Strongly correlated systems
in atomic and condensed matter physics

Lecture notes

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Chapter 3

Bose-Einstein condensation of weakly interacting atomic gases

3.1 Bogoliubov theory

Microscopic Hamiltonian for the uniform system of bosons with contact interaction is given by

$$\mathcal{H} = \sum_p \epsilon_p b_p^\dagger b_p + \frac{U_0}{2V} \sum_{pp'q} b_{p+q}^\dagger b_{p'-q}^\dagger b_{p'} b_p - \mu \sum_p b_p^\dagger b_p \tag{3.1}$$

Here b_p are boson annihilation operators at momentum p, $\epsilon_p = p^2/2m$ is kinetic energy, V-volume of the system. The strength of contact interaction U_0 is related to the s-wave scattering length

$$U_0 = \frac{4\pi\hbar^2 a_s}{m} \tag{3.2}$$

To relate the value of a_s to microscopic interactions requires solving for the scattering amplitude in the low energy limit. We will discuss this procedure in the sections dealing with Feshbach resonances. Note that we work in the grand canonical ensemble, i.e. we fix the chemical potential μ and calculate the number of particles N_0 that corresponds to it.

For non-interacting atoms at $T = 0$ all atoms are condensed in the state of lowest kinetic energy at $k = 0$

$$|\Psi_N\rangle = \frac{1}{\sqrt{N!}} (b_{p=0}^\dagger)^N |\text{vac}\rangle \tag{3.3}$$

where $|\text{vac}\rangle$ is the vacuum state. It is natural to take this state as zeroth order approximation for finite but small interactions. Expectation value of the

Hamiltonian (3.1 in this state is

$$E = -\mu N_0 + \frac{U_0}{2V} N_0^2 \tag{3.4}$$

Minimizing with respect to N_0 we find relation between the number of particles and the chemical potential

$$\frac{N_0}{V} = \frac{\mu}{U_0} \tag{3.5}$$

To proceed to the next order in the interaction it is convenient to introduce the idea of broken symmetry.

When we consider two point correlation functions for the state (3.3)

$$\langle \Psi_N | \Psi^\dagger(r_2) \Psi(r_1) | \Psi_N \rangle = \frac{N_0}{V} \tag{3.6}$$

$$\Psi(r) = \frac{1}{\sqrt{V}} \sum_p b_p e^{ipr} \tag{3.7}$$

they do not depend on the relative distance between the two points. This is the definition of the long range order. Naively one expects property (3.6) to hold when individual expectation values of $\Psi(r)$ and $\Psi^\dagger(r)$ are equal to $(N_0/V)^{1/2}$. However individual expectation values of these operators vanish since they change the number of particles by one and state $|\Psi_N\rangle$ has a well defined number of particles. Let us then consider a state

$$|\Psi_0\rangle \quad = \quad e^{-\frac{\alpha^2}{2}} e^{\alpha b^\dagger_{p=0}} |\text{vac}\rangle \tag{3.8}$$

If we choose $\alpha = N_0^{1/2}$ we find that

$$\langle \Psi_0 | \Psi(r) | \Psi_0 \rangle = \langle \Psi_0 | \Psi^\dagger(r) | \Psi_0 \rangle = (\frac{N_0}{V})^{1/2} \tag{3.9}$$

State (3.8) captures property (3.6) but does it in a more natural way. It has individual expectation values of $\Psi(r)$ and $\Psi^\dagger(r)$. One may be concerned by the fact that this state does not have a well defined number of particles, although Hamiltonian (3.1) commutes with the total number of particles $N = \sum_p b_p^\dagger b_p$. And according to the fundamental theorem in quantum mechanics, if some operator commutes with the Hamiltonian, then it can be made diagonal in the basis of energy eigenstates. This "violation" of the basic theorem of quantum mechanics is the essence of the idea of spontaneous symmetry breaking. In state (3.8) we have a non-vanishing expectation value of the order parameter $\langle \Psi_N | \Psi(r) | \Psi_N \rangle$ and this automatically means that state $|\Psi_N\rangle$ is not an eigenstate of the conserved operator N. Some justification for using wavefunction (3.8) instead of (3.3) is that it has the correct number of particles *on the average*

$$\langle \Psi_0 | N | \Psi_0 \rangle = N_0 \tag{3.10}$$

and relative fluctuations in the number of particles are negligible in the thermodynamic limit.

$$\Delta N = \left(\langle \Psi_N | (N - N_0)^2 | \Psi_N \rangle\right)^{1/2} = N_0^{1/2} \tag{3.11}$$

The benefit of using the state (3.8) is that it dramatically simplifies calculations.

