of particles N.

The energy of the bright soliton is

$$E = \int_{-\infty}^{\infty} \left(-\frac{\hbar^2}{2m} \psi \frac{d^2 \psi}{dz^2} - \frac{|g|}{2} \psi^4 \right) dz = -\frac{mg^2}{24\hbar^2} N^3.$$
(10.8)

This gives the chemical potential

$$\mu = -\frac{mg^2}{8\hbar^2}N^2 = -\frac{1}{2}n_0|g|.$$
(10.9)

Why do we have such a striking difference from the 3D case? Let us compare a 3D system which has a linear size L and with a 1D system of the same linear



Figure 10.1: Density profile $n(z) = \psi^2(z)$ for the bright soliton state. A change of colour from blue to red corresponds to an increase in the number of particles.

size. In both cases the kinetic energy is $\sim \hbar^2 N/mL^2$. However, in 3D the interaction energy is $\sim -|g_{3D}|N^2/L^3$, whereas in 1D it is $\sim -|g|N^2/L$. So, omitting numerical coefficients we can write

$$E_{1D}(L) = \frac{\hbar^2 N}{mL^2} - \frac{|g|N^2}{L^3};$$
(10.10)

$$E_{3D}(L) = \frac{\hbar^2 N}{mL^2} - \frac{|g_{3D}|N^2}{L}.$$
 (10.11)

The energies $E_{1D}(L)$ and $E_{3D}(L)$ are displayed in Fig.10.2. In the 3D case the energy decreases with decreasing L and this is the origin of collapse (the region to the right of the shallow maximum corresponds to the case where the level spacing in the finite size system is larger than the interaction energy per particle, and one expects a stable BEC at a relatively small number of particles $N \leq L/|a|$, with a being the 3D scattering length). In contrast, in 1D the energy $E_{1D}(L)$ has a minimum at $L \sim \hbar^2/m|g|N \sim \xi$, and it is this minimum that corresponds to the bright soliton state.

10.2 Dynamical stability. Moving bright soliton as a particlelike object

The bright soliton state is the ground state of the 1D Bose gas of N particles at g < 0. It is dynamically stable, which is seen from the solution of the



Figure 10.2: Energy E of a Bose-condensed state versus the linear system size L for the 1D and 3D cases.

Bogoliubov-de Gennes equations for the excitations. Using the Gross-Pitaevskii equation (10.1), in analogy with Eqs. (9.31) and (9.32) we write these equations in terms of the functions f_{ν}^{\pm} as

$$-\frac{\hbar^2}{2m}\frac{d^2f_{\nu}^+}{dz^2} + \frac{\hbar^2}{2m}\frac{f_{\nu}^+}{\psi(z)}\frac{d^2\psi(z)}{dz^2} = \epsilon_{\nu}f_{\nu}^-, \qquad (10.12)$$

$$-\frac{\hbar^2}{2m}\frac{d^2f_{\nu}^-}{dz^2} + \frac{\hbar^2}{2m}\frac{f_{\nu}^-}{\psi(z)}\frac{d^2\psi(z)}{dz^2} - 2|g|\psi^2(z)f_{\nu}^- = \epsilon_{\nu}f_{\nu}^+.$$
 (10.13)

One should simply put $\psi(z)$ instead of $\sqrt{n(z)}$ in Eqs. (9.31) and (9.32) and replace g by -|g|. The solutions of equations (10.12) and (10.13) read:

$$f_k^+ = \frac{k^2 \xi^2 - 1 + 2ik\xi \tanh(z/\xi)}{(k+i)^2} \exp ikz, \qquad (10.14)$$

$$f_k^- = \frac{k^2 \xi^2 - 1 + 2ik\xi \tanh(z/\xi) + 2/\cosh^2(z/\xi)}{(k+i)^2} \exp ikz, \qquad (10.15)$$

where we put the excitation momentum k at an infinite separation from the soliton as the index ν . The excitation spectrum is given by

$$\epsilon_k = \frac{\hbar^2 k^2}{2m} + |\mu| \tag{10.16}$$

and it has a gap equal to $|\mu|$. The derivation of equations (10.14), (10.15), and (10.16) is transferred to the problem section.

The energy of a bright soliton decreases with the number of particles N. So, one can think that the 1D system has a tendency to form one big soliton. However, if one creates several moving solitons they freely pass through each other. This property is a consequence of integrability of the system. There is an infinite number of the integrals of motion. The potential $g|\psi|^2$ is reflectionless: elementary excitations go through the soliton without reflection. Thus, the formation of one big soliton requires lifting the integrability.

Let us now write down the solution for a moving bright soliton. Writing the condensate wavefunction as $\Psi(z,t) \exp(-i\mu t/\hbar)$ we have the time-dependent Gross-Pitaevskii equation in the form:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial z^2} + g|\Psi|^2\Psi - \mu\Psi.$$
(10.17)

The solution of this equation reads:

$$\Psi = \frac{\sqrt{n}}{\cosh[(z - vt)/\xi]} \exp(imvz/\hbar), \qquad (10.18)$$

where v is the soliton velocity, and the chemical potential is given by

$$\mu = -\frac{1}{2}n_0g + \frac{mv^2}{2}.$$
(10.19)

Thus, the energy of the moving bright soliton is

$$E = -\frac{mg^2}{24\hbar^2}N^3 + \frac{mNv^2}{2}.$$
 (10.20)

So, we see that the form of the bright soliton is independent of its velocity, and it can be viewed as a particle-like object with mass Nm.

10.3 Dark solitons

We now turn to soliton solutions of the Gross-Pitaevskii equation at g > 0. Consider an infinite Bose-condensed gas and assume that far from the soliton the Schroedinger-picture condensate wavefunction is $\psi = \sqrt{n}$, where n is the density. Assuming that ψ is real, the stationary Gross-Pitaevskii equation reads:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + g\psi^2 - \mu\right)\psi = 0,$$
(10.21)

and considering this equation at an infinite separation from the soliton we see that $\mu = ng$. Multiplying Eq. (10.21) by $d\psi/dz$ and integrating over dz we find

$$-\frac{\hbar^2}{4m}\left(\frac{d\psi}{dz}\right)^2 + \frac{g}{4}\psi^4 - \frac{\mu}{2}\psi^2 = C.$$

Since $\mu = ng$ and at an infinite separation from the soliton we have $\psi^2 = n$, the integration constant should be put equal to $C = -n^2g/4$. This gives

$$\frac{d\psi}{dz} = \pm \left(\frac{mg}{\hbar^2}\right)^{1/2} (n - \psi^2). \tag{10.22}$$

Integrating Eq. (10.22) we immediately obtain

$$\psi = \pm \sqrt{n} \tanh(z/\xi), \qquad (10.23)$$

where $\xi = \hbar/\sqrt{mng}$ is the healing length at an infinite separation from the soliton, and we selected z = 0 as the point where the condensate wavefunction is equal to zero. This Bose-condensed state is called *dark soliton*. The condensate wavefunction (10.23) is shown in Fig.10.3. It can also be written in the density-phase representation:

$$\psi = \sqrt{n(z)} \exp i\phi(z). \tag{10.24}$$

Then, from equation (10.23) (with, for example, the sign +) we obtain the density and phase of the dark soliton:

$$n(z) = \tanh^2(z/\xi),$$
 (10.25)

$$\phi(z) = \pi (1 - \theta(z)). \tag{10.26}$$

Just the fact that the density vanishes at a certain point z = 0 has led to the term dark soliton. The phase of the dark soliton undergoes a jump by π at this point (see Fig.10.4).

10.4 Grey soliton. Particle-like object with a negative mass

Let us now analyze moving dark solitons which obey the time-dependent Gross-Pitaevskii equation. Writing the condensate wavefunction as $\Psi(z,t) \exp(-i\mu t/\hbar)$ this equation is similar to Eq. (10.17):

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial z^2} + g|\Psi|^2\Psi - \mu\Psi.$$
(10.27)

We then assume that the function Ψ depends only on the variable z - vt, where v is the soliton velocity and represent Ψ as $\sqrt{n}f[(z - vt)/\xi]$. So, we have $f \to 1$ and df/dx = 0 for $|x| = |z - vt|/\xi \to \infty$. Equation (10.27) then reduces to

$$i\frac{v}{c_s}\frac{df}{dx} = \frac{1}{2}\frac{d^2f}{dx^2} + (1 - |f|^2)f,$$
(10.28)

where we took into account that

$$\frac{\hbar v}{\xi ng} = \frac{v}{c_s},$$



Figure 10.3: Condensate wavefunction for the dark soliton state.

with $c_s = \sqrt{ng/m}$ being the velocity of sound. Writing $f = f_1 + if_2$, where f_1 and f_2 are real, we look for the solution with $f_2 = \text{const.}$ Then, equation (10.28) leads to two equations:

$$\frac{v}{c_s}\frac{df_1}{dx} = (1 - f_1^2 - f_2^2)f_2, \qquad (10.29)$$

$$\frac{1}{2}\frac{d^2f_1}{dx^2} + (1 - f_1^2 - f_2^2)f_1 = 0.$$
(10.30)

Integrating Eq. (10.30) we find

$$f_1 = \sqrt{1 - f_2^2} \tanh\left(\sqrt{1 - f_2^2} \frac{c_s f_2}{v} x\right),$$

and substituting this solution in Eq. (10.29) we obtain $f_2 = v/c_s$. Thus, returning to the variable z - vt the solution solution is

$$\Psi = \sqrt{n} \left(i \frac{v}{c_s} + \sqrt{1 - \frac{v^2}{c_s^2}} \tanh\left[\frac{(z - vt)}{\xi} \sqrt{1 - \frac{v^2}{c_s^2}}\right] \right).$$
(10.31)

The solution (10.31) is called *grey soliton*. In the density-phase representation where we write $\Psi(z,t) = \sqrt{n(z,t)} \exp\{i\phi(z,t)\}$, we obtain the following



Figure 10.4: Density and phase for the dark soliton state.

density and phase profiles for the grey soliton:

$$n(z,t) = |\Psi|^2 = n \left(1 - \frac{1 - v^2/c_s^2}{\cosh^2[(z - vt)\sqrt{1 - v^2/c_s^2}/\xi]} \right),$$
(10.32)

$$\phi(z,t) = \frac{\pi}{2} - \arctan\left\{\frac{c_s}{v}\sqrt{1 - v^2/c_s^2} \tanh[(z - vt)\sqrt{1 - v^2/c_s^2}/\xi]\right\}.$$
 (10.33)

These profiles are displayed in Fig.10.5 and Fig.10.6. With increasing velocity v the density dip becomes smaller and so does the phase change $\Delta \phi = \phi(-\infty) - \phi(\infty)$. For v = c the density dip is zero, as well as the phase change. The grey soliton transforms into a uniform BEC state with $\Psi = \sqrt{n}$.

So, the grey soliton exists at $v < c_s$. It is a macroscopically excited Bosecondensed state, the ground state being a uniform BEC. Using Ψ (10.31) in the Hamiltonian

$$H = \int_{-\infty}^{\infty} dz \left\{ -\frac{\hbar^2}{2m} \Psi^* \frac{d^2 \Psi}{dz^2} + \frac{g}{2} |\Psi|^4 \right\}$$

we calculate the expectation value $\langle H \rangle$. Then, substracting the ground state energy $E_0 = Nng/2$ we obtain the energy of the grey soliton:

$$E_s = \langle H \rangle - E_0 = \frac{Mc_s^2}{3} \left(1 - \frac{v^2}{c_s^2} \right)^{3/2}, \qquad (10.34)$$



Figure 10.5: Density profile for the grey soliton. A change of colour from blue to brown corresponds to increasing the soliton velocity v.



Figure 10.6: Phase profile for the grey soliton. A change of colour from blue to brown corresponds to increasing the soliton velocity v.

where the quantity

$$M = 4n\xi m \tag{10.35}$$

can be identified as the soliton mass. For $v \ll c_s$ the soliton energy (10.34) becomes

$$E_s = \frac{Mc_s^2}{3} - \frac{Mv^2}{2}.$$
 (10.36)

Thus, the grey soliton can be viewed as a particle-like object with a negative mass so that any friction force, if present, accelerates the soliton.

Equation (10.34) demonstrates an important kinematic property of the grey soliton. As the soliton momentum is

$$p = \frac{\partial E_s}{\partial v} = -M \left(1 - \frac{v^2}{c_s^2}\right)^{1/2} v,$$

the quantity $-M(1-v^2/c_s^2)$ can be considered as a kinematic mass of the soliton. Its modulus decreases with increasing v and it becomes easier to accelerate the soliton by applying a friction force. This is in contrast to the case of a relativistic particle, where the kinematic mass is increasing with v, and an infinite force is required to accelerate the particle to the speed of light. Here, the grey soliton can ultimately reach the velocity of sound and disappear.

However, the problem is integrable and the soliton is transparent for the excitations. So, in order to provide a friction force one should lift the integrability. In this respect, the situation is quite different from that in the case of vortices, where the decay in the bulk is prevented by the presence of the topological charge, circulation. The grey soliton does not have a topological charge, but its decay in the bulk requires to lift the integrability, for example by adding an extra non-linearity to the Gross-Pitaevskii equation.

Problems 10

10.1 Calculate the excitation spectrum and wavefunctions for a standing bright soliton.

We first use Eq. (10.3) and rewrite the Bogoliubov-de Gennes equations (10.12) and (10.13) in the form:

$$-\frac{\hbar^2}{2m}\frac{d^2f_k^+}{dz^2} + n_0|g|\left(\frac{1}{2} - \frac{1}{\cosh^2(z/\xi)}\right)f_k^+ = \epsilon_k f_k^-, \qquad (10.37)$$

$$-\frac{\hbar^2}{2m}\frac{d^2f_k^-}{dz^2} + n_0|g|\left(\frac{1}{2} - \frac{3}{\cosh^2(z/\xi)}\right)f_k^- = \epsilon_k f_k^+, \qquad (10.38)$$

where we again use the excitation momentum at an infinite separation from the soliton, k, as the excitation quantum number ν . Turning to the variable $x = z/\xi$

and introducing a dimensionless energy $\tilde{\epsilon}_k$ we reduce Eqs. (10.37) and (10.38) to

$$\hat{H}_+ f_k^+ = \tilde{\epsilon}_k f_k^-, \qquad (10.39)$$

$$\hat{H}_{-}f_{k}^{-} = \tilde{\epsilon}_{k}f_{k}^{+}, \qquad (10.40)$$

where the operators \hat{H}_{\pm} are given by

$$\hat{H}_{\pm} = \left(-\frac{1}{2} \frac{d^2}{dx^2} + \frac{-2 \pm 1}{\cosh^2 x} + \frac{1}{2} \right).$$
(10.41)

We then transform Eqs. (10.39) and (10.40) to two fourth order differential equations:

$$(\hat{H}_{-}\hat{H}_{+})f_{k}^{+} = \tilde{\epsilon}_{k}^{2}f_{k}^{+}, \qquad (10.42)$$

$$(\hat{H}_{+}\hat{H}_{-})f_{k}^{-} = \tilde{\epsilon}_{k}^{2}f_{k}^{-}.$$
(10.43)

The operator products read:

$$\hat{H}_{-}\hat{H}_{+} = \left\{ \frac{1}{4} \frac{d^{4}}{dx^{4}} + \left(\frac{2}{\cosh^{2} x} - \frac{1}{2} \right) \frac{d^{2}}{dx^{2}} - \frac{2\sinh x}{\cosh^{3} x} \frac{d}{dx} + \frac{1}{4} \right\}, (10.44)$$
$$\hat{H}_{+}\hat{H}_{-} = \left\{ \frac{1}{4} \frac{d^{4}}{dx^{4}} + \left(\frac{2}{\cosh^{2} x} - \frac{1}{2} \right) \frac{d^{2}}{dx^{2}} - \frac{6\sinh x}{\cosh^{3} x} \frac{d}{dx} + \left(\frac{1}{4} - \frac{2}{\cosh^{2} x} + \frac{6\sinh^{2} x}{\cosh^{4} x} \right) \right\}.$$
(10.45)

Differentiatiating equation (10.42) and using Eqs. (10.44), (10.45) we then obtain:

$$(\hat{H}_{+}\hat{H}_{-})\frac{df_{k}^{+}}{dx} = \tilde{\epsilon}_{k}^{2}\frac{df_{k}^{+}}{dx}.$$
(10.46)

This is the same equation as Eq. (10.43) for f_k^- , which allows us to conclude that we may put

$$f_k^- = C f_k^+, (10.47)$$

where C is a numerical constant. Then equation (10.39) reduces to

$$\left(-\frac{1}{2}\frac{d^2}{dx^2} - \tilde{\epsilon}_k C\frac{d}{dx} - \frac{1}{\cosh^2 x} + \frac{1}{2}\right)f_k^+ = 0.$$
(10.48)

For $|x| \to \infty$ one should have $f_k^+ \propto \exp iqx$, where $q = k\xi$ is a dimensionless momentum. We then set $f_k^+ = W_+(x) \exp iqx$, where $W_+ = \text{const}$ for $|x \to \infty$, and transform equation (10.48) to an equation for the function W_+ :

$$\left(-\frac{1}{2}\frac{d^2}{dx^2} - (iq + \tilde{\epsilon}_q C)\frac{d}{dx} + \frac{k^2}{2} + \frac{1}{2} - iq\tilde{\epsilon}_q C - \frac{1}{\cosh^2 x}\right)W_+ = 0, \quad (10.49)$$

where we changed the subscript from k to q. Since for $|x| \to \infty$ the function $W_+ = \text{const}$, we should have

$$C = -i\frac{1+q^2}{2q\tilde{\epsilon}_q},\tag{10.50}$$

which transforms Eq. (10.49) to

$$\left(-\frac{1}{2}\frac{d^2}{dx^2} - \frac{i(q^2 - 1)}{2q}\frac{d}{dx} - \frac{1}{\cosh^2 x}\right)W_+ = 0.$$
 (10.51)

Introducing a new variable $y = (1 - \tanh x)/2$ equation (10.51) becomes a hypergeometrical equation

$$y(1-y)\frac{d^2W_+}{dy^2} + \left(1 - \frac{i(q^2-1)}{2q} - 2y\right)\frac{dW_+}{dx} + 2W_+ = 0.$$
(10.52)

The solution of this equation that is analytical at $y \to 0$ $(x \to \infty)$ is a simple first order polynomial:

$$W_{+} = 1 - \frac{2y}{1 - i(q^2 - 1)/2q},$$

or

$$W_{+} = \frac{q^2 - 1 + 2iq \tanh x}{(q+i)^2}.$$

Accordingly, we have

$$f_q^+ = \frac{q^2 - 1 + 2iq\tanh x}{(q+i)^2} \exp iqx,$$
(10.53)

$$f_q^- = iqC \frac{q^2 - 1 + 2iq \tanh x + 2/\cosh^2 x}{(q+i)^2} \exp iqx.$$
(10.54)

The function $v_q = (f_q^+ - f_q^-)/2$ should tend to zero for $x \to \pm \infty$ since it is localized in the spatial area of the soliton (for $x \to \pm \infty$ the density vanishes and excitations are supposed to be single particles). This immediately gives

$$C = -\frac{i}{q}.$$
 (10.55)

Substituting this result into Eq. (10.54) and returning to the momentum k and coordinate z equations (10.53) and (10.54) become Eqs. (10.14) and (10.15). From Eqs. (10.50) and (10.55) we obtain the dispersion relation $\tilde{\epsilon}_q = (1+q^2)/2$, which in terms of the momentum k and excitation energy ϵ_k leads to equation (10.16):

$$\epsilon_k = \frac{\hbar^2 k^2}{2m} + |\mu|.$$

10.2 Calculate the wavefunctions of the excitations for the (standing) dark soliton.

Lecture 11. Strongly interacting 1D Bose gases

11.1 Two-particle problem in 1D. Transmission and reflection

In this *Lecture* we discuss the strongly interacting regime for 1D Bose gases, where the condition (9.6) is not fulfilled and, moreover, we have

$$\gamma = \frac{m|g|}{\hbar^2 n} \gg 1. \tag{11.1}$$

We consider g > 0 and focus on the case of *impenetrable bosons*, where $\gamma \to \infty$. Then, instead of the usual Hamiltonian which in first quantization has the form (1.59):

$$\hat{H} = \sum_{i} -\frac{\hbar^2}{2m} \frac{d^2}{dx_i^2} + g \sum_{i>j} \delta(x_i - x_j),$$

with indices i and j labeling particles, we consider only the kinetic energy part

$$\hat{H}_{K} = \sum_{i} -\frac{\hbar^{2}}{2m} \frac{d^{2}}{dx_{i}^{2}}$$
(11.2)

and put a constraint that the wavefunction vanishes when two particles approach each other to a zero distance (see Fig.11.1).



Figure 11.1: Behavior of the wavefunction of the 1D gas of impenetrable bosons when two of them (i and j) approach each other.

The behavior of the wavefunction displayed in Fig.11.1 is clearly seen from the solution of the Schroedinger equation for 2 particles interacting with each other via a potential $g\delta(x)$. The Schroedinger equation for their relative motion reads:

$$-\frac{\hbar^2}{m}\frac{d^2\psi}{dx^2} + g\delta(x) = E\psi.$$
(11.3)

Integrating equation (11.3) over dx from $x - \beta$ to $x + \beta$ ($\beta \rightarrow 0$) we obtain:

$$\lim_{\beta \to 0} [\psi'(\beta) - \psi'(-\beta)] = \frac{mg}{\hbar^2} \psi(0).$$
(11.4)

Considering E > 0 we actually have the scattering problem, where an incident particle with mass m/2 and momentum $k = \sqrt{mE}/\hbar$ is reflected (transmitted) by the potential $g\delta(x)$ (see Fig.11.2).



Figure 11.2: Reflection/transmission of a particle by the potential $\delta(x)$.

For x < 0 we have the incident and reflected waves, and for x > 0 the transmitted wave:

$$\psi = \exp(ikx) + R\exp(-ikx), \quad x < 0, \tag{11.5}$$

$$\psi = D \exp(ikx), \qquad x > 0, \tag{11.6}$$

with $|D|^2$ and $|R|^2$ being the transmission and reflection coefficients satisfying the relation $|D|^2 + |R|^2 = 1$. Since ψ is continuous at x = 0, we should have D = 1 + R. Then, from Eqs.(11.4), (11.5) and (11.6) we obtain:

$$D = \frac{2k}{2k + img/\hbar^2},\tag{11.7}$$

$$R = \frac{img/\hbar^2}{2k + img/\hbar^2}.$$
(11.8)

We thus see that for $g \to \infty$ the transmission coefficient $|D|^2 \to 0$ and $|R|^2 \to 1$. Bosons do not go through each other, which is the origin of the term "impenetrable bosons". We also see that

 $\psi \to 0 \quad \text{for} \quad x \to 0 \quad \text{if} \quad g \to \infty.$ (11.9)

11.2 Many-body wavefunction and energy

The results of the previous section have very important consequencies. Consider two impenetrable bosons in a large box (see Fig.11.3). One can not satisfy the condition (11.9) putting both bosons in the ground state (labeled 0). The lowest energy of the pair is achieved when one of the impenetrable bosons is in the state 0 and the other one in the first excited state labeled 1. The corresponding wavefunction is

$$\psi(x_1, x_2) = |\psi_0(x_1)\psi_1(x_2) - \psi_0(x_2)\psi_1(x_1)|, \qquad (11.10)$$

where ψ_0 and ψ_1 are the single-particle eigenfunctions of the states 0 and 1. The wavefunction ψ (11.10) is symmetrical with respect to interchanging the bosons and is tending to zero for $x_1 \to x_2$.



Figure 11.3: Two impenetrable bosons (red balls) in a large box.

In analogy with Eq. (11.10), considering N impenetrable bosons one can write their wavefunction as a modulus of the Slater determinant:

$$\psi(x_1, x_2, \dots x_N) = \text{Abs} \begin{vmatrix} \psi_0(x_1) & \psi_1(x_2) & \dots & \psi_{N-1}(x_N) \\ \psi_0(x_2) & \psi_1(x_3) & \dots & \psi_{N-1}(x_1) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_0(x_N) & \psi_1(x_1) & \dots & \psi_{N-1}(x_{N-1}) \end{vmatrix}$$
(11.11)

Note that for N free fermions the wavefunction is just the Slater determinant. So, $|\psi|^2$ is the same and in this sense an infinite repulsion plays a role of the Pauli principle. All thermodynamic quantities are the same since they are determined by $|\psi|^2$. The same statement holds for the energy spectrum.

Let us calculate the energy at T = 0. Free N fermions occupy the lowest N single-particle eigenstates. These are the states with momenta from k = 0 to $k = k_F$ and from k = 0 to $k = -k_F$, where k_F is called the Fermi momentum and is determined by the relation

$$\int_{-k_F}^{k_F} \frac{dk}{2\pi} L = N,$$

where L is the length of the box. Thus, $k_F = \pi N/L = \pi n$, and the corresponding eigenenergy $E_F = \hbar^2 k_F^2/2m$ is called Fermi energy (see Fig.11.4).



Figure 11.4: Distribution of impenetrable bosons (free fermions) over the energy states in a large box at T = 0

The total energy of the 1D gas of free fermions (impenetrable bosons) is given by

$$E = \int_{-k_F}^{k_F} \frac{\hbar^2 k^2}{2m} \frac{Ldk}{2\pi} = \frac{\hbar^2 k_F^3}{6\pi m} L = \frac{\hbar^2 \pi^2}{6m} \frac{N^3}{L^2}.$$
 (11.12)

The energy per particle, or chemical potential is

$$\mu = \frac{\partial E}{\partial N} = \frac{\hbar^2 \pi^2 n^2}{2m} = E_F. \tag{11.13}$$

11.3 Excitation spectrum

We now discuss the excitation spectrum of 1D impenetrable bosons relying on its analogy with the spectrum of free fermions. Consider T = 0 and put a particle out of the filled energy space in Fig.11.4 (filled momentum space in Fig.11.5) outside this space. Let say, put a particle with momentum $k_F - q$ to the state with momentum $k_F + k$ (q, k > 0, see Fig.11.5). Then the energy of the formed particle-hole pair is

$$\epsilon = \frac{\hbar^2}{2m} [(k_F + k)^2 - (k_F - q)^2].$$
(11.14)

For $k, q \ll k_F$ we then get

$$\epsilon = \hbar v_F(k+q) = \hbar v_F p, \qquad p \ll k_F, \tag{11.15}$$

where $v_F = \hbar k_F/m$ is the Fermi velocity. So, for small p the excitations are phonons and the "speed of sound" is the Fermi velocity v_F .



Figure 11.5: Creation of a particle-hole pair in the momentum distribution of free fermions at T = 0

For k, q comparable with k_F the situation changes. Putting k = p - q in Eq. (11.14) we have:

$$\epsilon_{pq} = \frac{\hbar^2}{2m} \left[(k_F + p - q)^2 - (k_F - q)^2 \right] = \frac{\hbar^2}{2m} [2k_F p + (p - q)^2 - q^2]. \quad (11.16)$$

As we see, the excitation energy also depends on q, and for this reason we write ϵ with the subscript pq. Note that $0 \leq q \leq 2k_F$ and for $p = 2k_F$ we have $0 \leq \epsilon_{pq} \leq 4E_F$. The energy spectrum is shown in Fig.11.6.



Figure 11.6: Excitation spectrum of 1D impenetrable bosons. Depending on the value of q the excitation energy can take any value in between the blue and brown curves.

11.4 Hydrodynamic equations. One-body density matrix

Since the low-energy excitations are phonons, the 1D gas of impenetrable bosons should obey hydrodynamic equations. In order to see this, we consider a general case of finite g > 0 and go back to equations (8.12) and (8.13) for the density and pghase operators. Assuming that at least on a long distance scale fluctuations of the phase gradient and density are small, we will only keep terms that are linear

in $\delta \hat{n}$ and $\nabla \phi$. Then, we put $\sqrt{\hat{n}} = \sqrt{n}$ in the right hand side of Eq. (8.12), where n is the mean density. In the left hand side of this equation we put $\sqrt{\hat{n}} = \delta \hat{n}/2\sqrt{n}$. In the right hand side of Eq. (8.13) we omit the first term which is quadratic in $\nabla \phi$. Multiplying both sides of this equation by $(\sqrt{\hat{n}})^{-1}$ and comparing the right hand side with that of Eq. (8.14) we then notice that it can be written as $\mu(\hat{n})$. The corresponding therm that is linear in $\delta \hat{n}$ is $(\partial \mu/\partial n)\delta \hat{n}$. For the uniform case, we thus obtain the continuity and Euler equations in the form:

$$\frac{\partial \delta \hat{n}}{\partial t} = -\frac{\hbar n}{m} \nabla^2 \hat{\phi}, \qquad (11.17)$$

$$\frac{\partial \hat{\phi}}{\partial t} = -\frac{1}{\hbar} \frac{\partial \mu}{\partial n} \delta \hat{n}, \qquad (11.18)$$

which allows us to consider the limit $g \to \infty$.

