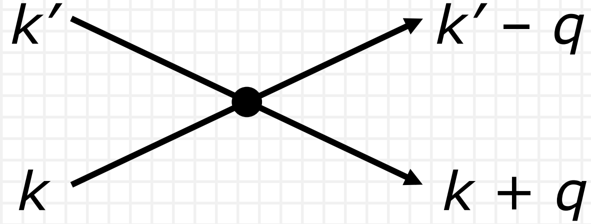
# Last lecture (#8):

We developed the 2nd quantized form of the Hamiltonian central to the microscopic theory of superfluidity and superconductivity, and other problems in Bose and Fermi systems

$$\hat{H} = \sum_k \varepsilon_k a_k^+ a_k + \frac{1}{2}\sum_q \left( g_q \hat{\rho}_q^+ \hat{\rho}_q - \frac{\hat{N}}{V} \right) \rightarrow \sum_k \varepsilon_k a_k^+ a_k + \frac{g}{2V} \sum_{kk'q} a_{k+q}^+ a_{k'-q}^+ a_{k'} a_k$$

$$\hat{\rho}_q^+ = \frac{1}{\sqrt{V}} \sum_k a_{k+q}^+ a_k$$ so that if $N_0 = V n_0 >> 1$

$$\hat{\rho}_q^+ \approx \frac{1}{\sqrt{V}} (a_q^+ a_0 + a_0^+ a_{-q}) = \sqrt{n_0}(a_q^+ + a_{-q})$$




The microscopic theory is based on the trial wave-function method. The trial ground state wavefunction is taken to be a coherent state: a BEC state for superfluids such as He-II and atomic gases and a BCS state for conventional superconductors and for superfluids such as liquid $^3$He. The elementary excitations above the ground states are then found via the Bogoliubov theory. We treat superfluidity in this lecture and then turn to superconductivity.

# Lecture 9:

I. Bogoliubov Theory
- IA. Effective Hamiltonian
- IB. Bogoliubov Transformation
- IC. Elementary Excitations and Superfluidity
- ID. Condensate Depletion

II. Connection to the Ginzburg-Landau Model
- IIA. Order Parameter $\psi_s(r)$
- IIB. Ginzburg-Landau Free Energy

Literature: Annett chs. 2 & 5, Pethick & Smith chs. 8 & 10, Waldram chs. 2 & 9

# I. Bogoliubov Theory
## IA. Effective Hamiltonian

Recall that in the limit of macroscopic occupation in the $k$=0 state (i.e., $N_0 \to \infty$) the leading terms in the potential energy operator will be those with the highest (even) powers of $a_0 \approx a_0^+ \approx \sqrt{N_0}$ . Retaining terms 2nd and 4th order in these quantities we arrive at a reduced or effective Hamiltonian of the form

$$\hat{H}_{eff} = \frac{1}{2}\sum_{k\neq 0}\left[ (\varepsilon_k + 2n_0 g)(a_k^+ a_k + a_{-k}^+ a_{-k}) + n_0 g(a_k^+ a_{-k}^+ + a_k a_{-k}) \right] + \frac{N_0^2 g}{2V}$$

$$= \frac{1}{2}\sum_{k\neq 0}\left[ (\varepsilon_k + n_0 g)(a_k^+ a_k + a_{-k}^+ a_{-k}) + n_0 g(a_k^+ a_{-k}^+ + a_k a_{-k}) \right] + \frac{N^2 g}{2V}$$

We have used the boson commutation rules, the relation

$$\hat{N} = \hat{N}_0 + \sum_{k\neq 0} a_k^+ a_k, \quad \text{so that} \quad \hat{N}^2 \approx \hat{N}_0^2 + 2\hat{N}_0 \sum_{k\neq 0} a_k^+ a_k$$

and replaced the number operators by real numbers $N$ & $N_0$. The Hartree-Fock chemical potential and energy spectrum are

$$\mu^{HF} = ng \approx n_0 g, \quad \xi_k = \varepsilon_k^{HF} - \mu^{HF} = \varepsilon_k + n_0 g$$

The anomalous *aa* and $a^+a^+$ terms in the effective Hamiltonian give crucially important corrections to Hartree-Fock theory for a boson system.