To continue perturbation theory in U we apply the traditional methodology of mean-field approaches. We replace $b^{\pm}_{p=0}$ operators by their expectation values in the ground state. The importance of different terms is determined by the number of $b^{\pm}_{p=0}$ factors, since each of them carries a large factor $N_0^{1/2}$. The most important terms, where all operators are at $p = 0$, are given by equation (3.4). The next contribution comes from terms that have two operators at non-zero momentum, which gives us the mean field Hamiltonian

$$\mathcal{H}_{\mathrm{MF}} = -\frac{N_0^2 U_0}{2V} + \sum_{p\neq 0} (\epsilon_p + 2n_0U_0 - \mu)(b_p^\dagger b_p + b_{-p}^\dagger b_{-p}) + n_0U_0 \sum_{p\neq 0} (b_p^\dagger b_{-p}^\dagger + b_p b_{-p}) \tag{3.12}$$

In summations $\sum_{p\neq 0}$ momentum pairs p, -p should be counted only once, $n_0 = N_0/V$.

We can diagonalize (3.12) using Bogoliubov transformation

$$\begin{aligned} b_p &= u_p \alpha_p + v_p \alpha_{-p}^\dagger \\ b_{-p} &= u_p \alpha_{-p} + v_p \alpha_p^\dagger \end{aligned} \tag{3.13}$$

Bosonic commutation relations are preserved when

$$u_p^2 - v_p^2 = 1 \tag{3.14}$$

The mean-field Hamiltonian becomes after substituting (3.13) and $\mu = n_0 U_0$

$$\begin{aligned} \mathcal{H}_{\mathrm{MF}} = -\frac{N_0^2 U_0}{2V} &+ \sum_{p\neq 0} (\alpha_p^\dagger \alpha_p + \alpha_{-p}^\dagger \alpha_{-p}) \left[(\epsilon_p + n_0U_0)(u_p^2 + v_p^2) + n_0U_0(2u_pv_p) \right] \\ &+ \sum_{p\neq 0} (\alpha_p^\dagger \alpha_{-p}^\dagger + \alpha_p \alpha_{-p}) \left[(\epsilon_p + n_0U_0)(2u_pv_p) + n_0U_0(u_p^2 + v_p^2) \right] \end{aligned} \tag{3.15}$$

Cancellation of the non-diagonal terms requires

$$(\epsilon_p + n_0U_0)(2u_pv_p) + n_0U_0(u_p^2 + v_p^2) = 0 \tag{3.16}$$

To satisfy equation (3.14) one can take

$$\begin{aligned} u_p &= \cosh \theta_p \\ v_p &= \sinh \theta_p \end{aligned} \tag{3.17}$$

Solution of these equations is

$$u_p = (\frac{\epsilon_p + n_0 U_0 + E_p}{2E_p})^{1/2} \tag{3.18}$$

$$v_p = -(\frac{\epsilon_p + n_0 U_0 - E_p}{2E_p})^{1/2} \tag{3.19}$$

which gives

$$\begin{aligned} \cosh 2\theta_p &= \frac{\epsilon_p + n_0 U_0}{E_p} \\ \sinh 2\theta_p &= -\frac{n_0 U_0}{E_p} \end{aligned}$$

$$E_p = \sqrt{(\epsilon_p + n_0 U_0)^2 - (n_0 U_0)^2} \tag{3.20}$$

The diagonal form of the mean-field Hamiltonian

$$\mathcal{H}_{\mathrm{MF}} = -\frac{N_0^2 U_0}{2V} \quad + \quad \sum_{p\neq 0} E_p(\alpha_p^\dagger \alpha_p + \alpha_{-p}^\dagger \alpha_{-p}) \tag{3.21}$$