Differentiating Eq. (11.17) with respect to t and substituting $\partial \hat{\phi} / \partial t$ from Eq. (11.18) we obtain:

$$\frac{\partial^2 \delta \hat{n}}{\partial t^2} = \frac{n}{m} \frac{\partial \mu}{\partial n} \frac{\partial^2 \delta \hat{n}}{\partial z^2} = v_F^2 \frac{\partial^2 \delta n}{\partial z^2}, \qquad (11.19)$$

where we used Eq. (11.13) for the chemical potential of a uniform gas of impenetrable bosons. Equation (11.19) immediately gives the energy spectrum (11.15): $\epsilon_k = \hbar v_F k$, and quantization relations for $\delta \hat{n}$ and ϕ :

$$\delta \hat{n} = \sum_{k} \left(\frac{k}{\pi L}\right)^{1/2} \exp(ikz - i\epsilon_k t/\hbar) \hat{b}_k + h.c.$$
(11.20)

$$\hat{\phi} = (-i)\sum_{k} \left(\frac{\pi}{kL}\right)^{1/2} \exp(ikz - i\epsilon_k t/\hbar)\hat{b}_k + h.c.$$
(11.21)

We can now calculate the long-distance form of the one-body density matrix assuming that fluctuations of the density are small on a large distance scale and writing the field operator in the form (8.22): $\hat{\Psi} = \sqrt{n} \exp(i\hat{\phi}_p)$. Like in previous lectures, the subscript p means that we have to restrict the summation in Eq. (11.21) only to the phonon part of the excitation spectrum. For impenetrable bosons this is equivalent to putting a high-momentum cut-off $k_{max} \sim k_F \sim 1/n$. For the mean square fluctuations of the phase we then have:

$$\langle [\hat{\phi}_p(z,0) - \hat{\phi}_p(0,0)^2 \rangle = \int_{-k_{max}}^{k_{max}} \frac{2\pi (1 - \cos kz)}{k} \frac{dk}{2\pi} \approx \ln n|z|, \quad |z| \gg n^{-1}.$$
(11.22)

This gives the long-distance form of the one-body density matrix at equal times:

$$g_1(z) = \langle \hat{\Psi}^{\dagger}(z,0)\hat{\Psi}(0,0)\rangle = n \exp\left\{-\frac{1}{2}\langle [\hat{\phi}_p(z,0) - \hat{\phi}_p(0,0)]^2 \rangle\right\} \propto \frac{1}{|z|^{1/2}}.$$
(11.23)

Accordingly, the momentum distribution of impenetrable bosons is

$$n(p) = \int_{-\infty}^{\infty} g_1(z) \exp ipz \, dz \propto \frac{1}{\sqrt{|p|}}, \qquad |p| \ll p_F.$$
(11.24)

This is very different from the Fermi-step n(p) of free fermions (see Fig.11.7). We thus conclude that although the thermodynamic quantities and excitation spectrum of impenetrable bosons are the same as those of free fermions, the correlation properties are quite different.



Figure 11.7: Momentum distribution of impenetrable bosons and free fermions.

Problems 11

11.1 Consider a 1D gas of impenetrable bosons in a harmonic potential $V(z) = m\omega^2 z^2/2$. Calculate the excitation spectrum and wavefunctions assuming the Thomas-Fermi regime.

The density profile in the Thomas-Fermi regime follows from the local density approximation:

$$\frac{m\omega^2 z^2}{2} + \mu(n(z)) = \mu.$$
(11.25)

In this approximation in every small piece of the system one has a local value of the chemical potential determined from the relation for a uniform system at density equal to the density in a given piece. For the case of impenetrable bosons we have $\mu = \pi^2 \hbar^2 n^2 / 2m$ and Eq. (11.25) yields

$$n(z) = n(0)(1 - z^2/L_{TF}^2)^{1/2}$$
(11.26)

for $|z| < L_{TF}$ and zero otherwise. The Thomas-Ferm size of the sample is given by $L_{TF} = (2\mu/m\omega^2)^{1/2}$. The continuity and Euler equations are obtained in the same way as equations (11.17) and (11.18), but taking into account that now the mean density is coordinate-dependent. This gives

$$\frac{\partial \delta \hat{n}}{\partial t} = -\frac{\hbar}{m} \nabla \left(n(z) \nabla \hat{\phi} \right), \qquad (11.27)$$

$$\frac{\partial \phi}{\partial t} = -\frac{1}{\hbar} \frac{\partial \mu}{\partial n} \delta \hat{n}. \tag{11.28}$$

Again, differentiating Eq. (11.27) with respect to t and substituting $\partial \hat{\phi} / \partial t$ from Eq. (11.28) we obtain

$$\frac{\partial^2 \delta \hat{n}}{\partial t^2} = \frac{\pi^2 \hbar^2}{m^2} \frac{\partial}{\partial z} n(z) \frac{\partial}{\partial z} n(z) \delta \hat{n}.$$
(11.29)

Writing quatization relations for the density and phase fluctuations in the form:

$$\delta \hat{n} = \sum_{j} A_j f_j(z) \exp(-i\epsilon_j t/\hbar) \hat{b}_j + h.c.$$
(11.30)

$$\hat{\phi} = (-i)\sum_{j} B_j f_j(z) \exp(-i\epsilon_j t/\hbar) \hat{b}_j + h.c.$$
(11.31)

where ϵ_j are eigenmode energies and $f_j(z)$ eigenfunctions, and using n(z) (11.26) we transform equation (11.29) into

$$v_F^2(0)\frac{d}{dz}\left(1-\frac{z^2}{L_{TF}^2}\right)^{1/2}\frac{d}{dz}\left(1-\frac{z^2}{L_{TF}^2}\right)^{1/2}f_j+\omega_j^2f_j=0,$$
(11.32)

with $\omega_j = \epsilon_j/\hbar$. Introducing a new variable $\tau = \arcsin(z/L_{TF})$ we reduce Eq. (11.32) to

$$\frac{d^2 f_j}{d\tau^2} + \frac{\omega_j^2}{\omega^2} f_j = 0 \tag{11.33}$$

and obtain odd and even solutions;

$$f_j = \sin\left(\frac{\omega_j}{\omega}\tau\right),$$
 (11.34)

$$f_j = \cos\left(\frac{\omega_j}{\omega}\tau\right). \tag{11.35}$$

Since

$$\frac{df_j}{dz} \propto \frac{1}{1 - z^2 / L_{TF}^2} \frac{df_j}{d\tau}$$

and it should be finite at the Thomas-Fermi boarder where $z = \pm L_{TF}$ and $\tau = \pm \pi/2$, the derivative $df_j/d\tau$ should be zero for this value of τ . This immediately gives the spectrum

$$\omega_j = \omega j, \tag{11.36}$$

with j being a positive integer, and the eigenfunctions (11.34) and (11.35) become

$$f_j = \sin(j \arcsin z/L_{TF}), \quad j \text{ odd}$$
 (11.37)

$$f_j = \cos(j \arcsin z/L_{TF}).$$
 j even (11.38)

Lecture 12. Rapidly rotating Bose gases

12.1 Single-particle problem for a rapidly rotating harmonically trapped atom

In this *Lecture* which is the last one in the part of Bose-condensed gases, we discuss rapidly rotating bosons. It will be shown that in some sense this problem also belongs to the class of one-dimensional problems.

Let us consider a Bose gas confined to two dimensions, x and y, and rotating with frequency Ω around the z axis in an external (shallow) harmonic potential $V(r) = m\omega^2 r^2/2$ ($r^2 = x^2 + y^2$). We first discuss the single-particle problem. The corresponding Hamiltonian reads:

$$\hat{H}^{(1)} = -\frac{\hbar^2}{2m} \Delta_{\mathbf{r}} + \frac{m\omega^2 r^2}{2} - \hbar \Omega \hat{L}_z, \qquad (12.1)$$

where the operator of orbital angular momentum is

$$\hat{L}_z = i \left(y \frac{\partial}{\partial x} - x \frac{\partial}{\partial y} \right).$$
(12.2)

We certainly consider $\Omega < \omega$, otherwise the centrifugal force exceeds the restoring force and the sample disintegrates.

The Hamiltonian (12.1) can be reduced to the form:

$$\hat{H}^{(1)} = -\frac{\hbar^2}{2m} (\nabla_{\mathbf{r}} - i\mathbf{A})^2 + (\omega^2 - \Omega^2) \frac{mr^2}{2}, \qquad (12.3)$$

where $\mathbf{A} = m\Omega(\hat{\mathbf{z}} \times \mathbf{r})/\hbar$ with $\hat{\mathbf{z}}$ being a unit vector in the *z* direction. Equation (12.3) is identical to the Hamiltonian of a particle with a unit charge in a uniform magnetic field $(2m\Omega/\hbar)\hat{\mathbf{z}}$ and confined in a harmonic potential $m(\omega^2 - \Omega^2)r^2/2$. A common eigenbasis of \hat{L}_z and $\hat{H}^{(1)}$ is (without a normalization coefficient):

$$\Phi_{jk}(\mathbf{r}) = \exp\left(\frac{r^2}{2l^2}\right) \left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)^j \left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)^k \exp\left(-\frac{r^2}{l^2}\right), \quad (12.4)$$

where $l = (\hbar/m\omega)^{1/2}$ is the (initial) harmonic oscillator length, and j, k are non-negative integers. The corresponding eigenenergies are given by

$$E_{jk} = \hbar\omega + \hbar(\omega - \Omega)j + \hbar(\omega + \Omega)k.$$
(12.5)

Let us consider ω very close to Ω so that $\delta \omega = (\omega - \Omega) \ll \Omega$. Then, for $\delta \omega = 0$ we have zero remaining confinement (put infinite walls at a large distance in order to prevent the disintegration of the cloud), which corresponds to a free charged particle in a uniform magnetic field and the well-known structure of Landau levels (see Fig.12.1):

$$E_k = \hbar \Omega (2k+1). \tag{12.6}$$



Figure 12.1: Structure of Landau levels for rotating trapped atom for $\Omega = \omega$ and for $\Omega < \omega$ ($\delta \omega = (\omega - \Omega) \ll \Omega$).

The distance between the lowest Landau levels is $2\hbar\Omega$. In the lowest Landau level (LLL, k = 0), the wavefunction of a particle is

$$\psi(\mathbf{r}) = f(z) \exp\left(-\frac{r^2}{2l^2}\right),\tag{12.7}$$

where z = x + iy, and f is any analytic function of z so that the LLL is infinitely degenerate.

If $\omega > \Omega$, then each Landau level has sublevels ($\delta \omega \ll \Omega$) and

$$E_{jk} = \hbar\omega + \hbar(\Omega + \omega)k + \hbar\delta\omega j.$$
(12.8)

So, the LLL is no longer degenerate (see Fig.12.1). For each j the wavefunction has the form (12.7) with

$$f_j(z) = \frac{z^j}{l^{j+1}\sqrt{\pi j!}}.$$
 (12.9)

The quantity z^j is equal to $r^j \exp(ij\phi)$, where ϕ is the asimuthal angle. So, the quantum number j is the orbital angular momentum of the eigenstate.

12.2 Rapidly rotating Bose-Einstein condensate

Let us now consider a rapidly rotating Bose-Einstein condensate at T = 0, assuming that $\delta \omega \ll \Omega$ and the interaction energy per particle is $ng \ll \hbar \Omega$. We then can say that there is a Bose-Einstein condensate in the lowest Landau level. The condensate wavefunction has to be of the form

$$\psi_0 = \sqrt{n}f(z)\exp\left(-\frac{r^2}{2l^2}\right),\qquad(12.10)$$

where again z = x + iy, and to zero order we do not distinguish between the total density n and the condensate density. The Gross-Pitaevskii equation reads:

$$\left[-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + \frac{m\omega^2 r^2}{2} - i\hbar\Omega\left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right) + ng|\psi_0^2 - \mu\right]\psi_0 = 0, \quad (12.11)$$

and substituting ψ_0 (12.10) we reduce it to

$$\exp\left(-\frac{r^2}{2l^2}\right) \left[\hbar\delta\omega z \frac{d}{dz} + ngf(z)f^*(\bar{z})\exp\left(-\frac{r^2}{l^2}\right) - \tilde{\mu}\right]f(z) = 0, \quad (12.12)$$

where $\bar{z} = x - iy$, and $\tilde{\mu} = \mu - \hbar \omega$. We can now write

$$f(z) = \sum_{j} C_{j} f_{j}(z), \qquad (12.13)$$

where $f_j(z)$ are given by Eq. (12.9). Then, multiplying Eq. (12.12) by $\psi_q^* = f_q^*(\bar{z}) \exp(-r^2/2l^2)$, where q is a non-negative integer, and integrating over d^2r we obtain:

$$\hbar \delta \omega \sqrt{q(q-1)} C_{q-1} - \tilde{\mu} C_q$$

$$+ \frac{ng}{\pi} \sum_{j_1, j_2, q} \frac{C_{j_1} C_{j_2} C^*_{j_1+j_2-q}}{\Gamma} (j_1 + j_2 + 1) 2^{-j_1-j_2-1} \sqrt{\Gamma(j_1+1)\Gamma(j_2+1)\Gamma(q+1)\Gamma(j_1+j_2-q+1)}$$

This is a 1D equation. It gives the coefficients C_j , which provides the wavefunction of the problem following from equations (12.10) and (12.13). Thus, in the space of orbital angular momenta the LLL problem becomes one-dimensional. However, being based on the solution of Eq. (12.14) it is a difficult problem, and in the next section we show a more convinient approach.

12.3 Projected Gross-Pitaevskii equation. Vortex lattice

The more convinient approach assumes that one first of all projects the mean field equation (12.12) onto the LLL. The projection operator has the form:

$$\hat{P} = \frac{1}{2\pi} \exp(z\bar{z}' - z'\bar{z}'/2), \qquad (12.15)$$

where we now use the coordinates z, \bar{z} in units of l, which is equivalent to putting l = 1. The action of \hat{P} on a certain function ψ reads:

$$\hat{P}\psi(z,\bar{z}) = \frac{1}{2\pi} \int \psi(z',\bar{z}') \exp(z\bar{z}' - z'\bar{z}'/2) \, dz' d\bar{z}', \qquad (12.16)$$

and it projects the function ψ onto the LLL. Acting with the operator \hat{P} on Eq. (12.12) we obtain:

$$\hbar\delta\omega z \frac{df(z)}{dz} + \frac{ng}{2\pi} \int f^2(z') f^*(\bar{z}') \exp(z\bar{z}' - 2z'\bar{z}') dz' d\bar{z}' - \tilde{\mu}f(z) = 0. \quad (12.17)$$

The easyest case is the one with $\delta \omega = 0$, i.e. in the absence of remaining trapping. Then the solution of Eq. (12.17) gives a vortex lattice described by the wavefunction

$$\psi_0 = \theta(z) \exp(z^2/2 - z\bar{z}/2), \qquad (12.18)$$

where $\theta(z)$ is the Jacobi θ -function which for a square lattice is given by

$$\theta(z) = \sum_{j=-\infty}^{\infty} (-1)^j \exp(-\pi (j+1/2)^2 + i\sqrt{\pi}(2j+1)z.$$
(12.19)

Actually, the ground state is a triangular lattice, with a somewhat more complicated expression for $\theta(z)$.

The mean-field approach for describing the vortex lattice is valid if the number of vortices is much smaller than the number of particles. The period of the vortex lattice and the size of the vortex core are of the order of l. Hence, the number of vortices is $N_v \sim A/l^2$, where A is the suerface area. The number of particles is $N \sim nA$. So, the condition $N_v \ll N$ takes the form

$$nl^2 \gg 1.$$
 (12.20)

Problems 12

12.1 Consider a 2D Bose-condensed gas trapped in a harmonic potential with frequency ω and rotating with frequency Ω such that $\delta \omega = (\omega - \Omega) \ll \Omega$. Find a condition under which the ground state is a condensate without vortices. Obtain a quantum transition to the state with one vortex and identify the order of the transition.

For the state without vortices we have $f_0(z) = 1/\sqrt{\pi}$, where the subscript of f indicates the number of vortices and the harmonic oscillator length l is again put equal to unity. From Eq. (12.17) we then find the chemical potential

$$\tilde{\mu}_0 = \frac{ng}{2\pi},\tag{12.21}$$

where n is the mean density equal to the number of particles N once l is set equal to unity. This corresponds to the energy

$$E = \frac{N^2 g}{4\pi}.\tag{12.22}$$

For the state with one vortex we have $f_1(z) = z/\sqrt{\pi}$, and equation (12.17) yields

$$\tilde{\mu}_1 = \hbar \delta \omega + \frac{ng}{4\pi},\tag{12.23}$$

which leads to the energy

$$E_1 = \hbar \delta \omega N + \frac{N^2 g}{8\pi}.$$
(12.24)

The state without vortices remains the ground state when $E_0 < E_1$, or

$$\hbar\delta\omega < \frac{ng}{8\pi}.\tag{12.25}$$

At the point where

$$\frac{ng}{8\pi} = \hbar\delta\omega, \qquad (12.26)$$

one has a quantum phase transition to the state with one vortex. The chemical potential undergoes a jump at this point (see Fig.12.2):

$$\tilde{\mu}_1 - \tilde{\mu}_0 = -\hbar\delta\omega. \tag{12.27}$$

The quantum phase transition, i.e. the transition at T = 0 under a change of one of the parameters of the system (for example, g in our particular case), at which the chemical potential has a jump is called first order quantum transition.



Figure 12.2: Energy of a rapidly rotating trapped Bose gas, E, versus the coupling constant g for the BEC state without vortices and for the one-vortex BEC in the lowest Landau level. The red ball shows the point of quantum transition between these states, which occurs at the coupling constant following from Eq. (12.26).

Ultracold quantum Gases Part 2 Degenerate Fermi gases

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Abstract

This is the second part of our lecturing course on ultracold quantum gases. It discusses ultracold degenerate gases of fermionic atoms and is focused on the role of interactions and on superfluidity. After creating quantum degenerate atomic Fermi gases, experiments have reached the so-called strongly interacting regime bringing analigies with neutron stars and high temperature superconductivity. Therefore, aside from an Introduction to the theory of degenerate fermions, the lecturing course includes several modern developments in this domain.

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Lecture 1. Key quantities. Elastic and inelastic interaction between atoms

1.1 Length and energy scales

Characteristic length scales for a gas of atomic fermions are the same as in the case of bosonic atoms. They have been introduced in *Part 1* of the lecturing course in section 1.1. So, there is the thermal de Broglie wavelength $\Lambda_T = (2\pi\hbar^2/mT)^{1/2}$, where *m* is the atom mass, and *T* the gas temperature, and this length scale is inversely proportional to the thermal wavevector of atoms, k_T . Then, there is a characteristic radius of interaction between atoms, R_e . The wavefunction of the atoms is influenced by the interaction only at interactomic distances of the order of or smaller than R_e , and at much larger distances their motion is free. The third length scale is the mean interatomic separation, $n^{-1/3}$, with *n* being the gas density.

The so-called dilute and ultracold limits have been also introduced in section 1.1 of *Part 1*. The dilute limit assumes that the mean interparticle distance is much larger than the characteristic radius of interaction, i.e. $n^{-1/3} \gg R_e$ or $nR_e^3 \ll 1$. Note that this condition is necessary for considering the system as a gas.

The ultracold limit relies on the condition $\Lambda_T \gg R_e$, i.e. it assumes that the de Broglie wavelength of particles greatly exceeds the radius of interaction between them. In a dilute ultracold gas we usually consider only pair interactions and collisions between the particles. The inequality $\Lambda_T \gg R_e$ provides the dominant role of *s*-wave collisions, that is the collisions with zero orbital angular momentum. However, for identical fermions the *s*-wave scattering is not possible because the wavefunction of the relative motion should change sign under permutation of the fermions. Thus, only the scattering with odd orbital angular momenta is allowed, and the leading channel is the *p*-wave scattering, i.e. the scattering with orbital angular momentum l = 1. We will see that this leads to a crucial difference of fermions from bosons with respect to collisional properties.

As well as in the case of bosons, we introduce the degeneracy parameter $n\Lambda_T^3$. When the de Broglie wavelength Λ_T is much smaller than the mean interparticle separation $n^{-1/3}$ and hence $n\Lambda_T^3 \ll 1$, then the gas is classical and it obeys the Boltzmann statistics. In the case of $n\Lambda_T^3 \gtrsim 1$, which in principle can be achieved either by decreasing the temperature or by increasing the density, the gas becomes *degenerate* and *quantum statistics* comes into play. For fermions this leads to the formation of *Fermi sea*.

Let us consider a gas of non-interacting single-component fermions in free space (the term *single-component* means that all particles are in the same internal quantum state). Then the particle wavevector \mathbf{k} is a good quantum number and the mean occupation number of the state with a given \mathbf{k} is governed by the Fermi distribution:

$$N_k = \frac{1}{\exp\{(E_k - \mu)/T\} + 1},$$
(1.1)

where μ is the chemical potential, and $E_k = \hbar^2 k^2 / 2m$ is the single particle kinetic energy. The dependence of the chemical potential on T and n follows from the normalization condition:

$$N = \sum_{\mathbf{k}} N_k = \int N_k \frac{V d^3 k}{(2\pi)^3},$$
 (1.2)

with N being the total number of particles, and V the volume of the system.

For T = 0 one has to have $\mu_0 > 0$ and

$$N_k = 0; \text{ for } E_k > \mu_0,$$

 $N_k = 1; \text{ for } E_k < \mu_0.$ (1.3)

In other words, N identical fermions in the ground state occupy N lowest quantum states, so that there is one fermion in each such state. This is clear from the idea of Fermi statistics, where due to the Pauli principle there is not more than one fermion in a given quantum state. Then, equation (1.2) at T = 0 takes the form:

$$N = \int_0^{k_F} V \frac{4\pi k^2 dk}{8\pi^3} = \frac{V k_F^3}{6\pi^2},$$
(1.4)

where the quantities $\hbar^2 k_F^2/2m = \mu_0 \equiv E_F$ and $\hbar k_F$ are called *Fermi energy* and *Fermi momentum*.

The zero-temperature distribution function N_k has a stepwise behavior and is shown in black in Fig 1.1. At a finite T such that $T \ll E_F$, the mean occupation number N_k is smaller than 1 at $k < k_F$, and there are occupied states $(N_k > 0)$ at $k > k_F$. The corresponding distribution function is given by the blue curve in Fig. 1.1.



Figure 1.1: The distribution function N_k as a function of the fermion momentum k at zero temperature (in black) and at a finite temperature $T \ll E_F$ (in blue).

From Eq. (1.4) we obtain the Fermi momentum as a function of the density at T = 0:

$$\hbar k_F = \hbar \left(\frac{6\pi^2 N}{V}\right)^{1/3} = \hbar (6\pi^2 n)^{1/3}.$$
(1.5)

Accordingly, for the Fermi energy we have:

$$E_F = \frac{(6\pi^2)^{2/3}}{2} \frac{\hbar^2 n^{2/3}}{m}.$$
 (1.6)

The de Broglie wavelength of particles with energies $\sim E_F$ is

$$\Lambda_F = \left(\frac{2\pi\hbar^2}{mE_F}\right)^{1/2} = n^{-1/3} \left(\frac{4}{3\sqrt{\pi}}\right)^{1/3}.$$
 (1.7)

So, we have $n\Lambda_F^3 \sim 1$, which is obvious as the Fermi energy is of the order of the temperature of quantum degeneracy. At $T \leq E_F$ the Fermi gas is degenerate

and for this reason the distribution function displayed in Fig. 1.1 is drastically different from that for the classical gas. It is called the *Fermi sea*.

We thus see that without interactions there are two energy scales in the Fermi gas, temperature T and Fermi energy E_F . The first quantum degenerate Fermi gas has been obtained at JILA in 1998 (D. Jin, ⁴⁰K), and presently tens of labs all over the world are working with degenerate fermions. As well as ultracold bosonic atoms, they are created by evaporative and optical cooling in magnetic and optical traps as discussed in the course of J.T.M. Walraven. Ongoing experiments are commonly dealing with temperatures from 100 nK to $1 \ \mu K$ and densities ranging from 10^{12} to 10^{14} cm⁻³. The number of fermionic atoms is usually in the range from 10^4 to 10^7 .

1.2 Interaction between identical fermions

The third energy scale is established by the interaction between particles. In the dilute limit where the condition $nR_e^3 \ll 1$ is satisfied, the total interaction energy in the system is the sum of all pair interactions, $E_{int} = (N^2/2)\epsilon_{int}$, where $N \gg 1$ is the number of particles, $N^2/2$ is the number of pairs, and ϵ_{int} is the interaction energy for a pair of atoms. Two important circumstances should be mentioned at this point. First of all, we consider here elastic interaction between particles, i.e. the interaction which does not change their internal states. Second, we assume the regime of weak interactions, where the interaction between particles can be taken into account in a sort of many-body perturbative approach. The related criterion will be discussed later in this *Lecture*.

The quantity ϵ_{int} has been calculated in section 1.2 of *Part 1* of the course. It is expressed through the phase shift (amplitude) of scattering of two particles with relative wavevector k and orbital angular momentum l. The derivation in section 1.2 of *Part 1* is given for the s-wave scattering (l = 0), but it remains exactly the same for $l \neq 0$. So, for given values of k and l we have:

$$\epsilon_{int}(l,k) = \frac{\langle g_l(k) \rangle}{V}; \quad g_l(k) = -\frac{4\pi\hbar^2}{m} \left(\frac{\delta_l(k)}{k}\right), \tag{1.8}$$

where $\delta_l(k)$ is the scattering phase shift for the orbital angular momentum l, and the symbol $\langle \rangle$ stands for the average over the momentum distribution of particles. Note that equation (1.8) does not take into account correlations between particles and for momentum-dependent g_l a special care should be taken in this respect.

The scattering phase shift follows from the condition that in the limit of interatomic separations $r \to \infty$ the wavefunction of the relative motion of two atoms with orbital angular momentum l takes the form

$$\psi_l(r) \sim \frac{\sin(kr - \pi l/2 + \delta_l)}{kr}$$

The calculation of δ_l relies on the knowledge of the potential of interaction between the atoms, U(r). This is done in *Problem 1.1* to this lecture. The

interaction potential U(r) for the atoms has a Van der Waals long-range tail, i.e. it decays at large distances as $1/r^6$. In this case, for identical fermions the leading interaction (scattering) channel is the *p*-wave scattering and away from resonances the corresponding phase shift is

$$\delta_1(k) = -\frac{(kb)^3}{3},$$
(1.9)

where b is a characteristic distance which depends on the shape of U(r), and we assume the inequality $k|b| \ll 1$.

For small k the p-wave scattering phase shift is much smaller than the phase shift for the s-wave scattering. The latter is given by $\delta_0 = -ka$, where a is the so-called scattering length. This is because for l = 1 the centrifugal barrier reduces the probability for particles to approach each other at short distances where the potential U(r) provides an efficient scattering (see *Problem 1.1* to this lecture).

In the case of identical fermions, using equations (1.8) and (1.9) we obtain

$$g(k) = \frac{4\pi\hbar^2}{3m} (k^2 b^3).$$
(1.10)

The total interaction energy then becomes

$$E_{int} = \frac{N^2}{2V} \langle g(k) \rangle = \frac{4\pi\hbar^2 b^3}{3mV} \langle k^2 \rangle \frac{N^2}{2}, \qquad (1.11)$$

and the interaction energy per particle is given by

$$\frac{\partial E_{int}}{\partial N} = n \langle g(k) \rangle, \tag{1.12}$$

assuming that $\langle g(k) \rangle$ is independent of the density. Note, however, that the presence of this dependence only changes the numerical coefficient.

