1 Lectures 4, 5. Bose condensation. Symmetry-breaking and quasiparticles.

In an ideal Bose gas, at sufficiently low temperature, the lowest energy state becomes occupied by a macroscopic number of particles (Bose-Einstein condensate). The density of a gas of free bosons, given by a sum of occupancies of different momentum states, has the form

$$n = \int \left(n_0 \delta(\mathbf{p}) + (2\pi\hbar)^{-3} n_{\mathbf{p}}^{(reg)} \right) d^3p \,, \quad n_{\mathbf{p}}^{(reg)} = \frac{1}{e^{\beta(p^2/2m-\mu)} - 1} \tag{1}$$

with m the particle mass and μ the chemical potential.

At high temperature $T > T_{BEC}$, with

$$T_{BEC} = \alpha \frac{\hbar^2}{m} n^{2/3} \,, \quad \alpha = \frac{2\pi}{\zeta^{2/3}(3/2)} = 3.3142... \tag{2}$$

at density n, there is no condensate: $n_0 = 0$, $\mu < 0$. On the other hand, at low temperature $T < T_{BEC}$, there is a macroscopic number of particles in the ground state, while the chemical potential is zero. In this case, the condensate density is

$$n_0 = n - n_c = n \left(1 - (T/T_{BEC})^{3/2} \right) \tag{3}$$

The question we shall discuss below is how this behavior is modified by the presence of interatomic interaction.

We shall focus on the problem of weakly nonideal Bose gas. This problem, due to the existence of a simple analytical method, serves well to illustrate the new features of Bose condensation of interacting particles: spontaneous symmetry breaking, the off-diagonal long-range order, and collective excitations.

1.1 Spontaneous symmetry breaking

Weakly interacting Bose gas with a short-range interaction,

$$\mathcal{H} = \int \left(-\hat{\varphi}^+(x) \frac{\hbar^2}{2m} \nabla_x^2 \hat{\varphi}(x) + \frac{\lambda}{2} \hat{\varphi}^+(x) \hat{\varphi}^+(x) \hat{\varphi}(x) \hat{\varphi}(x) \right) dx \tag{4}$$

where $x = \mathbf{r}$ in $D = 3$.

The coupling constant is the two-particle scattering amplitude in the Born approximation, $\lambda = \tilde{U}_{k=0} = \int U(x - x')dx$. A more accurate formula: $\lambda = 4\pi\hbar^2 a/m$, where a is the s-wave scattering length, to be discussed below.

The ground state at $T = 0$ is characterized by large occupation number of the $\mathbf{k} = 0$ state. In number representation, the BEC state of N particles is $|BEC\rangle = |N_{\mathbf{k}=0}, 0, 0, ...\rangle$, i.e.

$$a_{\mathbf{k}=0}|BEC_N\rangle = \begin{cases} \sqrt{N}|BEC_{N-1}\rangle, & \mathbf{k} = 0 \\ 0, & \mathbf{k} \neq 0 \end{cases} \tag{5}$$

This formula, at large N, suggests to replace the number state by a coherent state, $a_0|BEC\rangle = \sqrt{N}|BEC\rangle$, which is equivalent to replacing the operator $\hat{a}_0$ by a c-number $\sqrt{N}$.

This can be achieved if the BEC state is understood as a coherent state, which requires considering the problem (4) in the 'big' space with all particle numbers allowed. Such an approach gives results equivalent to that of the problem with fixed particle number N in the limit $N \to \infty$, since for a coherent state $\langle \delta N^2 \rangle^{1/2} = N^{1/2} \ll N$. Upon such a replacement, the field operator $\hat{\varphi} = V^{-1/2} \sum_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{kr}}$ turns into a classical field $\varphi = \sqrt{N/V}$, where V is system volume.