Dispersion of collective modes is given by

$$E_p = \sqrt{\epsilon_p(\epsilon_p + 2n_0 U_0)} \tag{3.22}$$

We can define the healing length from

$$\frac{1}{m\xi_h^2} = n_0 U_0 \tag{3.23}$$

In the long wavelength limit, $q\xi_h << 1$, we find sound-like dispersion $E_q = v_s|q|$. Sound velocity

$$v_s = \left(\frac{n_0 U_0}{m}\right)^{1/2} \tag{3.24}$$

We can interpret the appearance of the gapless mode as manifestation of spontaneously broken symmetry: this mode arises because the superfluid state spontaneously breaks the $U(1)$ symmetry corresponding to the conservation in the number of of particles. However sound mode by itself does not imply supefluidity. As we know, sound modes exist in room temperature gases.

In the short wavelength limit, $q\xi_h >> 1$, we find free particle dispersion $E_q = q^2/2m$.

It is natural to ask about the change in the wavefunction (3.8) implied by the Bogoliubov analysis. From the form of the mean-field Hamiltonian (3.12) we expect that it should have coherent superpositions of p, $-p$ pairs. So we expect the wavefunction to be of the form

$$|\Psi_{\mathrm{Bog}}\rangle = \mathrm{C}\, e^{\alpha b_{p=0}^\dagger + \sum_p f_p b_p^\dagger b_{-p}^\dagger} |\mathrm{vac}\rangle \tag{3.25}$$

where C is normalization constant. To find coefficients f_p one simply notes that state (3.25) should be a vaccum of Bogoliubov quasiparticles. Hence it should satisfy equations

$$\alpha_p|\Psi_{\rm Bog}\rangle = (u_p b_p + v_p b^\dagger_{-p})|\Psi_{\rm Bog}\rangle = 0 \tag{3.26}$$

for all momenta p. The last condition requires $f_p = -v_p/u_p$.

3.1.1 Experimental tests of the Bogoliubov theory

Information about collective modes of many body systems is contained in the response functions. Imaginary part of the density-density response function is called the dynamic structure factor

$$S(q,\omega) = \sum_n |\langle n|\rho^\dagger_q|0\rangle|^2 \delta(\omega - (E_n - E_0)) \tag{3.27}$$

Here $|0\rangle$ denotes the ground state, summation over n goes over all excited states $|n\rangle$, density operator at wavevctor q is given by

$$\rho^\dagger_q = \frac{1}{\sqrt{V}} \sum_k b^\dagger_{k+q} b_k \tag{3.28}$$

Note that the difference in momenta of states $|0\rangle$ and $|n\rangle$ must be q for the matrix element in (3.27) to be non-zero.

Two photon off-resonant light scattering shown in figure 3.1 can be used to measure the dynamic structure factor of the BEC [4]. By absorbing a photon from one laser beam an atom goes into an excited state (but only virtually since there is strong frequency detuning) and then gets de-excited by a photon from the other beam. By treating optical fields as classical, one can obtain effective Hamiltonian describing interaction of atoms with the laser fields

$$V_{\rm eff} = \frac{V_0}{2}(\rho^\dagger_q e^{-i\omega t} + \rho^\dagger_{-q} e^{i\omega t}) \tag{3.29}$$

Fermi's golden then gives the rate with which excitations are created in the system (this is linear response theory and applies only for exciting a relatively small number of atoms)

$$W = V_0^2 S(q,\omega) \tag{3.30}$$

What is being measured in experiments is the number of atoms excited into a state with finite momentum as a function of wavevector and frequency differences of the two laser beams (see figs 3.1 and 3.2).