At $T \ll E_F$ characteristic momenta of fermions are of the order of $\hbar k_F$ and from Eqs. (1.10) and (1.12) we find the interaction energy per particle $n\langle g(k)\rangle \sim E_F(nb^3)$. In the opposite limit of a classical Fermi gas, $T \gg E_F$, where characteristic particle momenta are of the order of the thermal momentum $\hbar k_T = \hbar (mT/\hbar^2)^{1/2}$, we obtain $n\langle g(k)\rangle \sim T(nb^3)$. The atomic distance |b| is generally of the order of R_e , and hence in the dilute limit we have the inequality $n|b|^3 \ll 1$. We thus see that at both low and high temperatures the interaction energy is smaller than the kinetic energy of particles by a factor of $n|b|^3$. At realistic densities $n \sim 10^{12} - 10^{14}$ cm⁻³ this factor is ranging from 10^{-9} to 10^{-5} (away from *p*-wave resonances) and therefore the interaction between identical fermions is usually omitted.

1.3 Elastic and inelastic collisions

The characteristic distance b is directly related to all parameters of elastic p-wave scattering. The two-body scattering problem has been discussed in detail

in section 1.3 of *Part 1* of the course. This problem is equivalent to the scattering of a particle with mass m/2 from a force center, due to the particle-center interaction via the potential U(r). As a result of the interaction, an incident particle moving along the axis z with momentum \mathbf{k} is scattered on an angle θ and acquires the momentum \mathbf{k}' (see section 1.3 of *Part 1*). For elastic scattering we have $|\mathbf{k}'| = |\mathbf{k}|$. At an infinite separation from the center the particle wavefunction is a superposition of the incident plane wave and scattered spherical wave:

$$\psi = \exp(ikz) + \frac{f(\theta)}{r} \exp(ikr), \qquad (1.13)$$

where $f(\theta)$ is called the scattering amplitude. The probability $\alpha(k)$ for the scattered wave to pass through the surface of a sphere of radius r per unit time is equal to the intensity of the scattered wave $|f(\theta)|^2/r^2$ multiplied by $vr^2d\Omega$ and integrated over the solid angle Ω . Here $v = 2\hbar k/m$ is the velocity of the incident particle or, returning to the two-body scattering problem, the relative velocity of colliding atoms. We thus have $\alpha(k) = \int v |f(\theta)|^2 d\Omega$, and this quantity is called the rate constant of elastic collisions. The number of scattering events per unit time and unit volume is given by $\bar{\alpha}N^2/2V$, where $\bar{\alpha}$ is the rate constant averaged over the momentum distribution of particles. The number of collisions that a given particle experiences per unit time is $\bar{\alpha}n$, and the quantity $(\bar{\alpha}n)^{-1}$ can be identified as a characteristic collisional or kinetic time τ_K . The quantity $\sigma(k) = \alpha(k)/v = \int |f(\theta)|^2 d\Omega$ has a dimension of surface area and is called the elastic cross section. The mean free path of a particle is $\lambda \sim 1/(n\sigma)$.

For finding the scattering amplitude $f(\theta)$ one commonly expands it in Legendre polynomials:

$$f(\theta) = \sum_{l=0}^{\infty} (2l+1) f_l P_l(\cos \theta),$$

where f_l are called partial scattering amplitudes. They correspond to the scattering with orbital angular momentum l. The solution of the two-body scattering problem in section 1.3 of *Part 1* and in *Problem 1.1* to this lecture establish a relation between the partial scattering amplitude f_l and the scattering phase shift δ_l :

$$f_l = \frac{\tan \delta_l}{k(1 - i \tan \delta_l)}.$$

For $k|b| \ll 1$, using Eq. (1.9) we immediately obtain the *p*-wave scattering amplitude

$$f_1 = -\frac{1}{3}b(kb)^2. \tag{1.14}$$

This amplitude is actually very small. Since the parameter b is generally of the order of R_e , we have $|f_1| \ll R_e$. The scattering cross section is $\sigma_1 \sim b^2(kb)^4$ and in the ultracold limit it is at least several orders of magnitude smaller than R_e^2 . The rate of elastic collisions is $\alpha_1 = \sigma_1 v \propto k^5$ and is generally very slow. For realistic parameters in cold gases we have the collisional time $\tau_K = (\bar{\alpha}n)^{-1}$ exceeding seconds. Therefore, elastic collisions between identical fermions usually do not play an important role.

We now discuss inelastic collisions, i.e. collisions changing the internal states of the colliding atoms. Consider a gas of atoms which can be in two different internal states, the ground state A_1 and an excited (hyperfine) state A_2 . Then, binary collisions involving atoms in the state A_2 can lead to their relaxation transition to the ground state. One may consider, for example, the following inelastic collisional process:

$$A_2 + A_2 \Rightarrow A_1 + A_1 + 2\Delta E,$$

where ΔE is the difference between energies of the internal states A_2 and A_1 . Usually in cold gases ΔE greatly exceeds the kinetic energy of colliding atoms, so that the final state of the pair is independent of the initial collision energy (momentum). In this respect, inelastic collisions in cold gases can be identified as "deep inelastic processes".

Inelastic collisions involving the s-wave in the incoming channel have been discussed in section 1.4 of Part 1 of the course. For collisions of identical fermions only odd angular momenta l in the incoming channel are possible and usually the p-wave (l = 1) is the most important. This makes inelastic collisions rather slow in the dilute ultracold limit, which is already seen without any calculations. Consider two fermions at large separations \mathbf{r} from each other, where the interaction potential U(r) is no longer important. Then the wavefunction of their relative motion is simply an antisymmetrized superposition of plane waves

$$\psi = \frac{1}{\sqrt{2}} \left[\exp(i\mathbf{kr}) - \exp(-i\mathbf{kr}) \right].$$

In the ultracold limit the inequality $kR_e \ll 1$ is satisfied, and there is a large interval of distances where $R_e \ll r \ll 1/k$ and the interaction is still not important. In this interval, expanding the exponents in powers of (\mathbf{kr}) we obtain $\psi \propto (\mathbf{kr})$. So, we may say that "cold identical fermions do not like to approach each other". The dependence $\psi \propto k$ is preserved with decreasing the interatomic separation r and making it of the order of or smaller than R_e . The interaction only changes the coordinate dependence of ψ irrespective of the value of k. The rate of an inelastic decay process is proportional to the square of the transition matrix element of an inelastic interaction between the initial and final states. For deep inelastic processes, the wavefunction and energy of the final state are practically independent of the initial momentum k. Thus, the only quantity that depends on k is the initial wavefunction ψ , which immediately shows that the inelastic rate is $\alpha_{in} \propto k^2$.

This conclusion is confirmed by calculations in *Problem 1.2* to this lecture. In general, the rate of inelastic processes depends on the shape of the interaction potential U(r) and on the interaction providing inelastic transitions. In order to obtain the dependence of the inelastic rate on the relative momentum k of colliding atoms we simplified the problem and assumed that the internal states of the atoms are completely changed once the interatomic distance reaches a certain value r_0 . At the same time it is assumed that inelastic transitions do not occur at $r > r_0$. This is equivalent to putting a perfectly absorbing wall
at $r = r_0$, so that there is only an incoming spherical flux at this point (see *Problem 1* to this *Lecture*).

As the rate of inelastic collisions between identical fermions is proportional to k^2 , it is usually not very important in ultracold gases.

1.4 Two-component Fermi gas. Weakly interacting regime.

The situation with interparticle interaction drastically changes in a two-component Fermi gas, i.e. when fermionic atoms in two different internal states are present. The interaction between fermions of different components originates from their *s*-wave scattering. The phase shift for the *s*-wave scattering is given by $\delta_0 = -ka$ assuming that $k|a| \ll 1$, where the quantity *a* is called the scattering length and it depends on the shape of the potential U(r) (see section 1.2 of *Part 1*). The *s*-wave scattering amplitude is $f_0 = -a$ as follows from equation (1.37) in *Part 1* at $k|a| \ll 1$ and *Problem 1.1* to this lecture. Accordingly, the contribution of the intercomponent interaction to the interaction energy in the system is

$$E_{int}^{0} = \frac{4\pi\hbar^2 a}{mV} N_1 N_2, \qquad (1.15)$$

where the first multiple is the interaction energy for an atomic pair consisting of fermions in different internal states, and the second multiple represents the number of such pairs, with N_1 and N_2 being the number of particles in the first and second component.

Let us now assume that $N_1 = N_2 = N$ and compare the energy of the intercomponent interaction (1.15) with the energy of interaction between fermions in the same internal state (intracomponent interaction). The latter originates from the *p*-wave scattering and follows from Eq. (1.11):

$$E_{int}^1 = \frac{4\pi\hbar^2 b^3}{3mV} \langle k^2 \rangle N^2, \qquad (1.16)$$

where N^2 appears as $(N_1^2/2 + N_2^2/2)$ for $N_1 = N_2 = N$. On the other hand, for $N_1 = N_2 = N$ equation (1.15) gives

$$E_{int}^{0} = \frac{4\pi\hbar^2 a}{mV} N^2.$$
 (1.17)

Generally, we have $|a| \sim |b| \sim R_e$ and in the ultracold dilute limit the ratio of the intra- to intercomponent interaction energy is

$$\frac{E_{int}^1}{E_{int}^0} \sim \langle k^2 \rangle R_e^2 \ll 1$$

The intercomponent interaction leads to the interaction energy per particle

$$ng = \frac{4\pi\hbar^2 a}{m}n \sim E_F(k_F a) \sim E_F(na^3)^{1/3}$$
(1.18)

and it can no longer be omitted. Moreover, as we will see later in the course, this interaction leads to all interesting physics in dilute Fermi gases.

Usually, the interaction between particles in quantum gases is treated within the many-body perturbation theory. For Fermi gases this assumes that the interaction energy per particle is much smaller than the characteristic kinetic energy of particles. In the case of quantum degenerate fermions, the latter is $\sim E_F$. Then, from Eq. (1.18) we immediately find the condition of such *weakly interacting* regime:

$$k_F|a| \ll 1 \rightarrow (n|a|^3)^{1/3} \ll 1.$$
 (1.19)

This condition should be certainly completed by the criterion of the dilute limit, $nR_e^3 \ll 1$, which is especially important if for a given potential U(r) the scattering length a turns out to be anomalously small.

Problems 1

1.1 Calculate the phase shift and scattering amplitude for elastic scattering with orbital angular momentum l in the limit of low collision energies. Show that the scattering with l > 0 is much weaker than the s-wave scattering (l = 0).

The scattering problem for two particles with equal masses m is equivalent to the scattering of a particle with mass m/2 from the force center, due to the particle-center interaction via the potential U(r). The Schroedinger equation for the relative motion of these particles then reads:

$$\left[-\frac{\hbar^2}{m}\Delta_{\mathbf{r}} + U(r)\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}),\tag{1.20}$$

where $E = \hbar^2 k^2 / m$ is the collision energy. We now expand the wavefunction of the relative motion of colliding atoms, $\psi(\mathbf{r})$ in Legendre polynomials:

$$\psi(\mathbf{r}) = \sum_{l} (2l+1) P_l(\cos\theta) \psi_l(r), \qquad (1.21)$$

where θ is the scattering angle, and $\psi_l(r)$ is the wavefunction of the relative motion with orbital angular momentum l. Since we took the z axis (the axis along the wave vector of the incident plane wave) as the axis of quantization, due to the axial symmetry of our scattering problem the wavefunction $\psi(\mathbf{r})$ (1.21) is independent of the azimuthal angle ϕ . Substituting $\psi(\mathbf{r})$ (1.21) into the Schroedinger equation (1.20), multiplying both sides of the equation by $P_{l'}(\cos \theta)$ and integrating over the solid angle we obtain an equation for the relative motion with a given orbital angular momentum l:

$$-\frac{\hbar^2}{m} \left[\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{l(l+1)}{r^2} \right] \psi_l(r) + U(r)\psi_l(r) = \frac{\hbar^2 k^2}{m} \psi_l(r).$$
(1.22)

When obtaining Eq. (1.22) we took into account the well-known expression for the Laplacian in spherical coordinates:

$$\Delta_{\mathbf{r}} = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{\partial^2}{\partial \theta^2} + \cot\theta\frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial \phi^2}\right)$$

and the fact that

$$\left(\frac{d^2}{d\theta^2} + \cot\theta \frac{d}{d\theta}\right) P_l(\cos\theta) = -l(l+1)P_l(\cos\theta).$$

Equation (1.22) can be rewritten in the form:

$$-\frac{\hbar^2}{m} \left[\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right] \psi_l(r) + U_{eff}(r)\psi_l(r) = \frac{\hbar^2 k^2}{m} \psi_l(r), \qquad (1.23)$$

with

$$U_{eff}(r) = U(r) + \frac{\hbar^2 l(l+1)}{mr^2}$$
(1.24)

being the so-called effective potential (see Fig. 1.2).



Figure 1.2: Effective potential $U_{eff}(r) = U(r) + \hbar^2 l(l+1)/mr^2$ for the relative motion with orbital angular momentum l.

At distances $r \gg R_e$ we can drop U(r) from Eq. (1.22), which transforms it to the equation of free motion with orbital angular momentum l. The solution then reads:

$$\psi \propto \left[j_l(kr) + C\eta_l(kr) \right]. \tag{1.25}$$

The spherical Bessel and Neumann functions, j_l and η_l , have the following asymptotic behavior at large arguments:

$$j_l(x) \Rightarrow \frac{\sin(x - \pi l/2)}{x}; \quad x \to \infty$$
 (1.26)

$$\eta_l(x) \Rightarrow -\frac{\cos(x-\pi l/2)}{x}; \quad x \to \infty$$
 (1.27)

The scattering phase shift δ_l is defined by writing ψ_l at $r \to \infty$ as

$$\psi_l \propto \frac{\sin(kr - \pi l/2 + \delta_l)}{kr}, \quad r \to \infty.$$
 (1.28)

For U(r) = 0 we have $\delta_l = 0$ and $\psi_l \propto j_l(kr)$. Comparing Eq. (1.28) with Eq. (1.25) we obtain:

$$\tan \delta_l = -C. \tag{1.29}$$

At distances where $R_e \ll r \ll k^{-1}$, we may drop both U(r) and $\hbar^2 k^2/m$ from the Schroedinger equation (1.22) and then obtain

$$\psi_l \propto \left(r^l - \frac{b^{2l+1}}{r^{l+1}} \right), \tag{1.30}$$

where the length b is independent of k. Importantly, we assume that U(r) decays faster than r^{-2l-3} and, hence, the term b^{2l+1}/r^{2l+3} originating from the kinetic energy exceeds the potential energy term $U(r)r^l$. Within a normalization coefficient, Eq. (1.30) should coincide with ψ_l following from Eq. (1.25) at $kr \ll 1$. Taking into account asymptotic expressions for the spherical Bessel and Neumann functions at small arguments:

$$j_l(x) \Rightarrow \frac{\sqrt{\pi}}{2^{l+1}\Gamma(l+3/2)} x^l \quad x \ll 1$$
 (1.31)

$$\eta_l(x) \Rightarrow (-1)^l \frac{2^l \sqrt{\pi}}{\Gamma(1/2 - l)} x^{-l-1}; \quad x \ll 1,$$
 (1.32)

we reduce ψ_l (1.25) at $kr \ll 1$ to

$$\psi_l \propto \left[\frac{\sqrt{\pi}}{2^{l+1}\Gamma(l+3/2)} (kr)^l + (-1)^l C \frac{2^l \sqrt{\pi}}{\Gamma(1/2-l)} (kr)^{-l-1} \right].$$

The comparison of this expression with Eq. (1.30) immediately gives

$$C = (-1)^{l} \left(\frac{bk}{2}\right)^{2l+1} \frac{\Gamma(1/2 - l)}{\Gamma(l+3/2)}$$
(1.33)

and Eq. (1.29) yields

$$\tan \delta_l = (-1)^{l+1} \left(\frac{kb}{2}\right)^{2l+1} \frac{\Gamma(1/2-l)}{\Gamma(l+3/2)}.$$
(1.34)

Using the expansion of the scattering amplitude in Legendre polynomials given by Eq. (1.21) and recalling that at $r \to \infty$ the total wavefunction ψ is given by Eq. (1.13), we write the *l*-wave part of ψ as

$$\psi_l = i^l \frac{\sin(kr - \pi l/2)}{kr} + \frac{f_l}{r} \exp(ikr)$$

and after a certain algebra transform it to

$$\psi_l \propto \frac{1}{kr} \{ (1 + ikf_l) \sin(kr - \pi l/2) + kf_l \cos(kr - \pi l/2) \}.$$

Since this expression should coincide within a normalization coefficient with ψ_l (1.28) we immediately find a relation between the scattering phase shift and scattering amplitude:

$$f_l = \frac{\tan \delta_l}{k(1 - i \tan \delta_l)} \equiv \frac{\exp(2i\delta_l) - 1}{2ik}.$$
(1.35)

In the limit of low collision energies we put $k|b| \ll 1$ and obtain;

$$f_l = \frac{\delta_l}{k} = (-1)^{l+1} \frac{b}{2} \left(\frac{kb}{2}\right)^{2l} \frac{\Gamma(1/2 - l)}{\Gamma(l + 3/2)}$$
(1.36)

then the l-wave scattering cross section is

$$\sigma_l = 4\pi (2l+1)|f_l|^2 = \frac{4\pi}{k^2} (2l+1)\sin^2 \delta_l \propto k^{4l}.$$
 (1.37)

We thus see that for slow particles the *l*-wave scattering (away from *l*-wave resonances) is much weaker than the *s*-wave scattering. The physical reason is that the centrifugal barrier of the effective potential $U_{eff}(r)$ reduces the amplitude of the wavefunction at short distances where the interaction potential U(r) acts.

1.2 Calculate the inelastic rate constant for collisions of identical ultracold fermions interacting with each other via the potential U(r) representing a perfectly absorbing wall at $r = r_0$ and having a deep potential well for $r_0 < r < R_0$ (see Fig. 1.3).

We start with Eq. (1.23) for the wavefunction $\psi_l(r)$ of the relative motion with orbital angular momentum l. We assume that the collision energy E_k and the centrifugal potential $\hbar^2 l(l+1)/mr_0^2$ are much smaller than the well depth U_0 . Then, for $r_0 < r < R_0$ the solution of Eq. (1.23) reads:

$$\psi_l(r) = A\{j_l(k_0 r) + Bh_l(k_0 r)\},\tag{1.38}$$



Figure 1.3: The interaction potential U(r) having a perfectly absorbing wall at $r = r_0$ and a deep potential well for $r_0 < r < R_0$. The brown curve shows the effective piotential $U_{eff}(r) = U(r) + \hbar^2 l(l+1)/mr^2$.

where j_l and h_l are spherical Bessel and Hankel functions, $k_0 = \sqrt{mU_0}/\hbar$, and the coefficients A and B have to be determined. The presence of the perfectly absorbing wall at $r = r_0$ means that for $r \to r_0$ we only have an incoming spherical flux and hence $\psi_l(r) \propto \exp[-ik_0(r-r_0)]$. The assumption $\hbar^2 l(l+1)/mr_0^2 \ll U_0$ is equivalent to $k_0 r_0 \gg 1$, i.e. the arguments of the Bessel and Hankel functions in Eq. (1.38) are large. This allows us to use the asymptotic expression (1.26) and a similar asymptotic expression for h_l :

$$h_l(x) \Rightarrow -i \frac{\exp(ix - i\pi l/2)}{x}; \quad x \to \infty.$$
 (1.39)

Then, in order to satisfy the boundary condition for $r \to r_0$ we should put B = -1/2, and the wavefunction in the interval of distances $r_0 < r < R_0$ takes the form

$$\psi_l(r) = \frac{iA}{2k_0 r} \exp(-ik_0 r + i\pi l/2).$$
(1.40)

For $r > R_0$ the motion is free and we write the solution as

$$\psi_l(r) = i^l [j_l(kr) + ik f_l h_l(kr)]$$
(1.41)

so that at $r \to \infty$ the second term in Eq. (1.41) becomes $(f_l/r) \exp(ikr)$ and thus describes an outgoing spherical wave with orbital angular momentum l,

with f_l being the *l*-wave scattering amplitude. Note that multiplying Eq. (1.41) by $(2l+1)P_l(\cos\theta)$, making the summation over *l*, and using the relations

$$\exp(ikz) = \sum_{l} i^{l}(2l+1)j_{l}(kr)P_{l}(\cos\theta); \quad f(\theta) = \sum_{l} (2l+1)f_{l}P_{l}(\cos\theta),$$

where $f(\theta)$ is the total scattering amplitude, we obtain the required expression for the wavefunction $\psi(\mathbf{r})$ at $r \to \infty$:

$$\psi(\mathbf{r}) = \exp(ikz) + \frac{f(\theta)}{r}\exp(ikr).$$

In the ultracold limit we have $kR_0 \ll 1$ and at r close to R_0 in Eq. (1.41) we may use the asymptotic expression (1.31) and the asymptotic expression

$$h_l(x) \Rightarrow \frac{i(-1)^{l+1}\sqrt{\pi}}{\Gamma(1/2-l)} \frac{2^l}{x^{l+1}}; \quad x \ll 1.$$
 (1.42)

Then, equalizing the wavefunctions (1.41) and (1.40) and their derivatives at $r = R_0$ and using the inequality $k_0 R_0 \gg 1$, we obtain:

$$f_{l} = \frac{ij_{l}(kR_{0})}{kh_{l}(kR_{0})} \left[1 - \frac{(2l+1)i}{k_{0}R_{0}} \right] = \frac{(-1)^{l+1}\Gamma(1/2-l)(kR_{0})^{2l}}{\Gamma(l+3/2)2^{2l+1}} \left[1 - \frac{(2l+1)i}{k_{0}R_{0}} \right] R_{0}, (1.43)$$
$$|A| = 2(2l+1)j_{l}(kR_{0}) = \frac{\sqrt{\pi}(2l+1)}{2^{l}\Gamma(l+3/2)}(kR_{0})^{l}.$$
(1.44)

The inelastic rate constant is equal to the incoming flux at $r \to r_0$, multiplied by the surface area $4\pi r_0^2$:

$$\alpha_{in} = \frac{\hbar}{im} \left\{ \left(\psi_l \frac{d\psi_l^*}{dr} - \psi_l^* \frac{d\psi_l}{dr} \right) \times 4\pi r^2 \right\}_{r \to r_0}.$$
 (1.45)

Using ψ_l (1.40) with |A| (1.44), we obtain

$$\alpha_{in} = \frac{2\pi\hbar|A|^2}{mk_0} = \frac{2\pi^2\hbar}{mk_0} \left[\frac{(2l+1)}{\Gamma(l+3/2)}\right]^2 \left(\frac{kR_0}{2}\right)^{2l}.$$
 (1.46)

For identical fermions only odd l are possible, and the leading decay channel is related to the *p*-wave scattering (l = 1). Thus, we have

$$\alpha_{in} \simeq \frac{8\pi\hbar}{mk_0} \, (kR_0)^2 \propto k^2. \tag{1.47}$$

Taking into account that for identical fermions the wavefunction should be antisymmetrized, we have to multiply Eq. (1.47) by a factor of 2.

The obtauined result (1.47) justifies the dimensional estimate $\alpha_{in} \propto k^2$ obtained in subsection 1.3.

1.3. Find the *l*-wave scattering amplitude and the inelastic rate constant in the limit of $k \to 0$ for the scattering potential which has the form $U(r) = -\beta/r^4$ at $r \ge r_0$ and and has a perfectly absorbing wall at $r = r_0$ (see Fig. 1.4). Assume the validity of the WKB approximation at $r \to r_0$.



Figure 1.4: The scattering potential $U(r) = -\beta/r^4$ $(r > r_0)$ with a perfectly absorbing wall at $r = r_0$ (brown curve). The effective potential $U_{eff}(r) = U(r) + \hbar^2 l(l+1)/mr^2$ is shown by the blue curve.

Lecture 2. Second quantization. Ideal Fermi gas

2.1 Second quantization

We now introduce the method of second quantization for fermions. For simplicity we first consider N identical fermions in a large but finite volume and assume that they do not interact with each other, so that the Hamiltonian is

$$\hat{H}_{kin} = -\frac{\hbar^2}{2m} \sum_{\alpha} \frac{\partial^2}{\partial \mathbf{r}_{\alpha}^2},\tag{2.1}$$

where particles are labelled by the index α and \mathbf{r}_{α} are their coordinates. The many-body wavefunction is antisymmetric with respect to an interchange of fermionic particles and has the form of a Slater determinant:

$$\psi = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_{p_1}(\mathbf{r}_1) & \psi_{p_1}(\mathbf{r}_2) & \dots & \psi_{p_1}(\mathbf{r}_N) \\ \psi_{p_2}(\mathbf{r}_1) & \psi_{p_2}(\mathbf{r}_2) & \dots & \psi_{p_2}(\mathbf{r}_N) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_{p_N}(\mathbf{r}_1) & \psi_{p_N}(\mathbf{r}_2) & \dots & \psi_{p_N}(\mathbf{r}_N) \end{vmatrix}$$
(2.2)

where $\psi_{p_i}(\mathbf{r}_k)$ are wavefunctions of single-particle states. In order to establish the sign of ψ we numerate the states by the numbers

$$p_1 < p_2 < p_3 < \dots < p_N. \tag{2.3}$$

All p_i (2.3) are different from each other so that the occupation numbers N_i can be only 1 or 0.

Consider now an operator

$$\hat{F}^{(1)} = \sum_{\alpha} \hat{f}(\mathbf{r}_{\alpha}).$$
(2.4)

Its matrix elements will be non-zero only between the states with the same $N_1, N_2, ...$ or between the states in which one of these numbers increases by 1 and another one decreases by 1. For the diagonal matrix element we have:

$$\bar{F}^{(1)} = \sum_{i} f_{ii}^{(1)} N_i, \qquad (2.5)$$

as well as in the case of bosons, and the notation

$$f_{ik}^{(1)} = \int \psi_i^*(\mathbf{r}) f^{(1)}(\mathbf{r}) \psi_k(\mathbf{r}) d^3r$$
 (2.6)

is again used for the matrix element between the single particle states i and k. For the matrix element between the many-body states 1_i , 0_k and 0_i , 1_k (in the initial state $N_k = 1$, $N_i = 0$ and in the final state $N_k = 0$, $N_i = 1$, and it is assumed that i < k) we have

$$\langle 1_i, 0_k | F^{(1)} | 0_i, 1_k \rangle = f_{ik}^{(1)} (-1)^{A_{ik}},$$
 (2.7)

where A_{ik} is the sum of the occupation numbers for the states from i + 1 to k - 1:

$$A_{ik} = \sum_{j=i+1}^{\kappa-1} N_j.$$
 (2.8)

For i = k - 1 one should put $A_{ik} = 0$.



Figure 2.1: Two identical fermions (red balls) in three possible single-particle states (blue lines). The configurations from left to right show two-particle states a), b), and c) (see text).

As an example, consider 2 identical fermions and assume that each of them can be in one of the 3 states as depicted in Fig. 2.1. There are 3 two-particle states:

(a)
$$\frac{1}{\sqrt{2}} \{ \psi_1(\mathbf{r}_1) \psi_2(\mathbf{r}_2) - \psi_1(\mathbf{r}_2) \psi_2(\mathbf{r}_1) \},$$
 (2.9)

(b)
$$\frac{1}{\sqrt{2}} \{ \psi_1(\mathbf{r}_1) \psi_3(\mathbf{r}_2) - \psi_1(\mathbf{r}_2) \psi_3(\mathbf{r}_1) \},$$
 (2.10)

(c)
$$\frac{1}{\sqrt{2}} \{ \psi_2(\mathbf{r}_1) \psi_3(\mathbf{r}_2) - \psi_2(\mathbf{r}_2) \psi_3(\mathbf{r}_1) \}.$$
 (2.11)

Matrix elements of the operator $\hat{F} = \hat{f}(\mathbf{r}_1) + \hat{f}(\mathbf{r}_2) + \hat{f}(\mathbf{r}_3)$ between these states are:

$$F_{ba} = f_{32}$$

$$F_{ca} = -f_{31}$$

$$F_{cb} = f_{21}$$

$$F_{aa} = f_{11} + f_{22}$$

$$F_{bb} = f_{11} + f_{33}$$

$$F_{cc} = f_{22} + f_{33}.$$

One can easily check that these relations coincide with what we get from Eqs. (2.5) and (2.7).