To that end, we are led to consider the coherent states

$$|\varphi\rangle = \exp\left(\sqrt{V}\left(\varphi \hat{a}_0^+ - \bar{\varphi}\hat{a}_0\right)\right)|0\rangle = e^{-\frac{1}{2}V|\varphi|^2} \sum_{m=0}^{\infty} \frac{\left(\sqrt{V}\varphi\right)^m}{\sqrt{m!}} |m\rangle \tag{6}$$

which have the desired property $\hat{\varphi}|\varphi\rangle = \varphi|\varphi\rangle$. These states do not correspond to any specific number of particles, in fact they are characterized by a distribution of particle numbers. Accordingly, the states $|\varphi\rangle$ are not invariant under the number operator $\hat{N} = \sum_{\mathbf{k}} a_{\mathbf{k}}^+ a_{\mathbf{k}}$, while the hamiltonian (4) commutes with $\hat{N}$. One has to understand why the BEC state apparently does not respect the particle number conservation.

We start by noting that

$$e^{i\alpha\hat{N}}|\varphi\rangle = |e^{i\alpha}\varphi\rangle\,, \quad e^{i\alpha\hat{N}}\mathcal{H}e^{-i\alpha\hat{N}} = \mathcal{H} \tag{7}$$

i.e. the operator $e^{i\alpha\hat{N}}$, applied to $|\varphi\rangle$, produces a state of the same energy, with a phase of φ shifted by α. Since the overlap of coherent states obeys $|\langle\varphi'|\varphi\rangle|^2 = e^{-V|\varphi'-\varphi|^2}$, any two different states $|\varphi\rangle$, $|\varphi'\rangle$ are orthogonal in the limit $V \to \infty$. Thus the states with different phase factors, $|\varphi\rangle$, $|e^{i\alpha}\varphi\rangle$, are macroscopically distinct. This observation demonstrates that the BEC states form a degenerate manifold parameterized by a phase variable $0 < \alpha < 2\pi$.

To clarify the origin of this degeneracy, let us find the states $|\varphi\rangle$ that provide minimum to the energy (4). Taking minimum at fixed particle density can be achieved by adding to $\mathcal{H}$ a term proportional to $\hat{N}$, $\mathcal{H} \to \mathcal{H} - \mu\hat{N}$. Taking the expectation value, obtain

$$U(\varphi) = \langle\varphi|\mathcal{H} - \mu\hat{N}|\varphi\rangle = \frac{\lambda}{2}|\varphi|^4 - \mu|\varphi|^2 \tag{8}$$

— the so-called Mexican hat potential. The energy minima are found on the circle $|\varphi|^2 = \mu/\lambda$, i.e. the phase of φ is arbitrary, while the modulus $|\varphi|$ is fixed, thereby giving a relation between the density and chemical potential, $\mu = \lambda n$.[1]

From the symmetry point of view, the systuation is quite interesting. The microscopic hamiltonian (4) has global $U(1)$ symmetry, since it is invariant under adding a constant phase factor to the wavefunction of the system, $\hat{\varphi} \to e^{i\alpha}\hat{\varphi}$. The ground states, however, do not possess this symmetry: adding a phase factor to the state $|\varphi\rangle$ produces a different ground state. This phenomenon, called *spontaneous symmetry breaking*, is absent in the noninteracting Bose gas. In the interacting system, the $U(1)$ symmetry breaking has a very fundamental consequence: it leads to *superfluidity*.

There is yet another way to understand the phenomenon of $U(1)$ symmetry breaking, due to Penrose and Onsager, that does not require to consider the states with fluctuating particle number. One can instead start with the density matrix of the Bose gas (4) ground state $|\Phi_\lambda\rangle$ in the coordinate representation,

$$R(x, x') = \langle \Phi_\lambda | \hat{\varphi}^+(x') \hat{\varphi}(x) | \Phi_\lambda \rangle \tag{9}$$

Using the translational invariance, one expects that the quantity (9) will depend only on the distance $x - x'$ between the two points. By going to Fourier representation, one can transform (9) to the form

$$R(x, x') = \int e^{-i\mathbf{k}(\mathbf{x}-\mathbf{x}')} n_{\mathbf{k}} \frac{d^3k}{(2\pi)^3}\,, \quad n_{\mathbf{k}} = \langle \Phi_\lambda | \hat{a}^+_{\mathbf{k}} \hat{a}_{\mathbf{k}} | \Phi_\lambda \rangle \tag{10}$$

In a Bose condensate, the particle distribution $n_{\mathbf{k}}$ has singularity at $\mathbf{k} = 0$,

$$n_{\mathbf{k}} = n_0 (2\pi)^3 \delta(\mathbf{k}) + f(\mathbf{k}) \tag{11}$$

where $f(\mathbf{k})$ is a smooth function. Accordingly, the density matrix (10) has two terms,

$$R(x, x') = n_0 + \tilde{f}(x - x')\,, \quad \tilde{f}(x - x') \int e^{-i\mathbf{k}(\mathbf{x}-\mathbf{x}')} f_{\mathbf{k}} \frac{d^3k}{(2\pi)^3} \tag{12}$$

the constant n_0, independent of point separtion, and the second part, $\tilde{f}(x - x')$, that vanishes at large $|x - x'|$.