To apply formulas (3.27), (3.29) to the BEC we write $\rho^\dagger_q$ in equation (3.28) using creation and annihilation operators of the Bogoliubov quasiparticles. The leading term in $N_0^{1/2}$

$$\rho^\dagger_q = \frac{1}{\sqrt{V}}(b_0 b^\dagger_q + b^\dagger_0 b_{-q}) = \left(\frac{N_0}{V}\right)^{1/2} (u_q + v_q)(\alpha^\dagger_q + \alpha_{-q}) \tag{3.31}$$

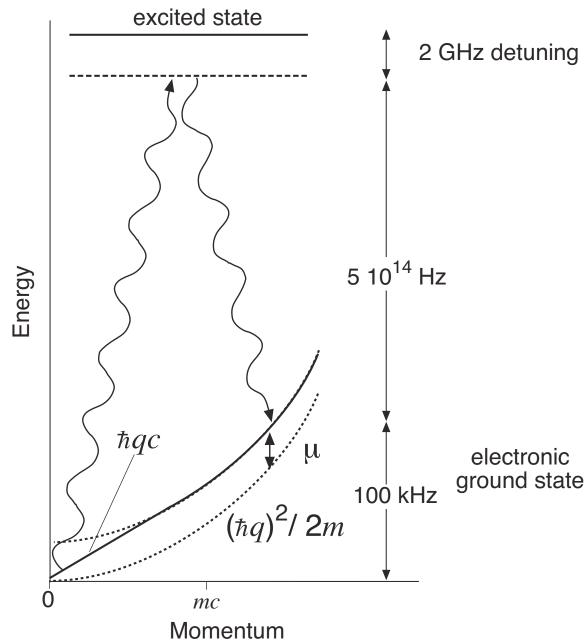

Figure 3.1: Experimental scheme for probing collective modes in a BEC using off-resonant light scattering. Figure taken from Ref. [4]. Excitations are created by stimulated light scattering using two laser which are both detuned from the atomic resonance. Absorption of one photon and emission of the other provides energy and momentum to create an excitation.

Ground state $|0\rangle$ is a vacuum of Bogoliubov quasiparticles. Hence state $|n\rangle$ in (3.27) should have one Bogoliubov quasiparticle and we obtain

$$S(q,\omega) = n_0\,(u_q + v_q)^2 \delta(\omega - E_q) = n_0\,\frac{\epsilon_q}{E_q}\,\delta(\omega - E_q) \tag{3.32}$$

For small q we find $\epsilon_q/E_q \propto |q|$. Results of experimental measurements of both the dispersion of Bogoliubov quasiparticles and the amplitude of the structure factor are shown in fig. 3.3.

3.2 Gross-Pitaevskii equation

In the Bogoliubov analysis we assumed macroscopic condensation of atoms into a single state and then found the state by minimizing the energy. We can also have macroscopic condensation of particles into a single state that is not stationary but undergoes dynamic evolution. This form of dynamics is exact for non-interacting particles, when all particles undergo identical evolution determined by the external fields (assuming that all atoms started in the same state). It is also a good approximation for weakly interacting particles. The role of interactions is to provide an effective field acting on the atoms. This effective field needs to be computed self-consistently according to the instantaneous value of the density. Equation describing such self-consistent dynamics is called the Gross-Pitaevskii (GP) equation.

We rewrite Hamiltonian (3.1) in real space rather than momentum space representations. We also add external potential $V_{\text{ext}}(r,t)$ for generality

$$\begin{aligned}\mathcal{H} = \frac{1}{2m}\int d^3r\,|\nabla\Psi|^2 \quad &+ \quad \int d^3r\, V_{\text{ext}}(r,t)\Psi^\dagger(r)\Psi(r) + \frac{U_0}{2}\int d^3r\,\Psi^\dagger(r)\Psi^\dagger(r)\Psi(r)\Psi(r) \\ &- \quad \mu\int d^3r\,\Psi^\dagger(r)\Psi(r)\end{aligned} \tag{3.33}$$