We now turn to the operators \hat{a}_i which act not on the functions of particle coordinates, but on the functions of occupation numbers:

$$\hat{a}_i | N_1, N_2, ..., N_i, ... \rangle \Rightarrow | N_1, N_2, ..., N_i - 1, ... \rangle,$$
 (2.12)

$$\hat{a}_{i}^{\dagger}|N_{1}, N_{2}, ...N_{i}, ...\rangle \Rightarrow |N_{1}, N_{2}, ...N_{i} + 1, ...\rangle.$$
 (2.13)

The operators \hat{a}_i and \hat{a}_i^{\dagger} are called annihilation and creation operators of particles. In order to write the operator $\hat{F}^{(1)}$ as

$$\hat{F}^{(1)} = \sum_{i,k} f_{ik}^{(1)} \hat{a}_i^{\dagger} \hat{a}_k, \qquad (2.14)$$

like in the case of bosons, the annihilation and creation operators should be determined as matrices with elements

$$\langle 0_i | \hat{a}_i | 1_i \rangle = \langle 1_i | \hat{a}_i^{\dagger} | 0_i \rangle = (-1)^{A_{0i}}.$$
 (2.15)

For the product of such matrices we find (for i < k):

$$\langle 1_i, 0_k | \hat{a}_i^{\dagger} \hat{a}_k | 0_i, 1_k \rangle = \langle 1_i, 0_k | \hat{a}_i^{\dagger} | 0_i, 0_k \rangle \times \langle 0_i, 0_k | \hat{a}_k | 0_i, 1_k \rangle = (-1)^{[A_{0i} + A_{0k}]}.$$
(2.16)

Since in the second matrix element the occupation number $N_i = 0$, we may write

$$A_{0k} = \sum_{j=1}^{k-1} N_j = \sum_{j=1}^{i-1} N_j + \sum_{j=i+1}^{k-1} N_j = A_{0i} + A_{ik}.$$

We then obtain

$$\langle 1_i, 0_k | \hat{a}_i^{\dagger} \hat{a}_k | 0_i, 1_k \rangle = (-1)^{A_{ik}}.$$
 (2.17)

For i = k the matrix $\hat{a}_i^{\dagger} \hat{a}_i$ is diagonal:

$$\hat{a}_i^{\dagger} \hat{a}_i = N_i \tag{2.18}$$

(zero element for $N_i = 0$ and unity for $N_i = 1$).

Reversing the order of the operators we again obtain the result of Eq. (2.16) (i < k):

$$\langle 1_i, 0_k | \hat{a}_k \hat{a}_i^{\dagger} | 0_i, 1_k \rangle = \langle 1_i, 0_k | \hat{a}_k | 1_i, 0_k \rangle \times \langle 1_i, 1_k | \hat{a}_i^{\dagger} | 0_i, 1_k \rangle = (-1)^{[A_{0i} + A_{0k}]}.$$

However, now in the first matrix element the occupation number $N_i = 1$ and, hence,

$$A_{0i} = \sum_{j=1}^{i-1} N_j = \sum_{j=1}^{k-1} N_j - \sum_{j=i}^{k-1} A_{0k} - A_{ik} - 1$$

Thus, we get

$$\langle 1_i, 0_k | \hat{a}_k \hat{a}_i^{\dagger} | 0_i, 1_k \rangle = (-1)^{2A_{0k} - A_{ik} - 1} = (-1) \times (-1)^{A_{ik}}$$
(2.19)

So, comparing Eq. (2.19) with Eq. (2.17) we see that

$$\hat{a}_{i}^{\dagger}\hat{a}_{k} + \hat{a}_{k}\hat{a}_{i}^{\dagger} = 0; \quad i \neq k.$$
 (2.20)

For the diagonal matrix we can write:

$$\hat{a}_i \hat{a}_i^{\dagger} = 1 - N_i,$$
 (2.21)

so that

$$\hat{a}_i \hat{a}_i^{\dagger} + \hat{a}_i^{\dagger} \hat{a}_i = 1.$$
(2.22)

A general relation can be written as

$$\hat{a}_i \hat{a}_k^{\dagger} + \hat{a}_k^{\dagger} \hat{a}_i = \delta_{ik}.$$
(2.23)

Similarly, we can obtain

$$\hat{a}_i \hat{a}_k + \hat{a}_k \hat{a}_i = 0. \tag{2.24}$$

The Hamiltonian (2.1) has only diagonal matrix elements. In free space the particle momentum is a good quantum number and plane waves form a complete set of basis functions. Thus, in terms of the operators $\hat{a}_{\mathbf{k}}$ and $\hat{a}_{\mathbf{k}}^{\dagger}$, equation (2.1) can be written as

$$\hat{H}_{kin} = \sum_{\mathbf{k}} E_k \hat{a}^{\dagger}_{\mathbf{k}} \hat{a}_{\mathbf{k}}, \qquad (2.25)$$

with $E_k = \hbar^2 k^2 / 2m$ being the single particle kinetic energy.

Relying on Eqs. (2.23) and (2.24) we can establish commutation relations for the field operators $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^{\dagger}(\mathbf{r})$ defined as

$$\hat{\psi}(\mathbf{r}) = \sum_{i} \hat{a}_{i} \psi_{i}(\mathbf{r}), \qquad (2.26)$$

$$\hat{\psi}^{\dagger}(\mathbf{r}) = \sum_{i} \hat{a}_{i}^{\dagger} \psi_{i}^{*}(\mathbf{r}), \qquad (2.27)$$

and representing annihilation and creation operators of a fermionic particle at the point \mathbf{r} . We have

$$\hat{\psi}^{\dagger}(\mathbf{r})\hat{\psi}(\mathbf{r}') + \hat{\psi}(\mathbf{r}')\hat{\psi}^{\dagger}(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}').$$
(2.28)

$$\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}') + \hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}) = 0.$$
(2.29)

In terms of the field operators $\hat{\psi}(\mathbf{r})$, $\hat{\psi}^{\dagger}(\mathbf{r})$ the Hamiltonian (2.25) takes the form:

$$\hat{H}_{kin} = -\int d^3 r \,\psi^{\dagger}(\mathbf{r}) \frac{\hbar^2}{2m} \Delta_{\mathbf{r}} \hat{\psi}(\mathbf{r}).$$
(2.30)

We thus see that the fermionic operators anticommute, in contrast to bosonic operators which commute. In a mixture of bosons and fermions, the operators of the fermions commute with bosonic operators. In a multicomponent Fermi system, the operators of different fermions can be considered as both commutative or anticommutative. The final results for physical quantities remain the same.

We finally present a useful relation for the square of the matrix element of the operator $\hat{a}_i^{\dagger} \hat{a}_k$ for $i \neq k$:

$$|\langle N_{i}+1, N_{k}-1|\hat{a}_{i}^{\dagger}\hat{a}_{k}|N_{i}, N_{k}\rangle|^{2} = \langle N_{i}, N_{k}|\hat{a}_{i}\hat{a}_{i}^{\dagger}\hat{a}_{k}^{\dagger}\hat{a}_{k}|N_{i}, N_{k}\rangle = N_{k}(1-N_{i}).$$
(2.31)

Let us now consider a two-component Fermi gas and omit the interaction between identical fermions. Then we only have the *s*-wave interaction between fermions of different components (internal states), which we denote as \uparrow and \downarrow . In the first quantization the interaction Hamiltonian reads:

$$\hat{H}_{int} = \sum_{\alpha\uparrow,\beta\downarrow} U(\mathbf{r}_{\alpha\uparrow} - \mathbf{r}_{\beta\downarrow}), \qquad (2.32)$$

where $\mathbf{r}_{\alpha\uparrow}$ and $\mathbf{r}_{\beta\downarrow}$ are coordinates of \uparrow and \downarrow fermions, and $U(\mathbf{r})$ is the potential of pair interaction between such fermions. The amplitude of the *s*-wave scattering in the ultracold limit is momentum independent and equal to -a, where *a* is the scattering length. The corresponding coupling constant for the interparticle interaction is $g = 4\pi\hbar^2 a/m$. Then, the secondly quantized interaction Hamiltonian in terms of the field operators $\hat{\psi}(\mathbf{r})$, $\hat{\psi}^{\dagger}(\mathbf{r})$ takes the form:

$$\hat{H}_{int} = g \int d^3 r \, \hat{\psi}_{\uparrow}^{\dagger}(\mathbf{r}) \hat{\psi}_{\downarrow}^{\dagger}(\mathbf{r}) \hat{\psi}_{\downarrow}(\mathbf{r}) \hat{\psi}_{\uparrow}(\mathbf{r}).$$
(2.33)

In free space, where the wavevector \mathbf{k} of a particle is a good quantum number, equation (2.33) can be rewritten through the creation and annihilation operators in the momentum space:

$$\hat{H}_{int} = \frac{g}{V} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3} \hat{a}^{\dagger}_{\mathbf{k}_3 \uparrow} \hat{a}^{\dagger}_{\mathbf{k}_4 \downarrow} \hat{a}_{\mathbf{k}_1 \downarrow} \hat{a}_{\mathbf{k}_2 \uparrow}, \qquad (2.34)$$

and there is a momentum conservation law $\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4$. The derivation of equations (2.34) and (2.33) is exactly the same as in the case of bosons in subsections 2.2 and 2.3 of *Lecture 2* in *Part 1* of the course and we do not repeat this derivation here.

2.2 Thermodynamics of an ideal Fermi gas

We now turn to thermodynamic properties of an ideal Fermi gas. For simplicity, we first consider a single-component Fermi gas in free space. It is described by the Hamiltonian (2.25). As we discussed in subsection 1.1 of *Lecture 1*, the distribution function (occupation number averaged over the ensemble) at T = 0is a filled Fermi sphere: $N_{\mathbf{k}} = \theta(k_F - k)$, where the Fermi wavevector k_F and Fermi energy E_F are given by Eqs. (1.5) and (1.6), and $\theta(x)$ is the step function equal to zero for negative arguments and to unity for positive ones. So, all states with $E < E_F$ or $k < k_F$ are occupied, and the states with higher energies (above the Fermi surface) are empty. The zero-temperature distribution function $N_{\mathbf{k}}$ is given in black in Fig. 1.1. It is the limiting case of the general Fermi distribution (1.1) at $T \to 0$, and the zero-temperature chemical potential is $\mu_0 = E_F$ (see subsection 1.1 of *Lecture 1*). The energy of the ideal single-component Fermi gas at T = 0 is

$$E = \int N_{\mathbf{k}} E_k \frac{V d^3 k}{(2\pi)^3} = \int_0^{k_F} \frac{\hbar^2}{m} k^4 \frac{V dk}{4\pi^2} = \frac{\hbar^2 k_F^5 V}{20\pi^2 m} = \frac{\hbar^2 V}{20\pi^2 m} \left(\frac{6\pi^2 N}{V}\right)^{5/3} = \frac{3}{5} E_F N, \quad (2.35)$$

where we used equation (1.4) providing a relation between the Fermi momentum $\hbar k_F$ and the total number of particles N.

Let us now consider temperatures $T \ll E_F$ and develop calculations of thermodynamic functions of the ideal Fermi gas. At these temperatures the chemical potential is close to the Fermi energy and our first step will be to find the deviation of μ from E_F . For this purpose we turn from the integration over k to the integration over $E_k = \hbar^2 k^2/2m$ in the expression providing a relation between the density and chemical potential through the Fermi distribution function. Using Eq. (1.1) we have:

$$n = \int \frac{d^3k}{(2\pi)^3} N_{\mathbf{k}} = \int_0^\infty \frac{4\pi k^2 dk}{(2\pi)^3} \frac{1}{\exp\{(E_k - \mu)/T\} + 1} = \int_0^\infty \frac{\nu(E) dE}{\exp\{(E - \mu)/T\} + 1}, \quad (2.36)$$

where

$$\nu(E) = \left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{E^{1/2}}{4\pi^2}$$
(2.37)

is the density of states. We then represent Eq. (2.36) as

$$n = \int_{-\mu}^{0} \frac{\nu(E - \mu + \mu)d(E - \mu)}{\exp\{(E - \mu)/T\} + 1} + \int_{0}^{\infty} \frac{\nu(E - \mu + \mu)d(E - \mu)}{\exp\{(E - \mu)/T\} + 1}$$

and write in the first integral

$$\frac{1}{\exp\{(E-\mu)/T\}+1} = 1 - \frac{\exp\{(E-\mu)/T\}}{\exp\{(E-\mu)/T\}+1} = 1 - \frac{1}{\exp(\epsilon/T)+1}$$

where $\epsilon = \mu - E$. In the second integral we write $E - \mu = \epsilon$. Then we have:

$$n = -\int_0^\mu \frac{\nu(\mu - \epsilon)d\epsilon}{\exp(\epsilon/T) + 1} + \int_0^\infty \frac{\nu(\mu + \epsilon)d\epsilon}{\exp(\epsilon/T) + 1} + \int_0^\mu \nu(E)dE.$$
 (2.38)

The values of ϵ which give the main contribution to the first two integrals are of the order of $T \ll \mu$. Therefore, we extend the integration to infinity in the first integral, and then we expand the density of states $\nu(\mu \pm \epsilon)$ in powers of ϵ up to the linear term:

$$u(\mu \pm \epsilon) = \nu(\mu) \pm \epsilon \frac{d\nu}{dE}.$$

This yields

$$n = \int_0^{\mu} \nu(E) dE + 2T^2 \frac{d\nu(\mu)}{d\mu} \int_0^{\infty} \frac{x dx}{\exp(x) + 1}.$$

Using Eq. (2.37) and the fact that $\int_0^\infty x [\exp(x) + 1]^{-1} dx = \pi^2/12$ we then find

$$n = \left(\frac{1}{6\pi^2} + \frac{T^2}{48\mu^2}\right) \left(\frac{2m\mu}{\hbar^2}\right)^{3/2}.$$
 (2.39)

The second term in Eq. (2.39) is much smaller than the first one and we may put $\mu = E_F$ in this term, whereas in the first term we should write $\mu = E_F + \delta$, where δ is a small deviation of the chemical potential from the Fermi energy. We thus obtain a linear equation for δ , which gives

$$\delta = -\frac{\pi^2}{12} \left(\frac{T}{E_F}\right)^2 E_F. \tag{2.40}$$

In a similar way we calculate the energy of the gas:

$$E = \int \frac{Vd^{3}k}{(2\pi)^{3}} \frac{E_{k}}{\exp\{(E_{k}-\mu)/T\}+1} = V \int_{0}^{\infty} \frac{E\nu(E)dE}{\exp\{(E-\mu)/T\}+1}$$
$$= V \int_{0}^{\mu} E\nu(E)dE \left[1 - \frac{\exp\{(E-\mu)/T\}}{\exp\{(E-\mu)/T\}+1}\right] + V \int_{0}^{\infty} \frac{E\nu(E)d(E-\mu)}{\exp\{(E-\mu)/T\}+1}$$
$$= V \int_{0}^{\mu} E\nu(E)dE + 2V \frac{d(E\nu(E))}{dE}|_{E=\mu} \times \int_{0}^{\infty} \frac{(E-\mu)d(E-\mu)}{\exp\{(E-\mu)/T\}+1}$$
$$= \frac{3}{5}E_{F}N \left(\frac{\mu}{E_{F}}\right)^{5/2} + \frac{\pi^{2}}{4}\nu(\mu)T^{2}V = \frac{3}{5}E_{F}N + \frac{3}{2}\delta N + \frac{3\pi^{2}}{8}\left(\frac{T}{E_{F}}\right)^{2}E_{F}N$$
$$= \frac{3}{5}E_{F}N + \frac{\pi^{2}}{4}\frac{T^{2}}{E_{F}}N.$$
(2.41)

The free energy F is related to the energy E by

$$E = -T^2 \left(\frac{\partial}{\partial T} \frac{F}{T}\right)_V \tag{2.42}$$

and the entropy is given by the relation

$$S = -\left(\frac{\partial F}{\partial T}\right)_V.$$
(2.43)

The relation for the pressure is

$$P = -\left(\frac{\partial F}{\partial V}\right)_T.$$
(2.44)

These thermodynamic quantities are easily calculated using Eq. (2.41) for the energy E.

The generalization to multicomponent ideal Fermi gases is straightforward. In the absence of interactions, fermionic components behave themselves as independent ideal gases. For example, in the case of two components which we again denote as \uparrow and \downarrow , the distribution of particles in these components is given by

$$N_{\mathbf{p}\uparrow} = \frac{1}{\exp\{(E_{\mathbf{k}\uparrow} - \mu_{\uparrow})/T\} + 1},$$
(2.45)

$$N_{\mathbf{p}\downarrow} = \frac{1}{\exp\{(E_{\mathbf{k}\downarrow} - \mu_{\downarrow})/T\} + 1},$$
(2.46)

where the corresponding chemical potentials are $\mu_{\uparrow} = E_{F\uparrow} + \delta_{\uparrow}$ and $\mu_{\downarrow} = E_{F\downarrow} + \delta_{\downarrow}$. The quantities δ_{\uparrow} and δ_{\downarrow} are given by Eq. (2.40) with $E_F = E_{F\uparrow}$ and $E_F = E_{F\downarrow}$, respectively. The Fermi energies of the two components, $E_{F\uparrow}$ and $E_{F\downarrow}$ follow from Eq. (1.6). One should simply put $n = n_{\uparrow} = N_{\uparrow}/V$ for the \uparrow -component, and $n = n_{\downarrow} = N_{\downarrow}/V$ for the \downarrow -component. The energy of the two-component gas is $E = E_{\uparrow} + E_{\downarrow}$, where E_{\uparrow} and E_{\downarrow} are given by Eq. (2.41) with $E_F = E_{F\uparrow}, N = N_{\uparrow}$ and $E_F = E_{F\downarrow}, N = N_{\downarrow}$ and $E_F = E_{F\downarrow}$.

2.3 Particle and hole excitations

We now consider T = 0 and discuss excitations of an ideal Fermi gas in free space. The ground state is a filled Fermi sphere, and let us create an excited state by transferring a particle with momentum $\hbar \mathbf{k}_1$ ($|\mathbf{k}_1| < k_F$) to the state with momentum $\hbar \mathbf{k}_2$ ($|\mathbf{k}_2| > k_F$) as depicted in Fig. 2.2. The change of the energy is

$$E - E_0 = \frac{\hbar^2 k_2^2}{2m} - \frac{\hbar^2 k_1^2}{2m},$$

and it can be written in the form

$$E - E_0 = \left(\frac{\hbar^2 k_2^2}{2m} - E_F\right) + \left(E_F - \frac{\hbar^2 k_1^2}{2m}\right).$$
(2.47)

By taking a particle out of the Fermi sphere and putting it into an excited state above the Fermi surface we create a hole in the Fermi sphere. Thus, we can distinguish between particle and hole excitations.

Consider first particle excitations. Acting with the operator $\hat{a}_{\mathbf{k}}^{\dagger}$ on the ground state of N particles we have $\hat{a}_{\mathbf{k}}^{\dagger}|N\rangle \neq 0$ only for $k > k_F$. In the latter case we create an excited state of the system of (N+1) particles. The excitation energy is given by

$$\epsilon_k = E_k + E_0(N) - E_0(N+1) = \frac{\hbar^2 k^2}{2m} - E_F > 0; \quad k > k_F, \tag{2.48}$$



Figure 2.2: The creation of particle and hole excitations.

i.e. it is represented by the first term in the right hand side of equation (2.47). So, for $k > k_F$ the quantity ϵ_k (2.48) can be identified as a particle excitation.

Let us now consider hole excitations. Acting with the operator $\hat{a}_{\mathbf{k}}$ on the ground state of N particles we have $\hat{a}_{\mathbf{k}}|N\rangle \neq 0$ only for $k < k_F$. Then, if $k < k_F$, we create an excited state of (N-1) particles. The corresponding excitation energy is

$$\epsilon_k = E_0(N) - E_0(N-1) - E_k = E_F - \frac{\hbar^2 k^2}{2m} > 0; \quad k < k_F,$$
 (2.49)

and is equivalent to the second term in the right hand side of Eq. (2.47). Thus, for $k < k_F$ the quantity ϵ_k (2.49) can be treated as a hole excitation. The particle and hole excitation branches are displayed in Fig. 2.3. In both cases one can write the excitation energy as

$$\epsilon_k = \frac{\hbar^2 |k^2 - k_F^2|}{2m}.$$
 (2.50)

Problems 2

2.1 Calculate the chemical potential and total energy of a single-component ideal two-dimensional Fermi gas at a finite temperature.

We first introduce the density of states in two dimensions (2D):

$$\nu(E) = \int \frac{d^2k}{(2\pi)^2} \delta(E - \hbar^2 k^2 / 2m) = \frac{m}{2\pi\hbar^2} = \text{const.}$$
(2.51)

Then, we obtain the following relation between the chemical potential and density:

$$n = \int_0^\infty \frac{\nu(E)dE}{\exp\{(E-\mu)/T\} + 1} = \frac{mT}{2\pi\hbar^2} \ln\left[1 + \exp(\mu/T)\right].$$
 (2.52)



Figure 2.3: The energies of particle and hole excitations versus the momentum $\hbar k$.

We thus obtain:

$$\mu = T \ln \left[\exp(T_d/T) - 1 \right], \qquad (2.53)$$

where the temperature of quantum degeneracy is given by

$$T_d = \frac{2\pi\hbar^2}{m}n\tag{2.54}$$

and is equal to the 2D Fermi energy E_F .

At high temperatures, $T \gg T_d$, equation (2.53) gives the well-known classical result:

$$\mu = -T \ln\left(\frac{T}{T_d}\right) = T \ln(n\Lambda_T^2). \tag{2.55}$$

At low temperatures, $T \ll T_d = E_F$, we have

$$\mu = E_F - T \exp(-E_F/T).$$
(2.56)

We thus see that the temperature-dependent part of μ is exponential, in contrast to the 3D case where it is proportional to T^2 .

For the total energy at $T \ll E_F$ we find

$$E = V \int_{0}^{\infty} \frac{\nu(E)EdE}{\exp\{(E-\mu)/T\} + 1} = \frac{mV\mu^{2}}{4\pi\hbar^{2}} + \frac{\pi T^{2}mV}{12\hbar^{2}}$$
$$= \frac{1}{2}E_{F}N + \frac{\pi^{2}}{6}\left(\frac{T}{E_{F}}\right)^{2}E_{F}N,$$
(2.57)

where we used the same method of integration as in 3D and omitted exponentially small corrections to μ .

2.2 Calculate the chemical potential and total energy for the one-dimensional ideal Fermi gas at temperatures $T \ll E_F$.

Lecture 3. Repulsively interacting Fermi gas. Landau's Fermi liquid theory

3.1 Weakly interacting Fermi gas with repulsion between particles

We now consider a degenerate interacting two-component Fermi system and start with the weakly interacting Fermi gas. We only include the *s*-wave interaction between fermions of different components and in this *Lecture* discuss the case where the interaction is repulsive. So, in free space the Hamiltonian is the sum of the kinetic and interaction energy terms which in the momentum space second quantization are given by Eqs. (2.25) and (2.34), respectively:

$$\hat{H} = \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} (\hat{a}_{\uparrow \mathbf{k}}^{\dagger} \hat{a}_{\uparrow \mathbf{k}} + \hat{a}_{\downarrow \mathbf{k}}^{\dagger} \hat{a}_{\downarrow \mathbf{k}}) + \frac{g}{V} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} \hat{a}_{\uparrow \mathbf{k}_3}^{\dagger} \hat{a}_{\downarrow \mathbf{k}_4}^{\dagger} \hat{a}_{\downarrow \mathbf{k}_2} \hat{a}_{\uparrow \mathbf{k}_1}, \qquad (3.1)$$

where $g = 4\pi\hbar^2 a/m$ with a > 0 being the scattering length, the symbols \uparrow and \downarrow label the two fermionic components, and the momentum conservation law $\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4$ is satisfied. As we discussed in subsection 1.4 of *Lecture* I, the weakly interacting regime is characterized by the condition $na^3 \ll 1$ which ensures that the interaction energy is much smaller than the Fermi energy (kinetic energy of particles) and allows one to treat the interaction part of the Hamiltonian within a many-body perturbation theory. To zero order the total energy of the system at T = 0 is equal to the ideal gas energy $E_0 = (3/5)[E_{F\uparrow}N_{\uparrow} + E_{F\downarrow}N_{\downarrow}]$, where $E_{F\uparrow}, N_{\uparrow}$ and $E_{F\downarrow}, N_{\downarrow}$ are Fermi energies and particle numbers in the \uparrow and \downarrow components (see subsection 2.2 of *Lecture 2*).

In the first order of perturbation theory, we have to add the diagonal matrix element of the interaction term (the second term of Eq. (3.1)). It is easy to see that then we should have $\mathbf{k}_3 = \mathbf{k}_1$ and $\mathbf{k}_4 = \mathbf{k}_2$, otherwise the diagonal matrix element is zero. So, the contribution of the interaction term to the total energy is

$$E_{int} = \frac{g}{V} \sum_{\mathbf{k}_1, \mathbf{k}_2} \langle \hat{a}_{\uparrow \mathbf{k}_1}^{\dagger} \hat{a}_{\uparrow \mathbf{k}_1} \rangle \langle \hat{a}_{\downarrow \mathbf{k}_2}^{\dagger} \hat{a}_{\downarrow \mathbf{k}_2} \rangle = \frac{g}{V} \sum_{\mathbf{k}_1, \mathbf{k}_2} N_{\uparrow \mathbf{k}_1} N_{\downarrow \mathbf{k}_2} = \frac{g}{V} N_{\uparrow} N_{\downarrow}.$$
(3.2)

Thus, the total energy of the Fermi gas is given by

$$E_0 = \frac{3}{5} (E_{F\uparrow} N_{\uparrow} + E_{F\downarrow} N_{\downarrow}) + \frac{g}{V} N_{\uparrow} N_{\downarrow}, \qquad (3.3)$$

and for the chemical potentials of the \uparrow and \downarrow components we have:

$$\mu_{\uparrow} = \frac{\partial E_0}{\partial N_{\uparrow}} = E_{F\uparrow} + n_{\downarrow}g, \qquad (3.4)$$

$$\mu_{\downarrow} = \frac{\partial E_0}{\partial N_{\downarrow}} = E_{F\downarrow} + n_{\uparrow}g, \qquad (3.5)$$

If the concentrations of the two fermionic components are equal, i.e. $N_{\uparrow} = N_{\downarrow} = N/2$ and $E_{F\uparrow} = E_{F\downarrow} = E_F$, then equations (3.3), (3.4), and (3.5) yield

$$E_0 = \left(\frac{3}{5}E_F + \frac{1}{4}ng\right)N = \frac{3}{5}E_F N\left(1 + \frac{5}{12}\frac{ng}{E_F}\right) = \frac{3}{5}E_F N\left(1 + \frac{10}{9\pi}k_F a\right), \quad (3.6)$$

$$\mu_{\uparrow} = \mu_{\downarrow} = \mu = E_F + \frac{1}{2}ng = E_F \left(1 + \frac{ng}{2E_F}\right) = E_F \left(1 + \frac{4}{3\pi}k_F a\right).$$
(3.7)

The small parameter of the perturbation theory is $(ng/E_F) \sim k_F a \ll 1$. As we see, the first order correction to the energy is $\sim k_F a$. The second order correction turns out to be $\sim (k_F a)^2$. The calculation of this correction is beyond the scope of the present course.



Figure 3.1: Particle and hole excitations in a two-component Fermi gas.

Let us now discuss excitations of a weakly interacting Fermi gas with interparticle repulsion. The picture of particle and hole excitations in the twocomponent gas remains the same as discussed in subsection 2.3 for a singlecomponent gas. For T = 0, transferring for example a \uparrow particle from the state with wavevector \mathbf{k}_1 inside the Fermi sphere to the state with wavevector \mathbf{k}_2 above the Fermi surface we change the energy by an amount $E - E_0 =$ $(\hbar^2 k_2^2/2m - \hbar^2 k_1^2/2m)$ and create both a particle and a hole excitation as shown in Fig.3.1. The particle excitation is an excited state of the system of (N + 1)particles. By bringing an extra \uparrow -particle from infinity and putting it above the Fermi surface we increase the energy by $(\hbar^2 k_2^2/2m - E_F)$ compared to the ground state of (N + 1) particles. The interaction energy does not change as it is momentum independent. The hole excitation is an excited state of (N-1) particles. Making a hole we increase the energy by $(E_F - \hbar^2 k_1^2/2m)$ compared to the ground state of (N-1) particles. Again, the interaction energy does not change. So, the excitation branches behave themselves exactly in the same way as depicted in Fig.2.2 for the ideal gas.