A density matrix that does not vanish at large point separtion represents an anomaly (recall that in any ordinary liquid all correlations vanish at several interatomic distances). The finite limit $n_0 = \lim_{|x-x'|\to\infty} \langle \Phi_\lambda | \hat{\varphi}^+(x') \hat{\varphi}(x) | \Phi_\lambda \rangle$ suggests that the quantities $\hat{\varphi}(x)$, $\hat{\varphi}^+(x')$ in some sense have finite expectation values: $\langle \hat{\varphi}(x) \rangle = e^{i\alpha}\sqrt{n_0}$, $\langle \hat{\varphi}^+(x) \rangle = e^{-i\alpha}\sqrt{n_0}$, with fixed modulus, but an undetermined phase. The name *Off-diagonal Long-range Order*, or ODLRO, associated with this phenomenon, expresses the fact that in the density matrix the ordering is revealed by the behavio of the off-diagonal component $R(x, x')_{|x-x'|\to\infty}$.

[1] In a finite, but large system, with fixed particle number, the true ground state (TGS) of a quantum-mechanical hamiltonian is nondegenerate. This TGS is isotropic in φ, due to boundary effects that split the circular manifold. The statement about the absence of degeneracy of TGS in a finite system is formally coirrect, but misleading, since this TGS is not 'pure'. Typically, at any moment of time the state is characterized by a global phase, changing slowly as a function of time. (In $D = 3$ the mixing of φ's with different phases results from vortices passing across the system, from one boundary to another.)

1.2 Quasiparticles

To study the excitations above the ground state, we substitute $\hat{a}_0 = \sqrt{N}$, a c-number, in the hamiltonian (4), and keep quadratic terms,

$$\mathcal{H} - \mu\hat{N} = \frac{1}{2}\lambda n^2 V + \sum_{\mathbf{k}\neq 0}\left(\epsilon^{(0)}_{\mathbf{k}} - \mu + 2\lambda n\right) a^+_{\mathbf{k}} a_{\mathbf{k}} + \frac{1}{2}\lambda n \sum_{\mathbf{k}\neq 0}\left(a^+_{\mathbf{k}} a^+_{-\mathbf{k}} + a_{\mathbf{k}} a_{-\mathbf{k}}\right) \quad (13)$$

$$= \frac{1}{2}\lambda n^2 V + \sum_{(\mathbf{k},-\mathbf{k})}\left(\epsilon^{(0)}_{\mathbf{k}}(a^+_{\mathbf{k}} a_{\mathbf{k}} + a^+_{-\mathbf{k}} a_{-\mathbf{k}}) + \lambda n (a_{\mathbf{k}} + a^+_{-\mathbf{k}})^+ (a_{\mathbf{k}} + a^+_{-\mathbf{k}})\right) \quad (14)$$

where the sum is taken over pairs $(\mathbf{k}, -\mathbf{k})$ Here we used the value $\mu = \lambda n$ obtained above.

At this stage, it is convenient to introduce the quantities $\hat{q}_{\mathbf{k}} = \frac{1}{\sqrt{2}}(a_{\mathbf{k}} + a^+_{-\mathbf{k}})$, $\hat{p}_{\mathbf{k}} = \frac{i}{\sqrt{2}}(a^+_{-\mathbf{k}} - a_{\mathbf{k}})$. These operators are non-hermitian, $\hat{q}^+_{\mathbf{k}} = \hat{q}_{-\mathbf{k}}$, $\hat{p}^+_{\mathbf{k}} = \hat{p}_{-\mathbf{k}}$, but obey the standard p, q algebra, $[\hat{q}_{\mathbf{k}}, \hat{p}_{\mathbf{k}'}] = \delta_{\mathbf{k}\mathbf{k}'}$, which allows to treat them as coordinate and momentum. In terms of the operators $\hat{p}_{\mathbf{k}}$, $\hat{q}_{\mathbf{k}}$ the hamiltonian is represented as a sum of independent harmonic oscillators. Indeed, since $a^+_{\mathbf{k}} a_{\mathbf{k}} + a^+_{-\mathbf{k}} a_{-\mathbf{k}} = \hat{p}^+_{\mathbf{k}} \hat{p}_{\mathbf{k}} + \hat{q}^+_{\mathbf{k}} \hat{q}_{\mathbf{k}}$, we can rewrite the hamiltonian as follows:

$$\mathcal{H} = \frac{1}{2}\lambda n^2 V + \sum_{(\mathbf{k},-\mathbf{k})}\left(\epsilon^{(0)}_{\mathbf{k}} \hat{p}^+_{\mathbf{k}} \hat{p}_{\mathbf{k}} + \left(\epsilon^{(0)}_{\mathbf{k}} + 2\lambda n\right) q^+_{\mathbf{k}} \hat{q}_{\mathbf{k}}\right) \quad (15)$$

This hamiltonian, quadratic in $\hat{q}_{\mathbf{k}}$, $\hat{p}_{\mathbf{k}}$, can be brought to the normal form by a rescaling (squeezing) transformation

$$\hat{q}_{\mathbf{k}} = e^{\theta_{\mathbf{k}}} \hat{q}'_{\mathbf{k}}\,, \quad \hat{p}_{\mathbf{k}} = e^{-\theta_{\mathbf{k}}} \hat{p}'_{\mathbf{k}}\,, \quad e^{4\theta_{\mathbf{k}}} = \frac{\epsilon^{(0)}_{\mathbf{k}}}{\epsilon^{(0)}_{\mathbf{k}} + 2\lambda n} \quad (16)$$

which acts on the operators $a_{\mathbf{k}}$, $a^+_{\mathbf{k}}$ as

$$a_{\mathbf{k}} = \cosh\theta_{\mathbf{k}} b_{\mathbf{k}} - \sinh\theta_{\mathbf{k}} b^+_{-\mathbf{k}}\,, \quad a^+_{-\mathbf{k}} = \cosh\theta_{\mathbf{k}} b^+_{-\mathbf{k}} - \sinh\theta_{\mathbf{k}} b_{\mathbf{k}} \quad (17)$$

(see Lecture 2). The transformation (17), called Bogoliubov transformation, can be shown to preserve the canonical commutation relations, $[b_{\mathbf{k}}, b^+_{\mathbf{k}}] = 1$.

The hamiltonian is now reduced to

$$\mathcal{H} = \frac{1}{2}\lambda n^2 V + \sum_{(\mathbf{k},-\mathbf{k})} E_{\mathbf{k}}\left(b^+_{\mathbf{k}} b_{\mathbf{k}} + b^+_{-\mathbf{k}} b_{-\mathbf{k}}\right) = \frac{1}{2}\lambda n^2 V + \sum_{\mathbf{k}\neq 0} E_{\mathbf{k}} b^+_{\mathbf{k}} b_{\mathbf{k}} \quad (18)$$

describing a gas of Bogoliubov quasiparticles, the noninteracting bosons created and annihilated by the operators $b^+_{\mathbf{k}}$, $b_{\mathbf{k}}$, having energy

$$E_{\mathbf{k}} = \sqrt{\left(\epsilon^{(0)}_{\mathbf{k}} + \lambda n\right)^2 - (\lambda n)^2} \quad (19)$$

The new ground state is annihilated by all the $b_{\mathbf{k}}$. Since for the ground state of the ideal Bose gas $a_{\mathbf{k}}|\Phi_0\rangle = 0$, and the transformation (17) can be represented as $b_{\mathbf{k}} = U a_{\mathbf{k}} U^{-1}$, $b^+_{\mathbf{k}} = U a^+_{\mathbf{k}} U^{-1}$, with

$$U = \exp\left(\sum_{\mathbf{k}\neq 0} \theta_{\mathbf{k}}\left(a^+_{\mathbf{k}} a^+_{-\mathbf{k}} - a_{\mathbf{k}} a_{-\mathbf{k}}\right)/2\right) \quad (20)$$

(see Lecture 2), one can write the new ground state as $|\Phi_\lambda\rangle = U|\Phi_0\rangle$.