We use canonical commutation relations of Ψ operators

$$[\Psi(r),\Psi(r')] = 0 \qquad\qquad \left[\Psi(r),\Psi^\dagger(r')\right] = \delta(r-r') \tag{3.34}$$

and write Heisenberg equations of motion

$$\begin{aligned} i\frac{\partial\hat\Psi(r)}{\partial t} &= -\left[\mathcal{H},\,\hat\Psi(r)\right] \\ &= -\frac{1}{2m}\nabla^2\hat\Psi(r) + V_{\text{ext}}(r,t)\hat\Psi(r) + U_0\hat\Psi^\dagger(r)\hat\Psi(r)\hat\Psi(r) - \mu\hat\Psi(r)\end{aligned} \tag{3.35}$$

We put $\hat\Psi$ to emphasize that at this point this is an *exact* operator equation of motion. However we want to describe states that have finite expectation values of $\langle\Psi(r,t)\rangle$. Thus we can turn this operator equation into classical differential equations

$$i\frac{\partial\Psi_{\text{cl}}(r)}{\partial t} = -\frac{1}{2m}\nabla^2\Psi_{\text{cl}}(r) + V_{\text{ext}}(r,t)\Psi_{\text{cl}}(r) + U_0\Psi^\dagger_{\text{cl}}(r)\Psi_{\text{cl}}(r)\Psi_{\text{cl}}(r) - \mu\Psi_{\text{cl}}(r) \tag{3.36}$$

Here Ψ_{cl} emphasizes that this is now differential equation on a *classical field*. Another way of thinking about the GP equation is to consider generalization of state (3.8) to time and space dependent wavefunction

$$|\Psi(t)\rangle = \frac{1}{\sqrt{N!}}\left(\int d^3r\Psi_{\text{cl}}(r,t)\hat\Psi^\dagger(r)\right)^N|\text{vac}\rangle \tag{3.37}$$

where wavefunction $\Psi_{\text{cl}}(r,t)$ is assumed to be normalized. We can think of state (3.37) as a time dependent variational wavefunction, and project dynamics under Hamiltonian (3.33) into this state . This procedure gives equation (3.36) (see problems for this section).

In the simplest case of $V_{\text{ext}} = 0$ we observe that equation (3.36) has a static solution $\Psi_{\text{cl}} = \sqrt{n_0}\,e^{i\phi}$, provided that equation (3.5) is satisfied. Phase ϕ can be arbitrary.

Equation (3.35) can be used to obtain an alternative derivation of the spectrum of Bogoliubov quasiparticles. For a system without an external potential we take $\Psi_0 = \sqrt{n_0}$ and then consider small fluctuations around this state $\Psi(r,t) = \Psi_0 + \delta\Psi(r,t)$. Linearized equations of motion are

$$\begin{aligned} i\,\delta\dot{\Psi} &= -\frac{1}{2m}\,\nabla^2\delta\Psi + U_0 n_0(\delta\Psi + \delta\Psi^*) \\ -i\,\delta\dot{\Psi}^* &= -\frac{1}{2m}\,\nabla^2\delta\Psi^* + U_0 n_0(\delta\Psi + \delta\Psi^*) \end{aligned} \tag{3.38}$$

Keeping in mind representation of the instantaneous wavefunction $\Psi(r,t) = \sqrt{n_0 + \delta n(r,t)}\, e^{i\delta\phi(r,t)}$, it is convenient to introduce

$$\begin{aligned} \delta\rho &= \sqrt{n_0}\,(\delta\Psi + \delta\Psi^*) \\ \delta\phi &= \frac{1}{2i\sqrt{n_0}}\,(\delta\Psi - \delta\Psi^*) \end{aligned} \tag{3.39}$$

Then the last two equations can be written as

$$\delta\dot{n} = -\vec{\nabla}(\,\frac{n_0}{m}\,\vec{\nabla}\delta\phi\,) \tag{3.40}$$

$$-\delta\dot{\phi} = U_0\delta n - \frac{1}{4mn_0}\,\nabla^2\delta n \tag{3.41}$$

The first equation can be understood as mass conservation. If we define the superfluid current as $\vec{j}_s = (n_0/m)\,\vec{\nabla}\delta\phi$, we can rewrite equation (3.40) as $\delta\dot{n} = -\vec{\nabla}\vec{j}_s$. Equation (3.41) is the so-called Josephson relation $\delta\dot{\phi} = \delta\mu$. Combining the two equations we obtain

$$\delta\ddot{\phi} = (U_0 n_0 - \frac{\nabla^2}{4m})\,\frac{\nabla^2}{m}\,\delta\phi \tag{3.42}$$

Taking $\delta\phi \sim \phi_p e^{ipx - iE_p t}$ we find the collective mode dispersion given by equation (3.20).