Does the interaction do something with the excitations? The answer is yes, it does. In contrast to the ideal gas, the excitations of an interacting Fermi gas interact with each other and have a finite lifetime, i.e. they are damped. Consider a particle excitation with momentum $\hbar \mathbf{k}_1$ $(k_1 > k_F)$ at T = 0. It interacts with a particle which has momentum $\hbar \mathbf{k}_2$ and is located inside the Fermi sphere $(k_2 < k_F)$, makes a hole and creates two particle excitations, with momenta $\hbar \mathbf{k}'_1$ and $\hbar \mathbf{k}'_2$. Using the terminology of the scattering theory, \uparrow and \downarrow particles with momenta $\hbar \mathbf{k}_1$ and $\hbar \mathbf{k}_2$, collide and go to the states with momenta $\hbar \mathbf{k}'_1$ and $\hbar \mathbf{k}'_2$. In the language of particle and hole excitations, a particle excitation with wavevector \mathbf{k}_1 (close to k_F) and energy $E = \hbar^2 k_1^2 / 2m - E_F$ decays into two particle excitations and one hole excitation. This process is caused by the interaction Hamiltonian (2.34):

$$\frac{g}{V}\sum_{\mathbf{k}_2,\mathbf{k}_1'}\hat{a}_{\uparrow\mathbf{k}_1'}^{\dagger}\hat{a}_{\downarrow\mathbf{k}_2'}^{\dagger}\hat{a}_{\downarrow\mathbf{k}_2}\hat{a}_{\downarrow\mathbf{k}_2}\hat{a}_{\uparrow\mathbf{k}_1}.$$

The decay rate is obtained by using the Fermi Golden rule:

$$\frac{1}{\tau} = \sum_{\mathbf{k}_{2},\mathbf{k}_{1}'} \frac{2\pi}{\hbar} \left| \langle \uparrow \mathbf{k}_{1}', \downarrow \mathbf{k}_{2}' | \hat{H}_{int} | \downarrow \mathbf{k}_{2}, \uparrow \mathbf{k}_{1} \rangle \right|^{2} \delta \left(\frac{\hbar^{2} k_{1}^{2}}{2m} + \frac{\hbar^{2} k_{2}^{2}}{2m} - \frac{\hbar^{2} k_{1}'^{2}}{2m} - \frac{\hbar^{2} k_{2}'^{2}}{2m} \right), \quad (3.8)$$

and there is a momentum conservation law $\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}'_1 + \mathbf{k}'_2$.

We now write $k_2'^2 = |\mathbf{k}_1 + \mathbf{k}_2|^2 + k_1'^2 - 2k_1'|\mathbf{k}_1 + \mathbf{k}_2|\cos\theta'$, where θ' is the angle between the vectors $(\mathbf{k}_1 + \mathbf{k}_2)$ and \mathbf{k}_1' . Since all momenta are close to $\hbar k_F$, we may put $k_1 = k_2 = k_1' = k_F$ and set $|\mathbf{k}_1 + \mathbf{k}_2| = 2k_F\cos\theta/2$ (θ is the angle between \mathbf{k}_1 and \mathbf{k}_2) in the energy conservation law, i.e. in the argument of the δ -function in Eq. (3.8). Then this argument becomes equal to $(2\hbar^2 k_F^2/m)[\cos^2\theta/2 - \cos\theta/2\cos\theta']$, and we rewrite Eq. (3.8) as

$$\frac{1}{\tau} = \frac{2\pi g^2}{\hbar} \int \frac{2\pi k_1'^2 dk_1' 2\pi k_2' dk_2 \sin\theta \, d\theta \, d\cos\theta'}{(2\pi)^6} N_{\downarrow}(k_2) (1 - N_{\uparrow}(k_1')) (1 - N_{\downarrow}(k_2')) \times \delta\left(\frac{2\hbar^2 k_F^2}{m} [\cos^2\theta/2 - \cos\theta/2 \, \cos\theta']\right),$$
(3.9)

where the occupation numbers $N_{\uparrow}(k)$ and $N_{\downarrow}(k)$ are equal to unity for $k < k_F$ and to zero for $k > k_F$, and $k'_2 = \sqrt{k_1^2 + k_2^2 - k'_1^2}$. The integration over $d \cos \theta'$ and then over $d\theta$ gives

$$\frac{1}{\tau} = \frac{2mg^2k_F^2}{(2\pi\hbar)^3} \int dq_1' dq_2 \, N_{\downarrow}(k_F + q_2)(1 - N_{\uparrow}(k_F + q_1'))(1 - N_{\downarrow}(k_F + q_1 + q_2 - q_1')). \tag{3.10}$$

Here $q_1 = k_1 - k_F$, $q_2 = k_2 - k_F$, $q'_1 = k'_1 - k_F$, and hence $q'_2 = q_1 + q_2 - q'_1$. In order to have $N_{\downarrow}(k_F + q_2) = 1$, $N_{\uparrow}(k_F + q'_1) = 0$, $N_{\downarrow}(k_F + q_1 + q_2 - q'_1) = 0$, the momenta should satisfy the inequalities

$$q_2 < 0; \quad q'_1 > 0; \quad q_1 + q_2 - q'_1 > 0.$$

Since we consider the decay of a particle excitation we have $q_1 > 0$, and these inequalities are equivalent to

$$0 < q_1' < q_1 + q_2, \tag{3.11}$$

$$-q_1 < q_2 < 0. \tag{3.12}$$

Equations (3.11) and (3.12) determine the limits of integration over dq'_1 and dq_2 in Eq. (3.10). We then obtain:

$$\frac{1}{\tau} = \frac{mk_F^2 g^2 q_1^2}{(2\pi\hbar)^3}.$$
(3.13)

As we consider the decay of an excitation with momentum k_1 close to the Fermi surface, the excitation energy can be written in the form $E = \hbar^2 k_1^2/2m - E_F = \hbar v_F q_1$, where $v_F = \hbar k_F/m$ is the Fermi velocity. Recalling that $k_F^3 = 3\pi^2 n$ and $g = 4\pi\hbar^2 a/m$ we then rewrite equation (3.13) as

$$\frac{1}{\tau} = \frac{3}{2} n \sigma v_F \left(\frac{E}{E_F}\right)^2, \qquad (3.14)$$

where $\sigma = 4\pi a^2$ is the cross section of elastic collisions. We thus see that the presence of the filled Fermi sphere (Pauli blocking) makes the lifetime of excitations rather large. It is clear that

$$\frac{1}{\tau} \ll \frac{E}{\hbar}.$$
(3.15)

The ratio $E\tau/\hbar$ is

$$\frac{E\tau}{\hbar} \simeq \frac{\pi}{4} \left(\frac{E_F}{E}\right) \frac{1}{(k_F a)^2} \gg 1.$$
(3.16)

3.2 Quasiparticles in Landau's Fermi liquid theory

We now turn to the discussion of Landau's Fermi liquid theory which was designed for the description of strongly (repulsively) interacting Fermi systems, such as liquid ³He. In a strongly interacting Fermi system instead of considering particles one introduces dressed particles, or *quasiparticles*. The number of quasiparticles is equal to the total number of particles and they also obey Fermi statistics. In free space each quasiparticle has momentum **p** and energy $\epsilon(\mathbf{p})$ (in the rest of this *Lecture* **p** is the true momentum, not the wavevector). Let $n(\mathbf{p})$ be the distribution function of quasiparticles. Then, in a two-component Fermi liquid, assuming that $\epsilon(\mathbf{p})$ and $n(\mathbf{p})$ are spin independent, we have

$$2\int n(\mathbf{p})\frac{d^3p}{(2\pi\hbar)^3} = \frac{N}{V},\tag{3.17}$$

where N is the total number of particles. However, the total energy E is not equal to $2 \int n(\mathbf{p}) \epsilon(\mathbf{p}) V d^3 p / (2\pi\hbar)^3$. The energy E is a functional of $n(\mathbf{p})$. Considering a change of E under an infinitesimally small variation δn of $n(\mathbf{p})$ we have

$$\frac{\delta E}{V} = 2 \int \epsilon(\mathbf{p}) \delta n(\mathbf{p}) \frac{d^3 p}{(2\pi\hbar)^3}.$$
(3.18)

So, $\epsilon(\mathbf{p})$ is a variational derivative of E with respect to $n(\mathbf{p})$.

The classification of energy levels in a Fermi liquid is similar to that in an ideal Fermi gas. The only difference is that particles are replaced by quasiparticles. Therefore, the entropy is given by the well-known expression:

$$\frac{S}{V} = -2 \int \frac{d^3 p}{(2\pi\hbar)^3} \left\{ n(\mathbf{p}) \ln n(\mathbf{p}) + (1 - n(\mathbf{p})) \ln (1 - n(\mathbf{p})) \right\}, \qquad (3.19)$$

and the distribution of quasiparticles at equilibrium obeys the Fermi-Dirac relation:

$$n(\mathbf{p}) = \frac{1}{\exp\{[\epsilon(\mathbf{p}) - \mu]/T\} + 1}.$$
(3.20)

At T = 0 the chemical potential coincides with the boundary energy at the Fermi sphere:

$$\mu_0 \equiv \mu(T=0) = \epsilon_F \equiv \epsilon(p_F). \tag{3.21}$$

Note, however, that $\epsilon(\mathbf{p})$ itself may depend on $n(\mathbf{p})$. The distribution of quasiparticles at T = 0 represents a step function:

$$n(\mathbf{p}) = \theta(p_F - p) \equiv \begin{cases} 1, & p < p_F \\ 0, & p > p_F \end{cases}$$
(3.22)

and the Fermi momentum is related to the total density n by the same expression as in an ideal Fermi gas: $p_F = \hbar (3\pi^2 n)^{1/3}$. At finite low temperatures the distribution function is different from the step function (3.22) in the energy interval ~ T near the boundary energy ϵ_F .

The fact that a quasiparticle has momentum and energy means, in particular, that the uncertainty in the energy should be smaller than the least of the important energy scales in the system. As we saw in previous lectures of the course, in a weakly interacting Fermi gas at temperatures $T \ll E_F$ only particles next to the Fermi surface participate in the response of the system to external perturbations. The energy width of the distribution function $n(\mathbf{p})$ where this happens is $\sim T$. The situation is similar in the Fermi liquid, so that the least important energy scale is T. The quantum uncertainty of the quasiparticle energy is $\sim \hbar/\tau$ where τ is the relaxation time of the quasiparticles. So, we should have the inequality

$$\frac{\hbar}{\tau} \ll T. \tag{3.23}$$

As we understand, only quasiparticles at energies within the width $\sim T$ next to the Fermi surface can scatter, and they stay in the same energy interval. Since

the scattering occurs in binary collisions, we have

$$\frac{1}{\tau} \sim T^2, \tag{3.24}$$

and the inequality (3.23) is surely satisfied at $T \to 0$. For a strongly interacting Fermi liquid at $T \to 0$ all energy parameters are $\sim \epsilon_F$. Hence, Eq. (3.24) may be written as $\tau^{-1} \sim T^2/\hbar |\epsilon_F|$, and the condition (3.23) is equivalent to

$$T \ll |\epsilon_F|. \tag{3.25}$$

Equations (3.24) and (3.25) are consistent with our discussion of the decay rate τ_E^{-1} of an excitation with energy E in a weakly interacting Fermi gas in the previous subsection. We found Eq. (3.14), and the finite-temperature relaxation rate that we discuss now is obtained by putting $E \sim T$. Then, with $\sigma = 4\pi a^2$, $v_F = p_F/m$, $p_F \sim \hbar n^{1/3}$, and $E \sim T$, equation (3.14) gives $\tau^{-1} \sim (na^3)^{2/3}T^2/\hbar E_F$. Approaching strong interactions one has $na^3 \sim 1$, so that we have $\tau^{-1} \sim T^2/\hbar E_F$ and the condition (3.23) reduces to $T \ll E_F$.

For low-temperature distributions which are close to the step-wise distribution (3.22), to first approximation one can take $n(\mathbf{p})$ in the form (3.22) for calculating $\epsilon(\mathbf{p})$. Then the latter becomes a definite function of p. Next to the Fermi surface where $\epsilon(p)$ makes sense, it can be expanded in powers of $(p - p_F)$. Confining ourselves to the linear term we have

$$\epsilon - \epsilon_F \simeq v_F (p - p_F), \tag{3.26}$$

where

$$\mathbf{v}_F = \frac{\partial \epsilon}{\partial \mathbf{p}} |_{p=p_F} \tag{3.27}$$

is the velocity of quasiparticles at the Fermi surface, and we may introduce an effective mass of a quasiparticle:

$$m^* = \frac{p_F}{v_F}.\tag{3.28}$$

Let us now briefly discuss the interaction between quasiparticles. The deviation δn of the distribution function $n(\mathbf{p})$ from the step-wise behavior (3.22) achieved for non-interacting quasiparticles, leads to a change in the quasiparticle energy. Assuming that both quantities are spin independent we have

$$\delta\epsilon(\mathbf{p}) = \int f(\mathbf{p}, \mathbf{p}') \delta n(\mathbf{p}') \frac{d^3 p'}{(2\pi\hbar)^3}.$$
(3.29)

The function $f(\mathbf{p}, \mathbf{p}')$ is called *interaction function* of quasiparticles. Then, near the Fermi surface the quasiparticle energy can be written as

$$\epsilon(\mathbf{p}) - \epsilon_F = v_F(p - p_F) + \int f(\mathbf{p}, \mathbf{p}') \delta n(\mathbf{p}') \frac{d^3 p'}{(2\pi\hbar)^3}.$$
 (3.30)

The deviation δn is significantly different from zero only near the Fermi surface. For this reason we may write

$$f(\mathbf{p}, \mathbf{p}') = \frac{\pi^2 \hbar^3}{2m^* p_F} F(\vartheta), \qquad (3.31)$$

where ϑ is the angle between **p** and **p**'. Taking into account the exchange interaction one adds the term $\sigma \sigma' G(\vartheta)$ to $F(\vartheta)$, where σ and σ' are Pauli matrices acting on spin variables corresponding to the momentum variables **p** and **p**'. Note that in the two-component liquid f represents the second variational derivative of the total energy with respect to the distribution functions of the components.

The interaction function f is a very important quantity and the knowledge of this function allows one to find many observables. In particular, using fone can establish a relation between the true particle mass m and the effective mass m^* . This is done in *Problem 1* to this *Lecture*. Here we consider a simple example of the weakly interacting two-component Fermi gas. To first order in the perturbation theory the total energy is

$$E_0 = \sum_{\mathbf{p}} \frac{p^2}{2m} (n_{\uparrow}(\mathbf{p}) + n_{\downarrow}(\mathbf{p})) + \frac{g}{V} \sum_{\mathbf{p},\mathbf{p}'} n_{\uparrow}(\mathbf{p}) n_{\downarrow}(\mathbf{p}').$$

Then, for the quasiparticle energies we have:

$$\begin{split} \epsilon_{\uparrow}(p) &= \frac{\delta E_0}{\delta n_{\uparrow}} = \frac{p^2}{2m} + \frac{g}{V} \sum_{\mathbf{p}} n_{\downarrow}(\mathbf{p}) = \frac{p^2}{2m} + n_{\downarrow}g = \mu_{\uparrow} + \frac{(p^2 - p_F^2)}{2m},\\ \epsilon_{\downarrow}(p) &= \frac{\delta E_0}{\delta n_{\downarrow}} = \frac{p^2}{2m} + n_{\downarrow}g = \mu_{\uparrow} + \frac{(p^2 - p_F^2)}{2m}. \end{split}$$

The interaction function is given by

$$f = \frac{\delta^2 E_0}{V \delta n_{\uparrow} \delta n_{\downarrow}} = g.$$

3.3 Hydrodynamic regime

Non-equilibrium states of the Fermi liquid are described by distribution functions which depend not only on momenta, but also on coordinates and time. Such functions $n(\mathbf{p}, \mathbf{r}, t)$ obey the kinetic equation:

$$\frac{dn}{dt} = \operatorname{St}n,\tag{3.32}$$

where Stn is the so-called collisional integral determining the rate of change of the quasiparticle number in a given element of the phase volume, due to their collisions with each other. For only slightly non-equilibrium states we have:

$$n(\mathbf{p}, \mathbf{r}, t) = n_0(\mathbf{p}) + \delta n(\mathbf{p}, \mathbf{r}, t), \qquad (3.33)$$

and the quasiparticle energy is $\epsilon = \epsilon_0 + \delta \epsilon$, where

$$\frac{\partial \epsilon}{\partial \mathbf{r}} = \frac{\partial \delta \epsilon}{\partial \mathbf{r}} = \int f(\mathbf{p}, \mathbf{p}') \frac{\partial \delta n(\mathbf{p}', \mathbf{r}, t)}{\partial \mathbf{r}} \frac{d^3 p'}{(2\pi\hbar)^3}.$$
(3.34)

The full time derivative of $n(\mathbf{p}, \mathbf{r}, t)$ is expressed through partial derivatives as

$$\frac{dn}{dt} = \frac{\partial \delta n}{\partial t} + \frac{\partial \delta n}{\partial \mathbf{r}} \,\dot{\mathbf{r}} + \frac{\partial n}{\partial \mathbf{p}} \,\dot{\mathbf{p}}.$$
(3.35)

For quasiparticles the role of the Hamiltonian function is played by ϵ . So, the Hamiltonian equations read:

$$\dot{\mathbf{r}} = \frac{\partial \epsilon}{\partial \mathbf{p}}; \tag{3.36}$$

$$\dot{\mathbf{p}} = -\frac{\partial\epsilon}{\partial\mathbf{r}}.\tag{3.37}$$

Then, confining ourselves to zero and linear order terms in δn we obtain:

$$\frac{\partial \delta n}{\partial t} + \frac{\partial \epsilon_0}{\partial \mathbf{p}} \frac{\partial \delta n}{\partial \mathbf{r}} - \frac{\partial \delta \epsilon}{\partial \mathbf{r}} \frac{\partial n_0}{\partial \mathbf{p}} = \mathrm{St}n.$$
(3.38)

Equations (3.36), (3.37), and (3.38) are classical. Hence, the de Broglie wavelength of quasiparticles \hbar/p_F should be much smaller than the characteristic distance L at which the distribution function changes: $L \gg \hbar/p_F$. So, the frequency of change of the distribution function, which is $\omega \sim v_F/L$, should satisfy the condition:

$$\hbar\omega \ll |\epsilon_F|. \tag{3.39}$$

Let us now discuss the limiting case where

$$\omega \tau \ll 1, \tag{3.40}$$

with $\tau^{-1} \propto T^2$ being the relaxation rate of quasiparticles. The criterion (3.40) corresponds to the *hydrodynamic regime*. Equation (3.40) is equivalent to the condition $l \ll \lambda$, where l is the mean free path of quasiparticles, and λ is their wavelength. In this case quasiparticle collisions establish a local thermal equilibrium in every elementary volume of the system. This means that we are dealing with ordinary *hydrodynamic waves* propagating with velocity

$$u = \sqrt{\frac{\partial P}{\partial \rho}},\tag{3.41}$$

where P is the pressure, ρ is the mass density, and at a finite temperature the partial derivative should be taken at a constant entropy. These waves have the dispersion relation

$$\omega = uk, \tag{3.42}$$

with k being their wavevector.

For the weakly interacting Fermi gas, where τ^{-1} is given by Eq. (3.14), the inequality (3.40) requires extremely small frequencies:

$$\omega \ll n\sigma v_F \left(\frac{T}{E_F}\right)^2 \sim (na^3)^{2/3} \left(\frac{T}{E_F}\right) T.$$

For realistic densities in the range from 10^{12} to 10^{14} cm⁻³ and typical values of the scattering length $a \sim 100$ Å, assuming $T \sim 0.1 E_F$ we obtain that ω should be smaller than T by more than 4 orders of magnitude. At commonly used temperatures ranging from 100 nK to 1 μ K this requires frequencies $\omega \ll 10$ s⁻¹. So, it is rather difficult to reach the hydrodynamic regime in the weakly interacting Fermi gas.

3.4 Collisionless regime. Zero sound

If the condition opposite to Eq. (3.40) is satisfied, i.e.

$$\omega \tau \gg 1, \tag{3.43}$$

then there is no equilibrium in each small volume of the system, and quasiparticle collisions do not play a role. This regime is identified as *collisionless*, and there is another type of waves called *zero sound*.

So, under the condition (3.43) we may neglect the collisional integral in the kinetic equation (3.38) and write it in the form:

$$\frac{\partial \delta n}{\partial t} + \mathbf{v} \frac{\partial \delta n}{\partial \mathbf{r}} - \frac{\partial \delta \epsilon}{\partial \mathbf{r}} \frac{\partial n_0}{\partial \mathbf{p}} = 0, \qquad (3.44)$$

where $\mathbf{v} = \partial \epsilon_0 / \partial \mathbf{p}$ is the unperturbed quasiparticle velocity, so that $\mathbf{v} = v_F \mathbf{n}$ with \mathbf{n} being a unit vector. Taking $n_0 = \theta(p_F - p)$ from Eq. (3.22) we have

$$\frac{\partial n_0}{\partial \mathbf{p}} = -\mathbf{n}\delta(p - p_F) = -\mathbf{v}\delta(\epsilon - \epsilon_F). \tag{3.45}$$

Then, assuming that

$$\delta n = \delta(\epsilon - \epsilon_F)\nu(\mathbf{n})\exp(i\mathbf{kr} - i\omega t), \qquad (3.46)$$

where $\nu(\mathbf{n})$ is an unknown function, and taking

$$\frac{\partial \delta \epsilon}{\partial \mathbf{r}} = \int f(\mathbf{p}, \mathbf{p}') \frac{\partial \delta n(\mathbf{p}', \mathbf{r}, t)}{\partial \mathbf{r}} \frac{d^3 p'}{(2\pi\hbar)^3},\tag{3.47}$$

we reduce Eq. (3.44) to

$$(\omega - v_F \mathbf{n} \mathbf{k}) \nu(\mathbf{n}) = \frac{(\mathbf{n} \mathbf{k}) p_F^2}{(2\pi\hbar)^3} \int f(\mathbf{n}, \mathbf{n}') \nu(\mathbf{n}') d\mathbf{O}_{\mathbf{p}'}, \qquad (3.48)$$

where \mathbf{n} and \mathbf{n}' are unit vectors in the directions of \mathbf{p} and \mathbf{p}' .

We now select **k** as a polar axis, and let θ , ϕ be the polar and azimuthal angles of **n**. Introducing the velocity of zero sound $u_0 = \omega/k$, from Eq. (3.48) we have:

$$\left(\frac{u_0}{v_F} - \cos\theta\right)\nu(\theta,\phi) = \cos\theta \int F(\varphi)\nu(\theta',\phi')\frac{\mathrm{dO}_{\mathbf{P}'}}{4\pi},\tag{3.49}$$

where φ is the angle between **p** and **p**', and the function $F(\varphi)$ is given by Eq. (3.31). Rewriting Eq. (3.49) as

$$\tilde{\nu}(\theta,\phi) = \cos\theta \int \frac{F(\varphi)\tilde{\nu}(\theta',\phi')}{u_0/v_F - \cos\theta'} \frac{d\mathcal{O}_{\mathbf{p}'}}{4\pi},$$
(3.50)

where $\tilde{\nu} = (u_0/k - \cos\theta)\nu$, we see that

$$u_0 > v_F, \tag{3.51}$$

otherwise there is a pole in Eq. (3.50) and ω will have an imaginary part for real k.

The zero sound waves deform the Fermi surface. Assuming that $f = f_0 = \text{const}$ ($F = F_0 = \text{const}$) we make sure that the Fermi surface becomes a surface of rotation elongated in the direction of the wave propagation. In this case we obtain

$$\nu = \operatorname{const} \frac{\cos \theta}{u_0/k - \cos \theta}.$$
(3.52)

Substituting Eq. (3.52) into Eq. (3.49) we find

$$F_0 \int_0^\pi \frac{\cos\theta}{u_0/k - \cos\theta} \frac{2\pi\sin\theta d\theta}{4\pi} = 1.$$
(3.53)

This gives

$$\frac{1}{F_0} = \frac{u_0}{2v_F} \ln\left(\frac{u_0 + v_F}{u_0 - v_F}\right).$$
(3.54)

For the weakly (repulsively) interacting two-component Fermi gas we have f = g and $m^* = m$ (see *Problem 1* to this *Lecture*). This yields

$$F = \frac{p_F m}{2\pi^2 \hbar^3} g = \frac{2}{\pi} \frac{p_F a}{\hbar} \ll 1.$$
(3.55)

Then, from Eq. (3.54) we obtain:

$$u_0 \approx v_F \left[1 + 2 \exp\left(-\frac{\pi\hbar}{p_F a}\right) \right].$$
 (3.56)

Thus, the velocity of zero sound in the weakly interacting Fermi gas almost coincides with the Fermi velocity.

Problems 3

3.1 Establish a relation between the true particle mass m and the effective mass m^* using the interaction function of quasiparticles.

The velocity of a quasiparticle is $\partial \epsilon / \partial \mathbf{p}$. Hence, the flux of quasiparticles is $\int n(\partial \epsilon / \partial \mathbf{p}) d^3 p / (2\pi)^3$. Since the number of quasiparticles coincides with the number of particles, the transfer of mass by quasiparticles is a product of their flux and the particle mass m. So, we have

$$\int \mathbf{p}n(\mathbf{p}) \frac{d^3p}{(2\pi\hbar)^3} = \int m \frac{\partial\epsilon}{\partial \mathbf{p}} n(\mathbf{p}) \frac{d^3p}{(2\pi\hbar)^3}.$$
(3.57)

Making a variation we obtain:

$$\int \mathbf{p}\delta n \frac{d^3 p}{(2\pi\hbar)^3} = m \int \frac{\partial \epsilon}{\partial \mathbf{p}} \delta n \frac{d^3 p}{(2\pi\hbar)^3} - m \int f(\mathbf{p}, \mathbf{p}') \frac{\partial n(\mathbf{p}')}{\partial \mathbf{p}'} \delta n(\mathbf{p}') \frac{d^3 p d^3 p'}{(2\pi\hbar)^6}.$$

As the quantity δn is arbitrary we find:

$$\frac{\mathbf{p}}{m} = \frac{\partial \epsilon}{\partial \mathbf{p}} - \int f(\mathbf{p}, \mathbf{p}') \frac{\partial n(\mathbf{p}')}{\partial \mathbf{p}'} \frac{d^3 p'}{(2\pi\hbar)^3}$$

Taking a step-wise distribution $n(\mathbf{p}) = \theta(p_F - p)$, using Eq. (3.26) for the quasiparticle energy, and putting $\mathbf{p} = p_F \mathbf{n}$ where \mathbf{n} is a unit vector, we then have

$$\frac{1}{m} = \frac{1}{m^*} + \frac{p_F}{(2\pi)^2 \hbar^3} \int_0^\pi f(\varphi) \cos\varphi \,\sin\varphi \,d\varphi, \qquad (3.58)$$

where φ is the angle between **p** and **p**'.

For the weakly interacting two-component Fermi gas we have f = g = const, and Eq. (3.58) gives $m^* = m$.

3.2 Consider a two-component Fermi gas with repulsive interaction between particles in an external harmonic potential $V(r) = m\omega^2 r^2/2$ at T = 0. Find the density distribution.

Lecture 4. Attractively interacting Fermi gas. Superfluid pairing

4.1 Cooper problem

This *Lecture* is dedicated to a weakly interacting two-component Fermi gas with attractive interaction between fermions of different components. We will discuss the phenomenon of superfluid pairing and superfluid phase transition.

In order to get a physical intuition we first consider two attractively interacting particles in vacuum. The wavefunction of their relative motion obeys the Schroedinger equation

$$\left\{-\frac{\hbar^2}{m}\Delta_{\mathbf{r}} + U(\mathbf{r})\right\}\psi(\mathbf{r}) = E\psi(\mathbf{r}),\tag{4.1}$$

where **r** is the relative coordinate. Representing the wavefunction $\psi(\mathbf{r})$ as

$$\psi(\mathbf{r}) = \sum_{\mathbf{k}} c_{\mathbf{k}} \exp(i\mathbf{k}\mathbf{r}), \qquad (4.2)$$

we have $\sum_{\mathbf{k}'} c_{\mathbf{k}'} [E - 2E_{k'} - U(\mathbf{r})] \exp(i\mathbf{k}'\mathbf{r}) = 0$ with $E_k = \hbar^2 k^2/2m$, and obtain a set of equations for the coefficients $c_{\mathbf{k}}$:

$$(E - 2E_k)c_{\mathbf{k}} = \frac{1}{\Omega} \sum_{\mathbf{k}'} U(\mathbf{k} - \mathbf{k}')c_{\mathbf{k}'}, \qquad (4.3)$$

where

$$U(\mathbf{k} - \mathbf{k}') = \int d\mathbf{r} U(\mathbf{r}) \exp[i(\mathbf{k}' - \mathbf{k})\mathbf{r}], \qquad (4.4)$$

and Ω is the volume.