The dispersion relation (19), for small $\mathbf{k}$, is linear,

$$E_{\mathbf{k}} = \hbar c|\mathbf{k}|\,, \quad c = \sqrt{\lambda n/m} \tag{21}$$

which is characteristic for sound waves in a fluid. For higher values of $\mathbf{k}$, the dispersion takes the form of a usual free-particle expression $E_{\mathbf{k}} = \hbar^2\mathbf{k}^2/2m + \lambda n$.

Remarkably, both the collective modes, sound waves, and the single-particle excitations appear on the same dispersion curve, gradually blending into one another at the energy *ca.* $E_{\mathbf{k}} \simeq \lambda n$. One can gain some insight into the difference of the modes at large and small $\mathbf{k}$ by considering the field equations

$$i\hbar\partial_t\hat{\varphi} = [\hat{\varphi}, (\mathcal{H} - \mu\hat{N})] = -\frac{\hbar^2}{2m}\nabla^2\hat{\varphi} + \lambda\hat{\varphi}^+\hat{\varphi}^2 - \mu\hat{\varphi} \tag{22}$$

$$-i\hbar\partial_t\hat{\varphi}^+ = [(\mathcal{H} - \mu\hat{N}), \hat{\varphi}^+] = -\frac{\hbar^2}{2m}\nabla^2\hat{\varphi}^+ + \lambda(\hat{\varphi}^+)^2\hat{\varphi} - \mu\hat{\varphi}^+ \tag{23}$$

It is instructive to treat these equations as a classical dynamics problem, linearizing near stationary solution, $\varphi = \varphi_0 + \eta$, where $\varphi_0 = \sqrt{\mu/\lambda}$. The linearized equation has solution of the form

$$\eta(\mathbf{r}, t) = a e^{i\mathbf{k}\mathbf{r} - i\omega t} + \bar{b} e^{-i\mathbf{k}\mathbf{r} + i\omega t} \tag{24}$$

with $\hbar\omega = \pm\sqrt{\left(\epsilon_{\mathbf{k}}^{(0)} + \lambda n\right)^2 - (\lambda n)^2}$ the same as Eq.(19). In other words, one can consider condensate with fluctuating amplitude and phase, and show that these fluctuations propagate in just the same way as the collective modes (19).

In such an approach, the difference between small and large $\mathbf{k}$ follows from the relation between the amplitudes a and b obtained from the dynamical equation. At small k, the sum $a + b$ is much smaller than the difference $a - b$. This means that the oscillations are predominantly *in the phase* of the field φ, not in the modulus, just as one expects from Goldstone theorem (and the above Mexican hat picture). At large $\mathbf{k}$, however, the normal modes have $a + b$ or $a - b$ nearly equal in magnitude, which means that the oscillation follows a small circle in the complex φ plane, i.e. the phase and the modulus of φ participate in the collective oscillations roughly equally.

We can use the above results to estimate the effect of condensate depletion due to interactions. The total density of all particles in the system can be written as

$$n = \langle\Phi_\lambda|a_0^+ a_0 + \sum_{\mathbf{k}\neq 0} a_{\mathbf{k}}^+ a_{\mathbf{k}}|\Phi_\lambda\rangle = n_0 + \sum_{\mathbf{k}\neq 0} \sinh^2\theta_{\mathbf{k}}\langle\Phi_\lambda|b_{\mathbf{k}} b_{\mathbf{k}}^+|\Phi_\lambda\rangle \tag{25}$$

$$= n_0 + \frac{1}{2}\sum_{\mathbf{k}\neq 0}\left(\frac{\epsilon_{\mathbf{k}}^{(0)} + \lambda n}{\sqrt{\left(\epsilon_{\mathbf{k}}^{(0)} + \lambda n\right)^2 - (\lambda n)^2}} - 1\right) \tag{26}$$

Estimating the sum as $O(\lambda^{3/2})$, we find that the condensate depletion is a small effect. In contrast, in superfuid ^{4}He only few percent of the helium atoms are in the single-particle ground state.