3.3 Problems for Chapter 3

Problem 1

Let $|\Psi_0\rangle$ be the Bogoliubov ground state of a BEC. Consider a state obtained from $|\Psi_0\rangle$ by creating l excitations with momentum $+q$

$$\frac{\alpha_{+q}^{\dagger l}}{\sqrt{l!}}\,|\Psi_0\rangle$$

Verify by explicit calculation that this state contains $lu_q^2 + v_q^2$ original (free) particles with momentum $+q$ and $(l+1)v_q^2$ original (free) particles with physical momentum $-q$. This effect was demonstrated experimentally in [2].

Problem 2
Show that wavefunction (3.25) solves equation (3.26) for $f_p = -v_p/u_p$.

Problem 3
Consider a sudden change of the scattering length in Bose gas from a_{s1} to a_{s2}. Both interactions are small. Within Bogoliubov theory, describe dynamics of the system.

Problem 4* (difficult problem). Alternative derivation of the Gross-Pitaevskii equation.

To project the Schroedinger equation into wavefunction (3.37) one defines the Lagrangian

$$L = -i\langle\Psi(t)|\frac{d}{dt}|\Psi(t)\rangle + \langle\Psi(t)|\mathcal{H}|\Psi(t)\rangle \tag{3.43}$$

Derive this Lagrangian and show that varying it with respect to Ψ^*_{cl} gives the GP equation (3.36).

Hint. It may be conceptually easier to discretize space when thinking about this problem.

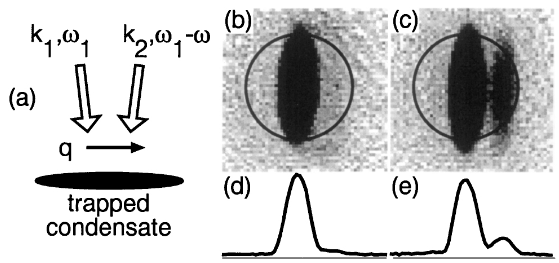

Figure 3.2: Experimental observation of momentum transfer to BEC by Bragg sattering. Atoms were exposed to laser beams as shown in fig 3.1. Time of flight technique converts momentum occupations into real space images. Figure taken from Ref. [1].

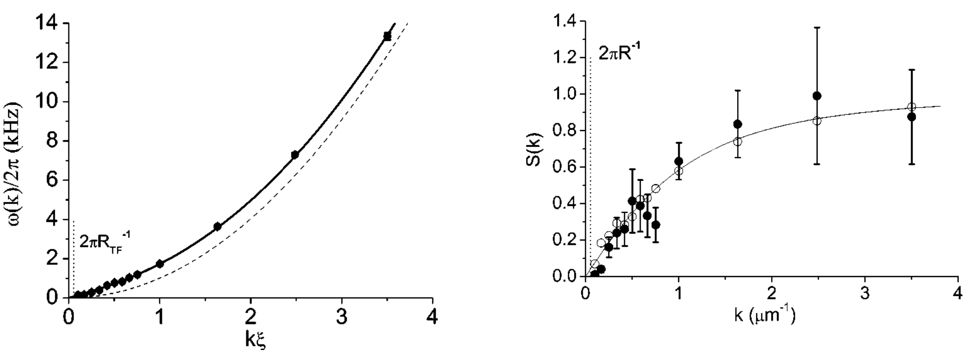

Figure 3.3: Experimental measurements of the dispersion of Bogoliubov quasiparticles and the dynamical structure factor in the BEC. Figure taken from [3].

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