We now use the model where

$$U(\mathbf{k} - \mathbf{k}') = \begin{cases} -V_0; & E_{k'} \le \tilde{\omega} \\ 0, & \text{otherwise} \end{cases}$$
(4.5)

Then we obtain

$$c_{\mathbf{k}} = \frac{-V_0}{E - 2E_k} \frac{1}{\Omega} \sum_{\mathbf{k}'} c_{\mathbf{k}'} \theta(\tilde{\omega} - E_{k'}),$$

where the θ -function is equal to unity for positive values of the argument and zero for negative arguments. Multiplying both sides of this equation by $\theta(\tilde{\omega} - E_k)$ and making a summation over **k** we arrive at the relation;

$$\sum_{\mathbf{k}} c_{\mathbf{k}} \theta(\tilde{\omega} - E_k) = \frac{1}{\Omega} \sum_{\mathbf{k}} \frac{-V_0 \theta(\tilde{\omega} - E_k)}{E - 2E_k} \sum_{\mathbf{k}'} c_{\mathbf{k}'} \theta(\tilde{\omega} - E_{k'})$$
$$-\frac{1}{\Omega} \sum_{\mathbf{k}} \frac{V_0 \theta(\tilde{\omega} - E_k)}{E - 2E_k} = 1.$$
(4.6)

or

Searching for the solution with a negative energy, that is $E = -2\Delta < 0$, we find:

$$\frac{V_0}{\Omega} \sum_{\mathbf{k}} \frac{\theta(\tilde{\omega} - E_k)}{2\Delta + 2E_k} = \int_0^{k_0} \frac{V_0}{(\hbar^2 k^2 / m + 2\Delta)} \, \frac{4\pi k^2 dk}{(2\pi)^3} = 1,$$

where $k_0 = \sqrt{2m\tilde{\omega}}/\hbar$. This gives

$$\frac{mV_0k_0}{2\pi^2\hbar^2}\left\{1-\frac{\sqrt{2m\Delta}}{\hbar k_0}\arctan\left(\frac{\hbar k_0}{\sqrt{2m\Delta}}\right)\right\} = 1.$$
(4.7)

Assuming that $\Delta \ll \tilde{\omega}$ and, hence, $k_0 = \sqrt{2m\tilde{\omega}}/\hbar \gg \sqrt{2\Delta m}/\hbar$, we have

$$\lambda \left(1 - \frac{\pi}{2} \sqrt{\frac{\Delta}{\tilde{\omega}}} \right) = 1, \tag{4.8}$$

where

$$\lambda = \frac{mk_0}{2\pi^2\hbar^2}V_0. \tag{4.9}$$

Equation (4.8) clearly shows that a bound state of two particles may exist only for $\lambda > 1$, which is a known result.

It is now easy to turn to the famous Cooper problem which lies in the basis of superfluid pairing phenomenon. Consider two attractively interacting fermions on top of a filled Fermi sphere, so that the states with wavevectors $k < k_F$ are filled and thus blocked for the occupation. Assume that the center of mass of the two fermions is at rest and, hence, their wavefunction is

$$\psi(\mathbf{r}) = \sum_{|\mathbf{k}| > k_F} c_{\mathbf{k}} \exp(i\mathbf{k}\mathbf{r}), \qquad (4.10)$$

with **r** being the separation between these fermions. We thus return to the already discussed problem, where now the coefficients $c_{\mathbf{k}}$ are given by

$$c_{\mathbf{k}} = \frac{1}{E - 2E_k} \sum_{|\mathbf{k}| > k_F, |\mathbf{k}'| > k_F} U(\mathbf{k} - \mathbf{k}') c_{\mathbf{k}'}.$$
(4.11)

We then use the following model:

$$U(\mathbf{k} - \mathbf{k}') = \begin{cases} -V_0; & E_k > E_F, \ E_F < E_{k'} \le E_F + \tilde{\omega} \\ 0, & \text{otherwise} \end{cases}$$
(4.12)

We search for the solution in the form $E = 2E_F - 2\Delta$ ($\Delta > 0$), i.e. for the bound state of the two fermions on top of the filled Fermi sphere and assume that the inequality $\Delta \ll \tilde{\omega} \ll E_F$ is satisfied. Then we have:

$$\int_{k_F}^{k_0} \frac{V_0}{(2\Delta + 2E_k - 2E_F)} \frac{4\pi k^2 dk}{(2\pi)^3} = 1,$$
(4.13)

where $k'_0 = \sqrt{2m(E_F + \tilde{\omega})} \approx k_F + m\tilde{\omega}/\hbar k_F$, and $(m\tilde{\omega}/\hbar k_F) \ll k_F$. Equation (4.13) then yields:

$$\frac{mV_0k_F^2}{2\pi^2\hbar^2} \int_0^{m\tilde{\omega}/\hbar k_F} \frac{d(k-k_F)}{(2m\Delta/\hbar^2) + 2k_F(k-k_F)} = \frac{\lambda}{2}\ln\left(\frac{\tilde{\omega}}{\Delta}\right) = 1.$$
(4.14)

So, we thus obtain

$$\Delta = \tilde{\omega} \exp\left\{-\frac{2}{\lambda}\right\} \neq 0.$$
(4.15)

In other words, two attractively interacting fermions on top of the filled Fermi sphere always form sort of bound pairs. This phenomenon is called *superfluid pairing*, and we will see later in the course how it leads to superfluidity. Note that it is a collective phenomenon. The presence of the filled Fermi sphere is crucial.

4.2 BCS approach. Gapped single-particle excitations

We now consider a weakly (attractively) interacting gas of \uparrow and \downarrow fermions with densities $n_{\uparrow} = n_{\downarrow} = n$. The grand-canonical Hamiltonian of this system is obtained by subtracting the term $\mu \hat{N}$ (\hat{N} is the operator of the total number of particles) from \hat{H} (3.1) and it reads:

$$\hat{H} = \sum_{\mathbf{k};\,\sigma=\uparrow,\downarrow} \xi_k \hat{a}^{\dagger}_{\sigma\mathbf{k}} \hat{a}_{\sigma\mathbf{k}} + \frac{g}{V} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3} \hat{a}^{\dagger}_{\uparrow\mathbf{k}_3} \hat{a}^{\dagger}_{\downarrow\mathbf{k}_4} \hat{a}_{\downarrow\mathbf{k}_2} \hat{a}_{\uparrow\mathbf{k}_1}, \qquad (4.16)$$

where $g = 4\pi \hbar^2 a/m < 0$, the chemical potential is $\mu = \hbar^2 k_F^2/2m$, and we introduced the notation

$$\xi_k = \frac{\hbar^2 k^2}{2m} - \mu = \frac{\hbar^2}{2m} (k^2 - k_F^2).$$
(4.17)

We will denote the first term of Eq. (4.16) as $\hat{H}_{0\mu}$, and the second (interaction) term as \hat{H}_{int} . In terms of the field operators $\hat{\psi}_{\uparrow}$, $\hat{\psi}_{\downarrow}$, the term $\hat{H}_{0\mu}$ is obtained by subtracting $\mu \sum_{\sigma} \int \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \hat{\psi}_{\sigma}(\mathbf{r}) d^3r$ from \hat{H}_K (2.30) and reads:

$$\hat{H}_{0\mu} = \int d^3r \sum_{\sigma} \hat{\psi}^{\dagger}_{\sigma}(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \nabla^2 - \mu \right) \hat{\psi}_{\sigma}(\mathbf{r}).$$
(4.18)

The interaction part of the Hamiltonian is given by equation (2.33) and we introduce a significant simplification writing \hat{H}_{int} in the form:

$$\hat{H}_{int} = \int d^3r \{ U(\mathbf{r}) [\hat{\psi}^{\dagger}_{\uparrow}(\mathbf{r}) \hat{\psi}_{\uparrow}(\mathbf{r}) + \hat{\psi}^{\dagger}_{\downarrow}(\mathbf{r}) \hat{\psi}_{\downarrow}(\mathbf{r})] + \Delta(\mathbf{r}) \hat{\psi}^{\dagger}_{\uparrow}(\mathbf{r}) \hat{\psi}^{\dagger}_{\downarrow}(\mathbf{r}) + \Delta^*(\mathbf{r}) \hat{\psi}_{\downarrow}(\mathbf{r}) \hat{\psi}_{\uparrow}(\mathbf{r}) \},$$
(4.19)

where the quantities $U(\mathbf{r})$ and $\Delta(\mathbf{r})$ are called the Hartree-Fock potential and pairing potential, respectively. They are given by the relations:

$$U(\mathbf{r}) = g\langle \hat{\psi}_{\uparrow}^{\dagger}(\mathbf{r}) \hat{\psi}_{\uparrow}(\mathbf{r}) \rangle = g\langle \hat{\psi}_{\downarrow}^{\dagger}(\mathbf{r}) \hat{\psi}_{\downarrow}(\mathbf{r}) \rangle, \qquad (4.20)$$

$$\Delta(\mathbf{r}) = g \langle \hat{\psi}_{\downarrow}(\mathbf{r}) \hat{\psi}_{\uparrow}(\mathbf{r}) \rangle.$$
(4.21)

In free space U and Δ are independent of **r** and are real, so that $\Delta = \Delta^*$.

Why do we write Eq. (4.19)? Note that there is Wick's theorem in an ideal gas (however, Δ in this case is zero):

$$\langle \hat{\psi}_{\uparrow}^{\dagger} \hat{\psi}_{\downarrow}^{\dagger} \hat{\psi}_{\downarrow} \hat{\psi}_{\uparrow} \rangle = \langle \hat{\psi}_{\uparrow}^{\dagger} \hat{\psi}_{\uparrow} \rangle \langle \hat{\psi}_{\downarrow}^{\dagger} \hat{\psi}_{\downarrow} \rangle + \langle \hat{\psi}_{\uparrow}^{\dagger} \hat{\psi}_{\downarrow}^{\dagger} \rangle \langle \hat{\psi}_{\downarrow} \hat{\psi}_{\uparrow} \rangle + \text{other pairs of averages.}$$

Assuming weak interactions we simply kept in mind this theorem and used a partial average in Eq. (4.19).

It is also important that the Hartree-Fock potential can be absorbed in the chemical potential by making a transformation $\mu \rightarrow \mu - U$, and it essentially drops out of the problem. We thus may restrict ourselves to the interaction Hamiltonian

$$\hat{H}_{int} = \Delta \int d^3 r [\hat{\psi}^{\dagger}_{\uparrow}(\mathbf{r}) \hat{\psi}^{\dagger}_{\downarrow}(\mathbf{r}) + \hat{\psi}_{\downarrow}(\mathbf{r}) \hat{\psi}_{\uparrow}(\mathbf{r})].$$
(4.22)

Then the momentum-space grand-canonical Hamiltonian (4.16) takes the form:

$$\hat{H}_{BCS} = \sum_{\mathbf{k};\,\sigma=\uparrow,\downarrow} \xi_k \hat{a}^{\dagger}_{\sigma\mathbf{k}} \hat{a}_{\sigma\mathbf{k}} + \Delta \sum_{\mathbf{k}} (\hat{a}_{\downarrow\mathbf{k}} \hat{a}_{\uparrow-\mathbf{k}} + \hat{a}^{\dagger}_{\uparrow-\mathbf{k}} \hat{a}^{\dagger}_{\downarrow\mathbf{k}}).$$
(4.23)

The approach based on the Hamiltonian (4.23) belongs to Bardeen, Cooper, and Schrieffer and is commonly identified as BCS approach.

The Hamiltonian (4.23) is bilinear in the particle operators $\hat{a}_{\sigma,\mathbf{k}}$ and hence can be reduced to a diagonal form by using a canonical Bogoliubov transformation. We employ the Bogoliubov transformation in the form:

$$\hat{b}_{\uparrow \mathbf{k}} = u_k \hat{a}_{\uparrow \mathbf{k}} + v_k \hat{a}_{\downarrow -\mathbf{k}}^{\dagger}, \qquad (4.24)$$

$$\hat{b}_{\downarrow \mathbf{k}} = u_k \hat{a}_{\downarrow \mathbf{k}} - v_k \hat{a}^{\dagger}_{\uparrow - \mathbf{k}}, \qquad (4.25)$$

where the new (quasiparticle) operators $\hat{b}_{\sigma \mathbf{k}}$ satisfy the same (anti)commutation relations as the particle operators $\hat{a}_{\sigma \mathbf{k}}$:

$$\hat{b}_{\sigma\mathbf{k}}\hat{b}^{\dagger}_{\sigma'\mathbf{k}'} + \hat{b}^{\dagger}_{\sigma'\mathbf{k}'}\hat{b}_{\sigma\mathbf{k}} = \delta_{\sigma\sigma'}\delta_{\mathbf{k}\mathbf{k}'}, \qquad (4.26)$$

$$\hat{b}_{\sigma\mathbf{k}}\hat{b}_{\sigma'\mathbf{k}'} + \hat{b}_{\sigma'\mathbf{k}'}\hat{b}_{\sigma\mathbf{k}} = 0.$$

$$(4.27)$$

From Eq. (4.24) we then have

$$\{\hat{b}_{\sigma\mathbf{k}}\hat{b}^{\dagger}_{\sigma'\mathbf{k}'}\} = u_k u_{k'}\{\hat{a}_{\sigma\mathbf{k}}\hat{a}^{\dagger}_{\sigma'\mathbf{k}'}\} + (2\delta_{\sigma\sigma'}-1)v_k v_{k'}\{\hat{a}^{\dagger}_{\sigma'-\mathbf{k}}\hat{a}_{\sigma-\mathbf{k}'}\} = (u_k^2 + v_k^2)\delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'},$$

where the symbol {} stands for the anticommutation: $\{\hat{a}_{\sigma \mathbf{k}}\hat{a}^{\dagger}_{\sigma'\mathbf{k}'}\} = \hat{a}_{\sigma \mathbf{k}}\hat{a}^{\dagger}_{\sigma'\mathbf{k}'} + \hat{a}^{\dagger}_{\sigma'\mathbf{k}'}\hat{a}_{\sigma \mathbf{k}}$. We thus obtain the normalization condition

$$u_k^2 + v_k^2 = 1. (4.28)$$

The inverse Bogoliubov transformation reads:

$$\hat{a}_{\uparrow \mathbf{k}} = u_k \hat{b}_{\uparrow \mathbf{k}} - v_k \hat{b}_{\downarrow - \mathbf{k}}^{\dagger}, \qquad (4.29)$$

$$\hat{a}_{\downarrow \mathbf{k}} = u_k \hat{b}_{\downarrow \mathbf{k}} + v_k \hat{b}^{\dagger}_{\uparrow - \mathbf{k}}.$$
(4.30)

Then, for reducing \hat{H}_{BCS} (4.23) to the diagonal form

$$\hat{H}_{\rm BCS} = E_0 + \sum_{\sigma, \mathbf{k}} \epsilon_k \hat{b}^{\dagger}_{\sigma \mathbf{k}} \hat{b}_{\sigma \mathbf{k}}, \qquad (4.31)$$

the functions u_k , v_k should satisfy the Bogoliubov-de Gennes equations

$$\xi_k u_k + \Delta v_k = \epsilon_k u_k, \tag{4.32}$$

$$-\xi_k v_k + \Delta u_k = \epsilon_k v_k. \tag{4.33}$$

Taking into account the normalization condition (4.28), equations (4.32) and (4.33) yield:

$$u_k^2 = \frac{1}{2} \left(1 + \frac{\xi_k}{\epsilon_k} \right), \tag{4.34}$$

$$v_k^2 = \frac{1}{2} \left(1 - \frac{\xi_k}{\epsilon_k} \right), \tag{4.35}$$



Figure 4.1: Spectrum of single-particle excitations for an attractively interacting two-component Fermi gas.

and lead to the dispersion relation



 $\epsilon_k = \sqrt{\xi_k^2 + \Delta^2}.\tag{4.36}$

Figure 4.2: The functions u_k (brown curve) and v_k (blue curve).

These quantities are shown in Fig. 4.1 and Fig. 4.2. Thus, the spectrum of single-particle excitations has a gap. This implies that the density of states for

the excitations has a singularity at $\epsilon = \Delta$ as shown in Fig. 4.3:

$$\nu(\epsilon) = \int \delta(\epsilon - \sqrt{\xi_k^2 + \Delta^2}) \, \frac{d^3k}{(2\pi)^3} = \nu(E_F) \, \frac{\epsilon}{\sqrt{\epsilon^2 - \Delta^2}}; \quad |\epsilon| > \Delta, \qquad (4.37)$$

where $\nu(E_F) = mk_F/2\pi^2\hbar^2$ is the particle density of states at the Fermi surface.



Figure 4.3: Density of states for single-particle excitations.

4.3 Order parameter and transition temperature

We now have to find the gap Δ . It is given by equation (4.21) and is, therefore, also termed *order parameter*. We write Eq. (4.21) in the form:

$$\Delta = g \langle \hat{\psi}_{\downarrow}(\mathbf{r}) \hat{\psi}_{\uparrow}(\mathbf{r}) \rangle = \frac{g}{V} \sum_{\mathbf{k}} \langle \hat{a}_{\downarrow - \mathbf{k}} \hat{a}_{\uparrow \mathbf{k}} \rangle = \frac{g}{V} \sum_{\mathbf{k}} \langle (u_k \hat{b}_{\downarrow - \mathbf{k}} + v_k \hat{b}_{\uparrow \mathbf{k}}^{\dagger}) (u_k \hat{b}_{\uparrow \mathbf{k}} - v_k \hat{b}_{\downarrow - \mathbf{k}}^{\dagger}) \rangle$$
$$= \frac{g}{V} \sum_{\mathbf{k}} (u_k v_k \langle (\hat{b}_{\uparrow \mathbf{k}}^{\dagger} \hat{b}_{\uparrow \mathbf{k}} - \hat{b}_{\downarrow - \mathbf{k}} \hat{b}_{\downarrow - \mathbf{k}}^{\dagger}) \rangle = -\frac{g}{V} \sum_{\mathbf{k}} u_k v_k (1 - 2N_k).$$
(4.38)

Single-particle excitations obey Fermi statistics and their occupation numbers N_k are given by the Fermi-Dirac relation:

$$N_k = \langle \hat{b}_{\sigma \mathbf{k}}^{\dagger} \hat{b}_{\sigma \mathbf{k}} \rangle = \frac{1}{\exp(\epsilon_k/T) + 1}.$$

Using the relation $u_k v_k = \Delta/2\epsilon_k$ following from Eqs. (4.34) and (4.35) we then transform Eq. (4.38) to

$$|g| \int \frac{\tanh(\epsilon_k/2T)}{2\epsilon_k} \frac{d^3k}{(2\pi)^3} = 1.$$

$$(4.39)$$

Equation (4.39) is called the gap equation. At T = 0 it becomes

$$|g| \int \frac{1}{2\sqrt{\Delta_0^2 + \xi_k^2}} \frac{d^3k}{(2\pi)^3} = 1.$$
(4.40)

The main contribution to the integral in Eq. (4.40) comes from momenta k close to k_F and we may write $|\xi_k| \simeq \hbar v_F |k - k_F| \ll E_F$. We thus obtain:

$$|g|\nu(E_F)\int_0^{\tilde{\omega}} \frac{d\xi}{\sqrt{\xi^2 + \Delta_0^2}} = \lambda \ln\left(\frac{\tilde{\omega}}{\Delta_0}\right) = 1, \qquad (4.41)$$

where recalling that $g = 4\pi\hbar^2 a/m$ we have $\lambda = 2k_F|a|/\pi$, and the high-energy cut-off $\tilde{\omega}$ may be put of the order of E_F . This gives the zero-temperature gap:

$$\Delta_0 \approx E_F \exp(-1/\lambda) = E_F \exp(-\pi/2k_F|a|) \ll E_F.$$
(4.42)

Let us now return to the initial gap equation (4.39). The highest temperature at which this equation has a non-trivial solution is the critical temperature T_c . Only below this temperature the spectrum of single-particle excitations has a gap. The calculation of T_c and $\Delta(T)$ is presented in *Problem 1* to this *Lecture*. The critical temperature is related to the zero-temperature gap as

$$T_c = 0.57\Delta_0,\tag{4.43}$$

and the temperature dependence of the gap is given by

$$\Delta = \Delta_0 \left[1 - \sqrt{\frac{2\pi T}{\Delta_0}} \exp(-\Delta_0/T) \right]; \quad T \ll \Delta_0, \quad (4.44)$$

$$\Delta = 3.06T_c \left(1 - \frac{T}{T_c}\right)^{1/2}; \qquad T \to T_c. \tag{4.45}$$

The dependence $\Delta(T)$ is displayed in Fig. 4.4.

The spectrum of single-particle excitations, $\epsilon(k)$, satisfies the Landau criterion of superfluidity discussed in *Lecture 6* of *Part 1* of the course. The minimum value of $\epsilon(k)/k$ is non-zero. Therefore, the weakly interacting two-component Fermi gas with intercomponent attraction is superfluid. We will discuss the issue of fermionic superfluidity in *Lecture 5*. Here we only mention that since $\Delta(T)$ decreases with increasing temperature and becomes zero for $T > T_c$, the temperature T_c is the superfluid transition temperature. For $T > T_c$ the spectrum is not gapped and is in some sense similar to the spectrum of an ideal gas (Fermi liquid), so that there is no superfluidity.

Note that the picture of pairing near the Fermi surface is better imaged as correlation between states in k-space, which allows two particles to have zero total momentum. The momentum interval δk in the region of correlations corresponds to the energy interval Δ . So, we have $\delta k \sim \Delta/\hbar v_F$. The related length is $\zeta \sim \hbar v_F/\Delta$. It determines a characteristic distance between particles with correlated momenta. At T = 0 it is called *coherence length* and is given by

$$\zeta_0 = \frac{\hbar v_F}{\Delta_0} \sim \frac{1}{k_F} \exp\left(\frac{\pi}{2|k_F|a}\right) \gg n^{-1/3}.$$
(4.46)



Figure 4.4: The gap in the spectrum of single-particle excitations as a function of temperature.

Problems 4

4.1 Find a relation between the zero-temperature gap Δ_0 and the critical temperature T_c . Calculate $\Delta(T)$ in the limit of ultralow temperatures $T \ll \Delta_0$.

At $T = T_c$ the gap vanishes and the excitation energy is $\epsilon_k = |\xi_k| = \hbar^2 |k^2 - k_F^2|/2m$. Thus the gap equation (4.39) becomes:

$$|g| \int \frac{\tanh(|\xi_k|/2T_c)}{2|\xi_k|} \frac{d^3k}{(2\pi)^3} = 1.$$
(4.47)

On the other hand, at T = 0 we have $\epsilon_k = \sqrt{\xi_k^2 + \Delta_0^2}$ and the gap equation (4.40). Subtracting Eq. (4.40) from Eq. (4.47) and turning to the integration over $d\xi_k$ we obtain:

$$\int_{-E_F}^{\infty} \left[\frac{\tanh(|\xi_k|/2T_c)}{2|\xi_k|} - \frac{1}{2\sqrt{\xi_k^2 + \Delta_0^2}} \right] \frac{mk}{2\pi^2\hbar^2} d\xi_k = 0.$$
(4.48)

Assuming that both Δ_0 and T_c are very small we divide the area of integration in Eq. (4.48) into two parts: from $-\omega$ to ω , and from ω to infinity plus from $-E_F$ to $-\omega$. The quantity ω is chosen such that $E_F \gg \omega \gg \Delta_0, T_c$. In the second area, i.e. from ω to ∞ and from $-E_F$ to $-\omega$, we may put $\tanh(|\xi_k|/2T_c) = 1$ and $\Delta_0 = 0$. Hence, the integrand vanishes, and we are left with the integration from $-\omega$ to ω for which we put $k = k_F$ outside the square brackets. Taking into
account that the integrand becomes an even function of ξ_k we reduce Eq. (4.48) to

$$\int_{0}^{\omega} \left[\frac{\tanh(\xi_k/2T_c)}{2\xi_k} - \frac{1}{2\sqrt{\xi_k^2 + \Delta_0^2}} \right] d\xi_k = 0.$$
 (4.49)

Integrating the first term in the square brackets we turn to the integration variable $\xi_k/2T_c$, and integrating the second term to the integration variable ξ_k/Δ_0 . The integration yields:

$$\ln\left(\frac{\omega}{2T_c}\right) \tanh\left(\frac{\omega}{2T_c}\right) - \int_0^{\omega/2T_c} \frac{\ln x}{\cosh^2 x} dx - \ln\left\{\frac{\omega}{\Delta_0} + \sqrt{1 + \frac{\omega^2}{\Delta_0^2}}\right\} = 0$$

Since $\omega \gg T_c, \Delta_0$, we may put $\tanh(\omega/2T_c) = 1$, set the upper limit of integration over dx equal to infinity, and write the last term as $\ln(2\omega/\Delta_0)$. This gives:

$$\ln \frac{\Delta_0}{4T_c} = \int_0^\infty \frac{\ln x}{\cosh^2 x} dx = \ln \pi - 2\ln 2 - C,$$

where C = 0.577 is the Euler constant. We thus obtain equation (4.43):

$$T_c = \frac{\exp C}{\pi} \Delta_0 = 0.57 \Delta_0.$$

For calculating $\Delta(T)$ at $T \ll \Delta_0$ we substract the gap equation (4.39) from the zero-temperature gap equation (4.40) and thus obtain:

$$\int_0^\infty \left[\frac{1}{2\sqrt{\xi_k^2 + \Delta_0^2}} - \frac{\tanh(\sqrt{\xi_k^2 + \Delta^2}/2T)}{2\sqrt{\xi_k^2 + \Delta^2}} \right] \frac{k^2 dk}{2\pi^2} = 0.$$

Again, turning to the integration over $d\xi_k$ and dividing the area of integration into two parts: from $-\omega$ to ω , and from ω to ∞ plus from $-E_F$ to $-\omega$, we select ω such that $\Delta_0 \ll \omega \ll E_F$ and find:

$$\int_{0}^{\omega} \left[\frac{1}{\sqrt{\xi_{k}^{2} + \Delta_{0}^{2}}} - \frac{\tanh(\sqrt{\xi_{k}^{2} + \Delta^{2}}/2T)}{\sqrt{\xi_{k}^{2} + \Delta^{2}}} \right] d\xi_{k} = 0.$$
(4.50)

Using a relation

$$\tanh x = 1 - \frac{2\exp(-x)}{\exp x + \exp(-x)}$$

we reduce equation (4.50) to

$$\ln \frac{\Delta}{\Delta_0} + 2 \int_0^\omega \frac{\exp(-\sqrt{\xi_k^2 + \Delta^2}/T)}{\sqrt{\xi_k^2 + \Delta^2}} d\xi_k = 0,$$

where we took into account that $\omega \gg \Delta_0$. Since $T \ll \Delta, \Delta_0$ the main contribution to the remaining integral over $d\xi_k$ comes from $\xi_k \ll \Delta$. We then represent $\sqrt{\xi_k^2 + \Delta^2}$ in the exponent as $\sqrt{\xi_k^2 + \Delta^2} = \Delta + \xi_k^2/2\Delta$ and put this quantity equal to ξ_k in the denominator of the integrand. After the integration over $d\xi_k$ we have:

$$\ln \frac{\Delta_0}{\Delta} = \sqrt{\frac{2\pi T}{\Delta}} \exp\left(-\frac{\Delta}{T}\right). \tag{4.51}$$

Writing $\Delta = \Delta_0 - \delta \Delta$ and assuming that $\delta \Delta \ll T$, from Eq. (4.51) we obtain:

$$\delta \Delta = \sqrt{2\pi\Delta_0 T} \exp\left(-\frac{\Delta_0}{T}\right)$$

This equation justifies the assumption that $\delta \Delta \ll T$. So, the final result is given by equation (4.44):

$$\Delta(T) = \Delta_0 \left[1 - \sqrt{\frac{2\pi T}{\Delta_0}} \exp\left(-\frac{\Delta_0}{T}\right) \right]$$

4.2 Calculate $\Delta(T)$ at temperatures near T_c , where $\Delta \ll T$ and $(T_c - T) \ll T_c$.

Lecture 5. Superfluidity in Fermi gases

5.1 Landau criterion in Fermi gases

In this Lecture we discuss the phenomenon of superfluidity in attractively interacting Fermi gases. As we have established in Lecture 4, the spectrum of single-particle excitations is $\epsilon(p) = \sqrt{\Delta^2 + \xi_p^2}$, where $\xi_p = v_F(p - p_F)$ (p is here the true momentum, not the wavevector). The gap Δ is exponentially small in the limit of weak interactions and becomes zero for $T > T_c = 0.57\Delta_0$, with Δ_0 being the zero-temperature gap. In Fig. 5.1 we compare the spectra of attractively and repulsively interacting Fermi gases. As we see, there is a drastic difference. For the attractively interacting gas there is a minimum value $(\epsilon(p)/p)_{min} > 0$, whereas for repulsive interactions it is zero.

Let us repeat the arguments given in *Lecture 6* of *Part 1* of the course, now on support of superfluidity in attractively interacting Fermi gases. Imagine that an excitation with energy $\epsilon(p)$ and momentum **p** appears in such a system. Then the energy and momentum of the gas become $\epsilon(p)$ and \hbar **p**. The excitation appears, for example, if the gas is in a capillary and the latter is moving with velocity $-\mathbf{v}$. Then, in the reference frame where the capillary is at rest but the gas is moving with velocity **v**, we have the energy and momentum:

$$E = \epsilon(p) + \mathbf{p}_0 \mathbf{v} + \frac{Mv^2}{2},$$

$$\mathbf{p}' = \mathbf{p} + M\mathbf{v},$$

where M is the mass of the gas. The term $Mv^2/2$ is the initial kinetic energy of the gas, and $\epsilon + \mathbf{pv}$ is the energy change due to the appearance of the excitation.



Figure 5.1: Spectrum of single-particle excitations for attractively and repulsively interacting Fermi gases.

So, at T = 0 we should have $\epsilon + \mathbf{pv} < 0$, otherwise the excitation can not appear. This is possible only if $v > (\epsilon/p)$. Thus, if there is a minimum value $(\epsilon/p)_{min} = v_c$, for velocities $v < v_c$ the excitations do not appear. Then, there is no friction between the capillary and the gas, and one has *superfluidity*.

So, the superfluidity requires the condition

$$\left(\frac{\epsilon(p)}{p}\right)_{min} > 0,$$

and the velocity of the motion

$$v < v_c = \left(\frac{\epsilon(p)}{p}\right)_{min}$$

For the attractively interacting Fermi gas we have a very small critical velocity:

$$v_c \approx \frac{\Delta}{v_F} \sim v_F \exp\left(-\frac{\pi}{2k_F|a|}\right).$$
 (5.1)

5.2 Superfluid current

Let us now discuss the superfluid current. First of all, we write the Bogoliubovde Gennes equations for the coordinate-space wavefunctions of the excitations. In free space they read (see *Problem 1* to this *Lecture*):

$$\hat{H}_0 u_\nu + \Delta v_\nu = \epsilon_\nu u_\nu, \tag{5.2}$$

$$-H_0 v_\nu + \Delta^* u_\nu = \epsilon_\nu v_\nu, \tag{5.3}$$

where $\hat{H}_0 = (-\hbar^2/2m)(d^2/d\mathbf{r}^2) - \mu$, and the index ν labels quantum states of the excitations. Assuming that in the presence of current the order parameter (gap) is complex we write

$$\Delta = \bar{\Delta} \exp(2i\phi). \tag{5.4}$$

Comparing equations (5.2) and (5.3) with the Bogoliubov-de Gennes equations for a Bose-condensed gas (see *Lecture 5* of *Part 1*) we see that Δ plays a role of the "wavefunction of a condensate of Cooper pairs". We now write

$$u_{\nu} = \bar{u}_{\nu} \exp(i\phi), \tag{5.5}$$

$$v_{\nu} = \bar{v}_{\nu} \exp(-i\phi). \tag{5.6}$$

For small gradients of ϕ and vanishingly low momenta of the excitations the quantities \bar{u} , \bar{v} coincide with u_k/\sqrt{V} , v_k/\sqrt{V} where $u_k v_k$ are given by Eqs. (4.34) and (4.35). This is clear from the Bogoliubov-de Gennes equations obtained after substituting u_{ν} (5.5) and v_{ν} (5.6) into Eqs. (5.2) and (5.3):

$$\begin{aligned} \hat{H}_0 \bar{u}_\nu + \bar{\Delta} \bar{v}_\nu + \text{gradients of } \phi &= \epsilon \bar{u}_\nu, \\ - \hat{H}_0 \bar{v}_\nu + \bar{\Delta}^* \bar{u}_\nu + \text{gradients of } \phi &= \epsilon \bar{v}_\nu. \end{aligned}$$

The operator of the current is given by

$$\hat{\mathbf{j}} = -\frac{i\hbar}{2m} \sum_{\sigma} \left[\hat{\psi}^{\dagger}_{\sigma} \nabla \hat{\psi}_{\sigma} - (\nabla \hat{\psi}^{\dagger}_{\sigma}) \hat{\psi}_{\sigma} \right].$$
(5.7)

Since the field operators $\hat{\psi}_{\sigma}$ can be expressed as (see *Problem 1* to this *Lecture*):

$$\begin{split} \hat{\psi}_{\uparrow} &= \sum_{\nu} (u_{\nu} \hat{b}_{\uparrow\nu} - v_{\nu}^{*} \hat{b}_{\downarrow\nu}^{\dagger}), \\ \hat{\psi}_{\downarrow} &= \sum_{\nu} (u_{\nu} \hat{b}_{\downarrow\nu} + v_{\nu}^{*} \hat{b}_{\uparrow\nu}^{\dagger}), \end{split}$$

at T = 0 we obtain the following expectation value

$$\langle j \rangle = -\frac{i\hbar}{2m} \sum_{\sigma\nu} (v_{\nu} \nabla v_{\nu}^* - v_{\nu}^* \nabla v_{\nu}) = \frac{\hbar}{m} \left(\sum_{\sigma\nu} \frac{v_{\nu}^2}{V} \right) \nabla \phi$$
(5.8)

Let us now recall the expression for v_k in the uniform case. It is given by Eq. (4.35). Except for a narrow vicinity of k_F , where the presence of the gap Δ in the expression for the excitation energy is important, we have $v_k = 1$ for $k < k_F$ and $v_k = 0$ for $k > k_F$. Thus, equation (5.8) gives:

$$\langle j \rangle = \frac{\hbar}{m} \nabla \phi \sum_{\sigma} \int_{0}^{k_{F}} \frac{k^{2}}{2\pi^{2}} dk = \frac{\hbar}{m} n \nabla \phi.$$
 (5.9)

where $n = \sum_{\sigma} n_{\sigma}$ is the total density. So, the quantity

$$\mathbf{v}_s = \frac{\hbar}{m} \nabla \phi \tag{5.10}$$

is the superfluid velocity.

The superfluid current is

$$\mathbf{j}_s = n\mathbf{v}_s. \tag{5.11}$$

Thus, at T = 0 the whole mass of the gas (liquid) is superfluid.

5.3 Bogoliubov-Anderson sound

We now consider hydrodynamic equations for the superfluid Fermi gas. They read:

$$\frac{\partial n}{\partial t} + \operatorname{div}(n\mathbf{v}) = 0, \qquad (5.12)$$

$$m\frac{\partial \mathbf{v}}{\partial t} + \nabla \left[\frac{1}{2}mv^2 + \mu(n)\right] = 0.$$
(5.13)

We then write $n = \bar{n} + \delta n$, where \bar{n} is the mean value of the density. Assuming small velocities **v** and density fluctuations δn , we confine ourselves only to terms that are linear in **v** and δn . Writing $\mathbf{v} = (\hbar/m)\nabla\phi$ we thus obtain linearized hydrodynamic equations:

$$\frac{\partial \delta n}{\partial t} + \nabla \left(\frac{\hbar \bar{n}}{m} \nabla \phi\right) = 0, \qquad (5.14)$$

$$\hbar \frac{\partial \nabla \phi}{\partial t} + \frac{\partial \mu}{\partial n} \Big|_{n=\bar{n}} \nabla \delta n = 0.$$
(5.15)

Taking the time derivative in Eq. (5.14) and substituting $\partial \nabla \phi / \partial t$ from Eq. (5.15) we obtain:

$$\frac{\partial^2 \delta n}{\partial t^2} = \frac{\bar{n}}{m} \frac{\partial \mu}{\partial n} \Big|_{n=\bar{n}} \nabla^2 \delta n.$$
(5.16)

The derivative of the chemical potential with respect to the density is given by

$$\frac{\partial \mu}{\partial n}\Big|_{n=\bar{n}} = \frac{\partial}{\partial n} \left(\frac{\hbar^2}{2m} (3\pi^2 n)^{2/3}\right)\Big|_{n=\bar{n}} = \frac{2E_F}{3\bar{n}}.$$

Writing small fluctuations of the density as

$$\delta n \propto \exp(-i\epsilon t/\hbar + i\mathbf{kr})$$

we then find

$$\left(\frac{\epsilon}{\hbar}\right)^2 = \frac{2E_F}{3m}k^2,$$

or

$$\epsilon = \hbar \sqrt{\frac{2E_F}{3m}} \, k = \frac{\hbar v_F}{\sqrt{3}} k. \tag{5.17}$$

We thus see that there is one more branch of excitations. It is related to fluctuations of the phase of Δ . These excitations obey the Bose statistics and are called Bogoliubov-Anderson sound. Note that for this branch of excitations we have $(\epsilon/\hbar k)_{min} = v_F/\sqrt{3}$ and they do not destroy superfluidity. They do not even change the critical velocity.

5.4 Superfluid and normal density. Thermodynamic quantities near T_c

At a finite temperature the superfluid gas can be implicitly divided into two parts: *superfluid* and *normal*. Repeating the arguments given in *Lecture* 6 of *Part* 1 of the course we now imagine that the "gas of excitations" is moving with respect to the liquid (gas) with velocity \mathbf{v} . The distribution function for the excitations is then obtained by replacing the excitation energy ϵ with $\epsilon - \mathbf{pv}$, where \mathbf{p} is the excitation momentum. So, the total momentum of the "gas of excitations" per unit volume will be:

$$\mathbf{P} = \int \mathbf{p} N(\epsilon - \mathbf{p}\mathbf{v}) \frac{d^3 p}{(2\pi\hbar)^3}.$$
(5.18)

Assuming a small velocity \mathbf{v} we expand the integrand of Eq. (5.18) in powers of (\mathbf{pv}) . Retaining only the linear term we have:

$$\mathbf{P} = -\int \mathbf{p}(\mathbf{p}\mathbf{v}) \frac{dN(\epsilon)}{d\epsilon} \frac{d^3p}{(2\pi\hbar)^3}.$$

Averaging over the directions of \mathbf{p} we then obtain:

$$\mathbf{P} = -\frac{\mathbf{v}}{3} \int \frac{dN(\epsilon)}{d\epsilon} p^2 \frac{d^3 p}{(2\pi\hbar)^3}.$$
(5.19)

The gas of excitations can collide with the walls, exchange energy and momentum, and eventually it will be stopped by the walls. The mass density of the liquid (gas) can be written as a sum of the superfluid and normal parts:

$$\rho = \rho_s + \rho_n. \tag{5.20}$$

The expression for the normal density follows from Eq. (5.19) treating **P** as the momentum of the system as a whole:

$$\rho_n = -\frac{1}{3} \int \frac{dN(\epsilon)}{d\epsilon} p^2 \frac{d^3 p}{(2\pi\hbar)^3}.$$
(5.21)

As we see, there are two contributions to ρ_n : the contribution of gapped single-particle excitations, and at sufficiently low temperatures we should take into account the contribution of Bogoliubov-Anderson sound. Both are zero at T = 0. At a finite temperature for the contribution of single-particle gapped excitations we have:

$$\rho_n = -\frac{2}{3} \int p^2 \frac{d}{d\epsilon} \left(\frac{1}{\exp(\epsilon/T) + 1} \right) \frac{d^3 p}{(2\pi\hbar)^3},\tag{5.22}$$

where $\epsilon = \sqrt{\Delta^2 + [(p^2 - p_F^2)/2m]^2}$, and an additional factor 2 comes from the summation over \uparrow and \downarrow excitation branches. The main contribution to the integral comes from momenta p close to the Fermi momentum p_F , and we obtain:

$$\rho_n = -\frac{p_F^4}{3\pi^2 v_F \hbar^3} \int_{-\infty}^{\infty} \frac{dN(\epsilon)}{d\epsilon} d\xi, \qquad (5.23)$$

with $\xi = v_F(p - p_F)$. Since the total density is $\rho = mp_F^3/3\pi^2$, we can write:

$$\rho_n = -2\rho \int_0^\infty \frac{dN(\epsilon)}{d\epsilon} d\xi.$$
(5.24)

We first notice that at the superfluid transition temperature, $T = T_c$, we have $\Delta = 0$ and $\epsilon = |\xi|$, so that

$$-2\int_0^\infty \frac{dN}{d\epsilon}\,d\xi = 1.$$

Just below T_c we may expand the integral in Eq. (5.24) in powers of Δ^2/T_c^2 . This gives

$$\frac{\rho_n}{\rho} = 1 - 2\frac{\Delta^2}{T_c^2} \frac{7\zeta(3)}{8\pi^2} = 1 - 2\frac{T_c - T}{T_c}; \quad 0 < (T_c - T) \ll T_c.$$
(5.25)

For very low temperatures, $T \ll \Delta_0$, we may write

$$\frac{dN}{d\epsilon} = -\frac{1}{T} \frac{\exp(\epsilon/T)}{\exp(\epsilon/T) + 1} \approx -\frac{1}{T} \exp\left(-\frac{\Delta_0}{T} - \frac{\xi^2}{2\Delta_0 T}\right),$$

and Eq. (5.24) yields

$$\frac{\rho_n}{\rho} = \left(\frac{2\pi\Delta_0}{T}\right)^{1/2} \exp(-\Delta_0/T); \quad T \ll \Delta_0.$$
(5.26)

The normal density decreases exponentially with temperature, and we have to take into account the contribution of bosonic Bogoliubov-Anderson sound.

For these excitations we have the dispersion relation (5.17) and the distribution function

$$N(\epsilon) = \frac{1}{\exp(\epsilon/T) - 1}$$

Then, equation (5.21) is transformed to

$$\rho_n = \frac{1}{6\pi^2 T} \int_0^\infty \frac{\exp(\epsilon/T)}{(\exp(\epsilon/T) - 1)^2} \frac{p^4 dp}{\hbar^3}$$

The integration with $\epsilon = v_F p / \sqrt{3}$ is straightforward and it yields:

$$\rho_n = \frac{1}{6\pi^2 T \hbar^3} \left(\frac{\sqrt{3}T}{v_F}\right)^5 \int_0^\infty \frac{x^4 \exp x}{(\exp x - 1)^2} dx = \frac{27\sqrt{3}}{4} \rho \left(\frac{T}{E_F}\right)^4 \zeta(4).$$
(5.27)

where $\zeta(4)$ is very close to unity. Thus, at $T \to 0$ the Bogoliubov-Anderson sound gives the leading contribution to the normal density.

We now show that the BCS superfluid transition is of the second order. Indeed, for $T = T_c$ we have $\Delta = 0$ and $\epsilon(p) = |p^2 - p_F^2|/2m$. This is the same as in the Fermi liquid. We should only renormalize the chemical potential in order to take into account the interactions, not more than that. Thus, the energy and other thermodynamic quantities are continuous at $T = T_c$. So, this is *not* the *first order* transition.

Let us focus on the derivatives of thermodynamic functions, for example on the heat capacity. Variation of the energy under variations of the occupation numbers is

$$\delta E = \sum_{\mathbf{p}} \epsilon(p) (\delta N_{\uparrow \mathbf{p}} + \delta N_{\downarrow \mathbf{p}}) = 2 \sum_{\mathbf{p}} \epsilon(p) \delta N_{\mathbf{p}}.$$
 (5.28)

Dividing Eq. (5.28) by δT we have

$$C = 2 \int \epsilon(p) \frac{\partial N(p)}{\partial T} \frac{V d^3 p}{(2\pi\hbar)^3} = \frac{V m p_F}{\pi^2} \int_{-\infty}^{\infty} \epsilon \frac{\partial N(\epsilon)}{\partial T} d\xi, \qquad (5.29)$$

where again $\xi = v_F(p-p_F)$ and we took into account that the main contribution to the integral comes from momenta near the Fermi surface.

Using the Fermi-Dirac relation for $N(\epsilon)$ we obtain;

$$\epsilon \frac{\partial N(\epsilon)}{\partial T} = \left[\frac{\epsilon^2}{T^2} - \frac{1}{2T} \frac{\partial \Delta^2}{\partial T}\right] \frac{\exp(\epsilon/T)}{(\exp(\epsilon/T) + 1)^2}.$$
 (5.30)

The result of the integration of the first term in the square brackets on the right hand side of Eq. (5.30) is continuous at $T = T_c$, and it gives the heat capacity in the normal (non-superfluid) phase, C_n . The second term is discontinuous at $T = T_c$. In the normal phase, i.e. for $T > T_c$, it is equal to zero. In the superfluid phase at $T \to T_c$, using Eq. (4.45) we have:

$$\frac{\partial \Delta^2}{\partial T} = -T_c \frac{8\pi^2}{7\zeta(3)}; \quad T \to T_c.$$
(5.31)

So, the result of the integration of the second term in the square brackets of Eq. (5.30) gives a jump in the heat capacity at $T = T_c$:

$$C_s - C_n = \frac{4Vmp_F}{7\zeta(3)} \int_{-\infty}^{\infty} \frac{\exp(\epsilon/T)}{(\exp(\epsilon/T) + 1)^2} d\xi.$$
 (5.32)

Putting $\epsilon = |\xi|$ in the integrand of Eq. (5.32) we find:

$$C_s - C_n = \frac{4Vmp_F}{7\zeta(3)}T_c \sim N\exp\left(-\frac{\pi}{2p_F|a|}\right),\tag{5.33}$$

where N is the total number of particles. We thus clearly see that the superfluid BCS transition is the transition of the second order.

Problems 5

5.1 Derive the Bogoliubov-de Gennes equations for the coordinate-space eigenfunctions of single-particle excitations. In terms of the field operators $\hat{\psi}^{\dagger}_{\sigma}(\mathbf{r})$, $\hat{\psi}_{\sigma}(\mathbf{r})$ the BCS Hamiltonian is the sum of $\hat{H}_{0\mu}$ (4.18) and \hat{H}_{int} (4.19) with $U(\mathbf{r}) = 0$:

$$\hat{H}_{\rm BCS} = \int d^3r \left[\sum_{\sigma} \hat{\psi}^{\dagger}_{\sigma}(\mathbf{r}) (\hat{H}_0 + V(\mathbf{r})) \hat{\psi}_{\sigma}(\mathbf{r}) + \Delta(\mathbf{r}) \hat{\psi}^{\dagger}_{\uparrow}(\mathbf{r}) \hat{\psi}^{\dagger}_{\downarrow}(\mathbf{r}) + \Delta^*(\mathbf{r}) \hat{\psi}_{\downarrow}(\mathbf{r}) \hat{\psi}_{\uparrow}(\mathbf{r}) \right], \quad (5.34)$$

where

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\nabla^2 - \mu, \qquad (5.35)$$

and we also included an external potential $V(\mathbf{r})$. We now write $\hat{\psi}_{\sigma}(\mathbf{r})$ in the form:

$$\hat{\psi}_{\uparrow}(\mathbf{r}) = \sum_{\nu} [u_{\nu}(\mathbf{r})\hat{b}_{\uparrow\nu} - v_{\nu}^{*}(\mathbf{r})\hat{b}_{\downarrow\nu}^{\dagger}], \qquad (5.36)$$

$$\hat{\psi}_{\downarrow}(\mathbf{r}) = \sum_{\nu} [u_{\nu}(\mathbf{r})\hat{b}_{\downarrow\nu} + v_{\nu}^{*}(\mathbf{r})\hat{b}_{\uparrow\nu}^{\dagger}], \qquad (5.37)$$

which is nothing else than the Bogoliubov transformation in the coordinate space. Substituting the field operators given by Eqs. (5.36) and (5.37) into $H_{\rm BCS}$ (5.34) we find that the latter reduces to the diagonal form

$$\hat{H}_{\rm BCS} = E_0 + \sum_{\sigma\nu} \epsilon_{\nu} \hat{b}^{\dagger}_{\sigma\nu} \hat{b}_{\sigma\nu}$$

if the functions $u_{\nu}(\mathbf{r}), v_{\nu}(\mathbf{r})$ satisfy the Bogoliubov-de Gennes equations:

$$[\hat{H}_0 + V(\mathbf{r})]u_\nu(\mathbf{r}) + \Delta(\mathbf{r})v_\nu(\mathbf{r}) = \epsilon_\nu u_\nu(\mathbf{r}), \qquad (5.38)$$

$$-[\hat{H}_0 + V(\mathbf{r})]v_{\nu}(\mathbf{r}) + \Delta^*(\mathbf{r})u_{\nu}(\mathbf{r}) = \epsilon_{\nu}v_{\nu}(\mathbf{r}).$$
(5.39)

In this respect, the functions $u_{\nu}(\mathbf{r})$, $v_{\nu}(\mathbf{r})$ can be called eigenfunctions of elementary excitations. In the absence of external potential $V(\mathbf{r})$ we immediately see that Eqs. (5.38) and (5.39) coincide with equations (5.2) and (5.3).

If the current is also absent, then putting the quantum number ν of an excitation as its wavevector **k** we have

$$u_{\mathbf{k}} = \frac{u_k}{\sqrt{V}} \exp(i\mathbf{k}\mathbf{r}),\tag{5.40}$$

$$v_{\mathbf{k}} = \frac{v_k}{\sqrt{V}} \exp(i\mathbf{k}\mathbf{r}),\tag{5.41}$$

where u_k , v_k are given by Eqs. (4.34) and (4.35). Substituting $u_{\mathbf{k}}$, $v_{\mathbf{k}}$ given by Eqs. (5.40) and (5.41) into Eqs. (5.36) and (5.37) and recalling that $\hat{\psi}_{\sigma}(\mathbf{r}) = \sum_{\mathbf{k}} \hat{a}_{\sigma \mathbf{k}} \exp(i\mathbf{kr})$, we arrive at the momentum-space Bogoliubov transformations (4.29), (4.30) and (4.24), (4.25).

5.2 Express the ratio ρ_n/ρ through $\Delta^{-1}d\Delta/dT$ in the entire range of temperatures $T < T_c$. Consider only the contribution of single-particle excitations.

Lecture 6. Gizburg-Landau approach. Vortices in Fermi gases

6.1 Landau-Ginzburg functional

In this Lecture we discuss the Ginzburg-Landau description of (two-component) Fermi superfluids and then turn to vortex structures in these systems. In previous lectures we introduced and found the order parameter (gap) $\Delta = g\langle \hat{\psi}_{\downarrow}(\mathbf{r}) \hat{\psi}_{\uparrow}(\mathbf{r}) \rangle$. In Lecture 5 we then showed that the gradient of the phase of Δ ($\Delta = \overline{\Delta} \exp(2i\phi)$) is related to the superfluid current $\mathbf{j} = n\mathbf{v}_s$, with nbeing the total density and $\mathbf{v}_s = (\hbar/m)\nabla\phi$ the superfluid velocity. The quantity $\langle \hat{\psi}_{\downarrow}(\mathbf{r}) \hat{\psi}_{\uparrow}(\mathbf{r}) \rangle$ plays a role of the wavefunction of the "condensate of Cooper pairs". In many cases it is more convinient to introduce the order parameter Ψ in such a way that its phase coincides with the phase of Δ , but the amplitude is $|\Psi|^2 = n_s/2$, where n_s is the superfluid density. Then the superfluid current is

$$\mathbf{j}_s = \frac{\hbar}{2mi} (\Psi \nabla \Psi^* - \Psi^* \nabla \Psi) = \frac{\hbar}{m} n_s \nabla \phi = n_s \mathbf{v}_s.$$
(6.1)

At T = 0 where $n_s = n$, equation (6.1) exactly coincides with Eq. (5.11) which we derived in *Lecture 5*.

As we have shown, at $T = T_c$ the system undergoes the second order phase transition. The physical nature of this transition lies in an anomalous growth of the fluctuations of the order parameter. Let us consider the spatially uniform system and write the free energy per unit volume as an expansion in powers of Ψ :

$$F = F_n + \alpha (T - T_c) |\Psi|^2 + \frac{b}{2} |\Psi|^4, \qquad (6.2)$$

where F_n is the free energy in the normal (non-superfluid) phase. In the presence of currents we have to add the term with the gradient of the order parameter. So, we have

$$F = F_n + \frac{\hbar^2}{4m} |\nabla \Psi|^2 + \alpha (T - T_c) |\Psi|^2 + \frac{b}{2} |\Psi|^4.$$
(6.3)

Equation (6.3) is usually called the Ginzburg-Landau functional. The coefficient $\alpha > 0$, so that the superfluid phase is at $T < T_c$. At $T = T_c$ the term $\alpha(T-T_c) = 0$, and the difference between the free energies of superfluid and normal phases is $(F_s - F_n) \propto |\Psi|^4$. The equilibrium value of $|\Psi|^2$ at $T < T_c$ is determined by the minimization of F (6.2) and is equal to

$$|\bar{\Psi}|^2 = \frac{\alpha(T_c - T)}{b}.$$
(6.4)

In the uniform case this gives:

$$F_s - F_n = -\frac{\alpha^2}{2b}(T_c - T)^2$$
(6.5)

and leads to the temperature independent heat capacity per unit volume:

$$C_s - C_n = -T \left(\frac{\partial^2 (F_s - F_n)}{\partial T^2}\right)_V = \frac{\alpha^2 T_c}{b},$$
(6.6)

as it should be according to our derivation in Lecture 5.

For a weakly interacting two-component Fermi gas we have:

$$\alpha = \frac{6\pi^2 T_c}{7\zeta(3)\mu},\tag{6.7}$$

$$b = \frac{\alpha T_c}{n}.\tag{6.8}$$

This follows from the expression for the energy

$$E = \langle \hat{H} \rangle = \langle \sum_{\sigma \mathbf{k}} E_k \hat{a}^{\dagger}_{\sigma \mathbf{k}} \hat{a}_{\sigma \mathbf{k}} + \Delta \sum_{\mathbf{k}} (\hat{a}_{\downarrow \mathbf{k}} \hat{a}_{\uparrow - \mathbf{k}} + \hat{a}^{\dagger}_{\uparrow - \mathbf{k}} \hat{a}^{\dagger}_{\downarrow \mathbf{k}}) \rangle$$

using the Bogoliubov transformation (4.29), (4.30) and the expression for the entropy:

$$S = -\sum_{\sigma \mathbf{k}} [N_{\sigma \mathbf{k}} \ln N_{\sigma \mathbf{k}} + (1 - N_{\sigma \mathbf{k}}) \ln(1 - N_{\sigma \mathbf{k}})].$$
(6.9)

Then, the free energy F = E - TS will be given by Eq. (6.2) with α , b from Eqs. (6.7) and (6.8).

6.2 Critical fluctuations

Let us now consider fluctuations of the order parameter. Under a small deviation of $|\Psi|$ from the equilibrium value $|\bar{\Psi}|$ the change of F is

$$\delta F = \frac{1}{2} (|\Psi| - |\bar{\Psi}|)^2 \left(\frac{\partial^2 F}{\partial |\Psi|^2}\right). \tag{6.10}$$

For the quantity $\partial^2 F/\partial |\Psi|^2$ we have:

$$\frac{\partial^2 F}{\partial |\Psi|^2} = 2\alpha (T - T_c); \quad T > T_c, \quad |\bar{\Psi}| = 0.$$
(6.11)

$$\frac{\partial^2 F}{\partial |\Psi|^2} = 4\alpha (T_c - T); \quad T < T_c, \quad |\bar{\Psi}| = \frac{\alpha (T_c - T)}{b}. \tag{6.12}$$

The probability of the fluctuation is

$$w \sim \exp\left\{-\frac{V\delta F}{T}\right\} = \exp\left\{-\frac{V(|\Psi| - |\bar{\Psi}|)^2}{2T}\frac{\partial^2 F}{\partial|\bar{\Psi}|^2}\right\}.$$
(6.13)

We then obtain the mean square fluctuation of $|\Psi|$:

$$\langle (|\Psi| - |\bar{\Psi}|)^2 \rangle = \frac{T_c}{2\alpha |T - T_c|V} \times \begin{cases} 1; & T > T_c \\ 1/2; & T < T_c \end{cases}$$
(6.14)

From Eq. (6.3) we can establish the correlation radius r_c of the fluctuations. It follows from the condition that the gradient term is of the order of the $|\Psi|^2$ term:

$$r_c \sim \sqrt{\frac{\hbar^2}{m\alpha |T_c - T|}}.$$
(6.15)

In order to still apply the theory that we discussed in previous lectures, we should have small fluctuations over the volume r_c^3 , compared to $|\bar{\Psi}|^2 = \alpha (T_c - T)/b$:

$$\left\langle (|\Psi| - |\bar{\Psi}|)^2 \right\rangle \Big|_{V=r_c^3} \ll |\bar{\Psi}|^2.$$

This leads to the inequality:

$$\frac{T_c}{\alpha |T_c - T| r_c^3} \ll \frac{\alpha}{b} |T_c - T|.$$
(6.16)

Substituting r_c from Eq. (6.15) we obtain the famous Ginzburg criterion:

$$\alpha |T_c - T| \gg T_c^2 b^2 \left(\frac{m}{\hbar^2}\right)^3.$$
(6.17)

For the weakly interacting Fermi gas, with $\alpha \sim T_c/\mu$; $b \sim T_c^2/\mu n$ from Eqs. (6.7), (6.8) and $\mu = E_F \sim \hbar^2 n^{2/3}/m$, we find:

$$|T_c - T| \gg T_c \left(\frac{T_c}{E_F}\right)^4.$$
(6.18)

Thus, in a very narrow interval of temperatures near T_c the theory is not applicable. This interval is called the *region of critical fluctuations*. A theory for this region is beyond the scope of the present course.

6.3 Vortex state

We now turn to the discussion of vortices in the two-component superfluid Fermi gas. What is the vortex state? Assume that in free space the complex order parameter Δ (or Ψ) is of the form

$$\Delta(\mathbf{r}) = \Delta(\boldsymbol{\rho}) \exp(i\phi), \tag{6.19}$$

where ρ is the vector in the $\{x, y\}$ plane and ϕ is the asimuthal angle $(x = \rho \cos \phi, y = \rho \sin \phi)$. The velocity field **v** as derived in *Lecture 5*, then is

$$\mathbf{v} = \frac{\hbar}{2m} \nabla \phi. \tag{6.20}$$

An extra factor 2 in the denominator is related to the fact that now we write the phase ϕ instead of 2ϕ before. Now it is even more convinient, since the factor

2m shows that the mass of a Cooper pair is twice the mass of a particle. The velocity field has a tangential form ($\rho \mathbf{v} = 0$):

$$\mathbf{v} = -\frac{[\boldsymbol{\rho}\hat{\mathbf{z}}]}{\rho^2} \frac{\hbar}{2m},\tag{6.21}$$

where $\hat{\mathbf{z}}$ is a unit vector perpendicular to the $\{x, y\}$ plane. So, we have

$$|\mathbf{v}| = \frac{\hbar}{2m\rho} \tag{6.22}$$

and clearly see that the velocity increases on approach to the vortex line, i.e. to the line where $|\mathbf{v}| \rightarrow \infty$. The circulation is quantized:

$$\oint \mathbf{v} d\mathbf{l} = \frac{\pi \hbar}{m}.$$
(6.23)

The angular momentum carried by the vortex is

$$\langle \hat{L}_z \rangle = m \int [\mathbf{r} \times \mathbf{v}] n(\mathbf{r}) d^3 r = \frac{\hbar N}{2},$$
 (6.24)

with N being the total number of particles, and $n(\mathbf{r})$ the density distribution. The energy E_v acquired by the vortex is mainly determined by the hydrodynamic kinetic energy $(m/2) \int nv^2 d^3r$. In a non-rotating cylinder of radius R we have:

$$E_v = \frac{N\hbar}{4mR^2} \ln\left(\frac{R}{\xi}\right),\tag{6.25}$$

where ξ is the radius of the vortex core, which is of the order of the coherence length $\hbar v_F / \Delta$.

Let us now discuss the form of $\Delta(\mathbf{r})$ in the case of the vortex state. For this purpose we write the Bogoliubov-de Gennes equations where we still keep the Hartree-Fock terms:

$$\begin{bmatrix} \mathcal{H} - \mu & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -(\mathcal{H} - \mu) \end{bmatrix} \begin{bmatrix} u_{\sigma}(\mathbf{r}) \\ v_{\sigma}(\mathbf{r}) \end{bmatrix} = \epsilon_{\sigma} \begin{bmatrix} u_{\sigma}(\mathbf{r}) \\ v_{\sigma}(\mathbf{r}) \end{bmatrix}, \qquad (6.26)$$

where

$$\mathcal{H} = -\frac{\hbar^2}{2m} - gn(\boldsymbol{\rho}), \tag{6.27}$$

and $g = -4\pi\hbar^2 a/m > 0$ for a < 0.

For simplicity we consider T = 0 and assume that the system is a very large cylinder and is not rotating. The density profile is given by

$$n(\boldsymbol{\rho}) = \sum_{\sigma \mathbf{k}} |v_{\sigma \mathbf{k}}(\boldsymbol{\rho})|^2 = 2 \sum_{\mathbf{k}} |v_{\mathbf{k}}(\boldsymbol{\rho})|^2, \qquad (6.28)$$

and the gap equation reads:

$$\Delta(\boldsymbol{\rho}) = g \sum_{\sigma \mathbf{k}} u_{\sigma \mathbf{k}}(\boldsymbol{\rho}) v_{\sigma \mathbf{k}}^*(\boldsymbol{\rho}).$$
(6.29)

The lowest energy solution $(\epsilon > 0)$ corresponds to

$$u = u(\rho); \quad v = \tilde{v}(\rho) \exp(-i\phi). \tag{6.30}$$

Since the order parameter is exponentially small in the BCS regime, the density is practically not affected by the vortex. However, Δ vanishes at the vortex line. The solution of this problem is quite combersome and requires numerics. Therefore, we only present the dependence $|\Delta(\rho)|$ in Fig. 6.1.



Figure 6.1: Modulus of the order parameter $|\Delta|$ as a function of the distance from the vortex core, ρ .

In a non-rotating cylinder the vortex state is an excited state of the system. We now briefly discuss the case of a rotating cylinder. Let Ω be the rotation frequency. In the rotating reference frame the energy associated with the appearance of the vortex is

$$E = E_v - \Omega \langle L_z \rangle, \tag{6.31}$$

where E_v is given by Eq. (6.25), and $\langle L_z \rangle$ by Eq. (6.24). The critical frequency Ω_c at which the vortex state becomes the ground state of the system is obtained from the condition E = 0. We thus have:

$$\Omega_c = \frac{\hbar}{2mR^2} \ln\left(\frac{R}{\xi}\right). \tag{6.32}$$

6.4 Vortices near T_c

Let us now discuss vortices at temperatures close to T_c and employ the Ginzburg-Landau functional (6.3). In the spatially non-uniform system we have to write it in the form:

$$F = \int d^3r \left\{ \frac{\hbar^2}{4m} (\nabla \Psi^* \nabla \Psi) - \alpha (T_c - T) |\Psi|^2 + \frac{b}{2} |\Psi|^4 \right\}.$$
 (6.33)

The first term in curly brackets can also be written as $-(\hbar^2/4m)\Psi^*\nabla^2\Psi$, which is clearly seen after performing the integration by parts. Let us make a variation of F. Note that we should vary Ψ^* and Ψ separately. Consider variations $\delta\Psi^*$ we have:

$$\delta F = \int d^3r \,\delta \Psi^* \left\{ -\frac{\hbar^2}{4m} \nabla^2 \Psi - \alpha (T_c - T) \Psi + b |\psi|^2 \Psi \right\}.$$

So, setting $\delta F = 0$ we obtain an equation:

$$-\frac{\hbar^2}{4m}\nabla^2\Psi - \alpha(T_c - T)\Psi + b|\Psi|^2\Psi = 0.$$
 (6.34)

Equation (6.34) looks exactly the same as the Gross-Pitaevskii equation for the condensate wavefunction in the case of bosons (see *Lecture 3* of *Part 1* of the course). In order to make the analogy explicit we should treat $\alpha(T_c - T)$ as the "chemical potential", and b as the "coupling constant". Since $\alpha \sim T_c/E_F$, $b \sim T_c^2/nE_F$ (see Eqs. (6.7) and (6.8)), we obtain the "healing length":

$$\xi \sim \sqrt{\frac{\hbar^2}{m\mu}} \sim \sqrt{\frac{\hbar E_F}{mT_c(T_c - T)}} \sim \frac{\hbar v_F}{\sqrt{T_c(T_c - t)}} \sim \frac{\hbar v_F}{\Delta},$$

where we took into account that $\Delta(T) \sim \sqrt{T_c(T_c - T)}$ at $T \to T_c$.

For the vortex state of bosons, Ψ has been obtained in *Lecture* 7 of *Part 1*. It is presented in Fig. 6.2.

All other solutions at temperatures near T_c are obtained in the same way as in the case Bose-Einstein condensates in *Part 1* of the course.

Problems 6

6.1 Obtain the Ginzburg-Landau functional for the free energy F = E - TS from the microscopic theory for the weakly interacting two-component Fermi gas. Use the following expessions for the energy and entropy:

$$E = 2 \int \epsilon(k) N_{\mathbf{k}} \frac{V d^3 k}{(2\pi)^3},$$

$$S = -2 \int [N_{\mathbf{k}} \ln N_{\mathbf{k}} + (1 - N_{\mathbf{k}}) \ln(1 - N_{\mathbf{k}})] \frac{V d^3 k}{(2\pi)^3}$$



Figure 6.2: Modulus of the order parameter $|\Psi|$ (or $|\Delta|$) as a function of the distance from the vortex core, ρ , at temperatures $T \to T_C$.

Lecture 7. Strongly interacting regime in Fermi gases

7.1 Anomalously large scattering length

We now arrive at the discussion of the so-called strongly interacting regime in dilute Fermi gases. In previous lectures we were writing the interaction term in the Hamiltonian as

$$\hat{H}_{int} = g \int \hat{\psi}_{\uparrow}^{\dagger}(\mathbf{r}) \hat{\psi}_{\downarrow}^{\dagger}(\mathbf{r}) \hat{\psi}_{\downarrow}(\mathbf{r}) \hat{\psi}_{\uparrow}(\mathbf{r}) \, d^3r,$$

where $g = 4\pi\hbar^2 a/m$, with a being the scattering length for the interaction between \uparrow and \downarrow atoms. We were considering the weakly interacting regime, where $n|a|^3 \ll 1$ and the interaction energy per particle is much smaller than the Fermi energy, so that the interactions can be taken into account within the many-body perturbation theory. What happens if $|a| \to \infty$, but the gas is still dilute and $nR_e^3 \ll 1$, where R_e is the radius of the interaction potential U(r)?

First of all, why and how this can happen? Consider U(r) such that there is a very weakly bound state with zero orbital angular momentum (s-state) and binding energy $\epsilon_0 \to 0$ (see Fig. 7.1). At $r \gg R_e$ the wavefunction of the bound s-state is governed by the Schroedinger equation for the free motion:

$$-\frac{\hbar^2}{m}\left(\frac{d^2\psi_0}{dr^2} + \frac{2}{r}\frac{d\psi_0}{dr}\right) = -\epsilon_0\psi_0\tag{7.1}$$

and reads:

$$\psi_0 = C \frac{\exp(-\kappa r)}{r},\tag{7.2}$$

where $\kappa = \sqrt{m\epsilon_0}/\hbar$, and C is the normalization coefficient.



Figure 7.1: Interaction potential U(r) supporting a weakly bound state with zero orbital angular momentum.

On the other hand, the wavefunction of continuum states with zero orbital angular momentum and energy $\epsilon \to 0$ is

$$\psi = \left(1 - \frac{a}{r}\right),\tag{7.3}$$

where a is the scattering length. In the interval of distances where $\kappa^{-1} \gg r \gg R_e$, equation (7.2) becomes $\psi_0 \propto (1-1/\kappa r)$ and it should coincide with Eq. (7.3), except for the normalization coefficient. This is because at such distances in both cases the wavefunction is governed by the Schroedinger equation for free motion with zero energy: $\psi_{rr}'' + (2/r)\psi_r' = 0$. So, we thus obtain:

$$a = \frac{1}{\kappa} = \frac{\hbar^2}{\sqrt{m\epsilon_0}} > 0. \tag{7.4}$$

The scattering length is positive and large $(a \gg R_e)$.

Note that we obtained Eq. (7.4) in the presence of a very weakly bound state. The case of a large but negative scattering length corresponds to the presence of the so-called virtual bound state (just make the potential U(r) slightly deeper and the bound state appears). So, we see that one can have $n|a|^3$ large, but $nR_e^3 \ll 1$. For $\epsilon_0 \to 0$ we have $|a| \to \infty$.

7.2 Fano-Feshbach resonance

Is there a possibility to manipulate the interaction and modify the scattering length a, thus changing the coupling constant g and influencing the many-body physics? Imagine that there is a collision between two atoms in certain hyperfine states along the potential curve $U_1(r)$. The hyperfine interaction can change the internal state of one of the colliding atoms or even the internal states of both of them, thus transferring the system to the motion along the potential curve $U_2(r)$ (see Fig. 7.2). Assume now that there is a bound state in the potential $U_2(r)$, which almost coincides with the bottom of continuum states of $U_1(r)$ so that the corresponding energy difference E_0 is small.



Figure 7.2: The picture of interaction potentials and bound state(s) showing the presence of a Fano-Feshbach resonance.

We then consider the s-wave scattering and write the wavefunction of the

scattering state at large distances as

$$\psi(r) = \frac{1}{r} [A \exp(ikr) + B \exp(-ikr)], \qquad (7.5)$$

with $k = \sqrt{mE/\hbar^2}$. Treat now the scattering energy E as a complex quantity. This is because the energy of the bound state E_0 is in fact complex and equal to $E_0 - i\Gamma/2$. This state is actually quasibound as it can decay into free atoms, and the quantity Γ is the corresponding width. The condition determining complex eigenstates is that there is no incoming wave at large distances. This means that we should have zero coefficient B for $E = E_0 - i\Gamma/2$:

$$B(E_0 - i\Gamma/2) = 0. (7.6)$$

For the scattering energy E close to E_0 we may expand B in powers of $(E - E_0 + i\Gamma/2)$ and confine ourselves to the linear term of the expansion, which gives

$$B = \left(E - E_0 + i\frac{\Gamma}{2}\right)b,$$

where b is a constant. So, taking into account that $A = B^*$ the wavefunction (7.5) becomes

$$\psi(r) = \frac{1}{r} \left[\left(E - E_0 - i\frac{\Gamma}{2} \right) b^* \exp(ikr) + \left(E - E_0 + i\frac{\Gamma}{2} \right) b \exp(-ikr) \right].$$
(7.7)

The phase δ of this function is given by

$$\exp(2i\delta) = \frac{E - E_0 - i\Gamma/2}{E - E_0 + i\Gamma/2} \exp(2i\delta^{(0)}),$$
(7.8)

where $\exp(2i\delta^{(0)}) = -b^*/b$. For $|E - E_0| \gg E_0$ we have $\delta = \delta^{(0)}$. So, $\delta^{(0)}$ is the phase far from resonance. For simplicity we put $\delta^{(0)} = 0$, thus omitting the potential scattering. Then, using the well-known formula for the scattering amplitude (see *Lecture 1*):

$$f = \frac{\tan \delta}{k(1 - i \tan \delta)}$$

we obtain:

$$f = -\frac{\Gamma/2}{k(E - E_0 + i\Gamma/2)}.$$
(7.9)

For E and E_0 tending to zero the function B(E) can be expanded in powers of E. The point E = 0 is the branching point of B(E) so that going from the upper part of the complex half-plane to the lower part transforms B to B^* . Therefore, the expansion of B should be in powers of \sqrt{E} , and we have

$$B(E) = (E - E_0 + i\gamma\sqrt{E})b.$$
 (7.10)

Thus, we have a relation

$$\frac{\Gamma}{2} = \gamma \sqrt{E} = \gamma \frac{\hbar}{\sqrt{m}}k.$$

We then rewrite equation (7.9) in the form

$$f = -\frac{\hbar\gamma}{\sqrt{2m}(E - E_0 + i\gamma\sqrt{E})},$$

$$f = -\frac{1}{a^{-1} + R^*k^2 + ik},$$
 (7.11)

or

where $a^{-1} = -E_0\sqrt{2m}/\hbar\gamma$, and $R^* = \hbar/(\gamma\sqrt{2m})$. For $k \to 0$ we have f = -aand we see that the scattering length is $a \propto E_0^{-1}$. In our derivation we assumed that $E_0 > 0$ and obtained a < 0. For $E_0 < 0$ the derivation is similar and one obtains a > 0. The original description of the discussed resonance scattering belongs to Fano and to Feshbach and it is usually identified as Fano-Feshbach resonance.

The spacing between the potentials $U_1(r)$ and $U_2(r)$ is equal to the difference in the energies of the involved internal (hyperfine) states of the atoms and depends on the magnetic field. As a result, the scattering length becomes field dependent and tends to infinity when $E_0 \rightarrow 0$ (see Fig. 7.3).

7.3 BCS-BEC crossover

Let us now consider T = 0 and make a qualitative sketch of the phase diagram. Namely, we find out what kind of ground state we have depending on the value of the scattering length a (or magnetic field B). For a small negative a satisfying the condition $k_F|a| \ll 1$ there is a BCS superfluid that we discussed in the previous lectures. For $|a| \to \infty$ we have the so-called strongly interacting regime, which we can not treat on the basis of the many-body perturbation theory. For a large positive a still satisfying the inequality $na^3 \ll 1$, \uparrow and \downarrow fermions form a weakly bound state as we discussed in subsection 7.1. So, we have diatomic molecules representing composite bosons, and they should bosecondense. The wavefunction of each composite boson is given by equation (7.2) and the corresponding momentum distribution is

$$G(k) = \int \psi_0(\mathbf{r}_1 - \mathbf{r}_2) \exp[i\mathbf{k}(\mathbf{r}_1 - \mathbf{r}_2)] d(\mathbf{r}_1 - \mathbf{r}_2) \propto \frac{1}{a^{-2} + k^2}.$$
 (7.12)

Considering a Bose-Einstein condensate of the molecules at T = 0 we may say that the system consists of real-space pairs of \uparrow and \downarrow fermions, with momentum distribution (7.12). This is an argument on support of the statement that going from BCS (small negative *a*) to BEC of molecules (positive *a* and $na^3 \ll 1$) simply transforms Cooper pairs to real space diatomic molecules. The symmetry of the system does not change and we have a *crossover*, not a quantum transition. The phase diagram is displayed in Fig. 7.4



Figure 7.3: The magnetic field dependence of the scattering length for a Fano-Feshbach resonance. The field B_0 corresponds to $|a| \to \infty$.

7.4 Description of the strongly interacting regime. Unitarity limit

We now treat all regimes shown in Fig. 7.4 on equal footing by using a sort of BCS approach at T = 0. So, we again write the BCS Hamiltonian (4.23)

$$\hat{H}_{\rm BCS} = \sum_{\mathbf{k};\,\sigma=\uparrow,\downarrow} \xi_k \hat{a}^{\dagger}_{\sigma\mathbf{k}} \hat{a}_{\sigma\mathbf{k}} + \Delta \sum_{\mathbf{k}} (\hat{a}_{\downarrow\mathbf{k}} \hat{a}_{\uparrow-\mathbf{k}} + \hat{a}^{\dagger}_{\uparrow-\mathbf{k}} \hat{a}^{\dagger}_{\downarrow\mathbf{k}}),$$

where $\hat{a}_{\sigma \mathbf{k}}$ are the particle operators, and $\xi_{\mathbf{k}} = (\hbar^2 k^2 / 2m - \mu)$. We then employ the Bogoliubov transformation (4.24), (4.25):

$$\begin{split} \hat{b}_{\uparrow \mathbf{k}} &= u_k \hat{a}_{\uparrow \mathbf{k}} + v_k \hat{a}_{\downarrow - \mathbf{k}}^{\dagger}, \\ \hat{b}_{\downarrow \mathbf{k}} &= u_k \hat{a}_{\downarrow \mathbf{k}} - v_k \hat{a}_{\uparrow - \mathbf{k}}^{\dagger}, \end{split}$$

thus reducing \hat{H}_{BCS} to the diagonal form (4.31):

$$\hat{H}_{\rm BCS} = E_0 + \sum_{\sigma, \mathbf{k}} \epsilon_k \hat{b}^{\dagger}_{\sigma \mathbf{k}} \hat{b}_{\sigma \mathbf{k}}.$$

For the ground state energy we have:

$$E_0 = \sum_{\mathbf{k}} \left(2E_k v_k^2 - \frac{\Delta^2}{2\epsilon_k} \right), \qquad (7.13)$$



Figure 7.4: Phase diagram for a two-component atomic Fermi gas at T = 0.

where $E_k = \hbar^2 k^2 / 2m$, and the normalization condition reads:

$$n = \frac{2}{V} \sum_{\mathbf{k}} v_k^2 = \int \frac{d^3k}{(2\pi)^3} \left(1 - \frac{\xi_k}{\epsilon_k} \right).$$
(7.14)

However, in contrast to the standard BCS approach we now do not assume that only momenta close to k_F are important in the integral over d^3k in Eq. (7.14) and use the exact expression $\xi_k = \hbar^2 k^2/2m - \mu$.

The zero-temperature gap equation (4.40) we now write using the so-called renormalized coupling constant:

$$\frac{1}{|g|} = \int \frac{d^3k}{2(2\pi)^3} \left(\frac{1}{\epsilon_k} - \frac{1}{E_k}\right).$$
(7.15)

The renormalization of the coupling constant is needed in order to circumvent the divergence of the integral at large k in Eq. (7.14). In the standard BCS approach in *Lecture* 4 we did this "by hands", saying that there should be a natural high-energy cut-off which is of the order of the Fermi energy. The rigorous renormalization procedure is beyond the scope of the present course, and we only give supporting arguments. Imagine that we have two particles with very low momenta and treat g as the Fourier transform of the interaction potential. Then, to first order in perturbation theory the coupling constant is g, and the second order gives the contribution $-\sum_{\mathbf{k}} g^2/2E_k V$. So, we have to make a replacement $g \to g(1 - \sum_{\mathbf{k}} g/2E_k V)$, or

$$\frac{1}{g} \to \frac{1}{g} + \sum_{\mathbf{k}} \frac{1}{2E_k V}.$$

For a negative g this is exactly what we have done in Eq. (7.15).

The functions u_k , v_k are still determined by the Bogoliubov-de Gennes equations (4.32), (4.33) and are given by Eqs. (4.34), (4.35):

$$u_k^2 = \frac{1}{2} \left(1 + \frac{\xi_k}{\epsilon_k} \right),$$
$$v_k^2 = \frac{1}{2} \left(1 - \frac{\xi_k}{\epsilon_k} \right)$$

The excitation energy ϵ_k follows from equation (4.36):

$$\epsilon_k = \sqrt{\xi_k^2 + \Delta^2}.$$

Then, using Eqs. (7.14) and (7.15), for small a < 0 we recover the earlier obtained result for the gap in the BCS limit. We even find a numerical coefficient in front of the exponent. However, this coefficient has to be corrected by including second order many-body processes.

In the limit of molecular BEC $(a > 0 \text{ and } na^3 \ll 1)$ equations (7.14), (7.15) and (7.13) give the ground state energy

$$E_0 = -\frac{\hbar^2}{2ma^2}N + \frac{\pi\hbar^2 a}{2m}\frac{N^2}{V},$$
(7.16)

where N is the number of fermionic atoms. Accordingly, the number of molecules is $N_m = N/2$, and the first term in Eq. (7.16) is nothing else than the binding energy of a molecule, $\epsilon_0 = \hbar^2/ma^2$, multiplied by the number of molecules. The second term corresponds to the interaction between the molecules. Taking into account that the molecular mass is 2m, we see that the molecule-molecule scattering length $a_m = 2a$. This because the molecule-molecule interaction energy should be equal to $(4\pi\hbar^2 a_m/2m)N_m^2/2V$. Note that the exact result following from the solution of the 4-body problem gives $a_m = 0.6a$.

The chemical potential following from Eq. (7.16) is

$$\mu = -\frac{\epsilon_0}{2} + \frac{\pi\hbar^2}{m}an. \tag{7.17}$$

The order parameter Δ then turns out to be much smaller than $|\mu|$, but the gap in the excitation spectrum is provided by the binding energy of a molecule and is equal to $\epsilon_0/2$.

In the unitarity limit, that is at $|a| \to \infty$, one finds $\Delta = 0.69E_F$, $E_0 = 0.6(3E_F/5)N$, and $\mu = 0.6E_F$. The latter result is 40% larger than the result of the exact Monte Carlo calculation.

We thus see that even using the BCS theory one can qualitatively recover the physics. The discussed approach for describing the BCS-BEC crossover has been proposed by Leggett. Note that the unitarity limit is universal. There is only one energy scale, the Fermi energy E_F , and only one distance scale, the mean interparticle separation $n^{-1/3}$.

Monte Carlo studies have obtained the superfluid transition temperature T_c as a function of the scattering length a, which for a given system is easily transformed into the dependence of T_c on the magnetic field. This dependence is sketched in Fig. 7.5. In the unitarity limit we have $T_c \approx 0.15 E_F$. Experimental studies have achieved the strongly interacting regime, and Monte Carlo calculations of T_c and μ are consistent with the experiments. The presence of superfluidity in the strongly interacting regime has been proven in MIT experiments (W. Ketterle) by creating a lattice of quantum vortices.



Figure 7.5: Superfluid transition temperature as a function of the magnetic field for the BCS-BEC crossover in a two-component atomic Fermi gas.

Problems 7

7.1 Calculate the spectrum of collective excitations for a 2-component Fermi gas in the unitarity limit and in the regime of molecular BEC.

We rely on the hydrodynamic equations (5.12), (5.13):

$$\frac{\partial n}{\partial t} + \operatorname{div}(n\mathbf{v}) = 0,$$

$$m\frac{\partial \mathbf{v}}{\partial t} + \nabla \left[\frac{1}{2}mv^2 + \mu(n)\right] = 0.$$

and assume small fluctuations of the density, $\delta n = n - \bar{n}$, where \bar{n} is the mean density. Then, writing the velocity as $\mathbf{v} = (\hbar/m)\nabla\phi$, with ϕ being the phase of the order parameter, we arrive at the linearized equations (5.14), (5.15):

$$\begin{split} & \frac{\partial \delta n}{\partial t} + \nabla \left(\frac{\hbar \bar{n}}{m} \nabla \phi \right) = 0, \\ & \hbar \frac{\partial \nabla \phi}{\partial t} + \frac{\partial \mu}{\partial n} \Big|_{n = \bar{n}} \nabla \delta n = 0. \end{split}$$

Reducing them to Eq. (5.16):

$$\frac{\partial^2 \delta n}{\partial t^2} = \frac{\bar{n}}{m} \frac{\partial \mu}{\partial n} \Big|_{n=\bar{n}} \nabla^2 \delta n,$$

we then write small fluctuations of the density as $\delta n \propto \exp(-i\omega t + i\mathbf{kr})$. This gives

$$\omega^2 = \left(\frac{\bar{n}}{m} \left. \frac{\partial \mu}{\partial n} \right|_{n=\bar{n}} \right) k^2. \tag{7.18}$$

In the unitarity limit we have $\mu = 0.4E_F$ and

$$\frac{\partial \mu}{\partial n}\Big|_{n=\bar{n}} = 0.4 \times \frac{2E_F}{3\bar{n}} = 0.267 \frac{E_F}{\bar{n}},$$

which yields

$$\omega = \left(\frac{0.4}{\sqrt{3}}\right) v_F k = 0.231 v_F k. \tag{7.19}$$

In the regime of molecular BEC we have

$$\mu = -\frac{\epsilon_0}{2} + \frac{\pi\hbar^2}{2m}n \times 0.6a$$

and

$$\left. \frac{\partial \mu}{\partial n} \right|_{n=\bar{n}} = 0.3 \frac{\pi \hbar^2 a}{m}.$$

Then equation (7.18) yields

$$\omega = \left(0.3 \frac{\pi \hbar^2 \bar{n}a}{m^2}\right)^{1/2} k \simeq 3 v_F (\bar{n}a^3)^{1/3} k.$$
(7.20)

7.2 Calculate the lowest frequencies of collective excitations of a 2-component Fermi gas in the unitarity regime in a harmonic potential $V(r) = m\omega_0^2 r^2/2$.