The effective Hamiltonian is a quadratic form that can be diagonalized by a linear transformation from the Bose operators ($a_k$, $a_k^+$) to new Bose operators ($\alpha_k$, $\alpha_k^+$) so that

$$\hat{H}_{eff} = E_{zp} + \sum_{k\neq 0} E_k \, \alpha_k^+ \alpha_k$$

where $E_{zp}$ is the zero point energy and $E_k$ is the excitation energy spectrum of interest here. (For a discussion of $E_{zp}$ see, e.g., Pethick & Smith p. 212.)

An excited state of the Bose system may be described in terms of elementary excitations with number density $\alpha_k^+\alpha_k$ and energy $E_k$. We need to find the new boson operators and then $E_k$ in terms of $\varepsilon_k$ & $g$.

# IB. Bogoliubov Transformation

We might expect $\alpha_k^+$ to be a linear superposition of a single-particle creation operator $a_k^+$ and a density-fluctuation creation operator $\rho_k^+$. In our model, $\rho_k^+$ is just a superposition of $a_k^+$ and $a_{-k}$ and thus we assume that $\alpha_k^+$ is of the form

$$\alpha_k^+ = u_k a_k^+ + v_k a_{-k}$$

where the coefficients $u_k$ and $v_k$ can be taken to be real and must be adjusted to diagonalize $\hat{H}_{eff}$ .

This is the Bogoliubov transformation. As can be confirmed by direct substitution in $\hat{H}_{eff}$ the solutions for these coefficients and for the excitation energy spectrum are as given below (see examples sheet 3 and, e.g., Pethick & Smith §8.1):

$$u_k^2 = \frac{1}{2}\left(\frac{\xi_k}{E_k} + 1\right) \qquad v_k^2 = \frac{1}{2}\left(\frac{\xi_k}{E_k} - 1\right)$$

$$E_k^2 = \xi_k^{\ 2} - (n_0 g)^2, \quad \xi_k = \varepsilon_k + n_0 g$$

where $\xi_k$ is the excitation energy measured from the chemical potential in the Hartree-Fock approximation (p3). The excitation energies in the Bogoliubov theory at low and high $k$ are then

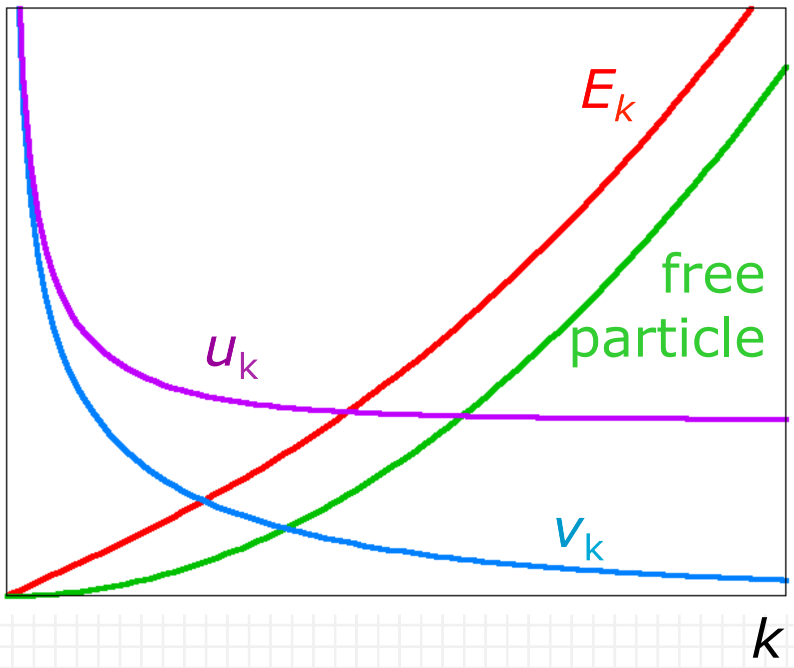
$$E_k = \begin{cases} \hbar\sqrt{\dfrac{n_0 g}{m}}\,k & \varepsilon_k << n_0 g \\ \dfrac{\hbar^2 k^2}{2m} & \varepsilon_k >> n_0 g \end{cases}$$

Thus, at low $k$ (i.e., $\varepsilon_k << n_0 g$) the spectrum is linear and the elementary excitations are collective density fluctuations ($u_k \approx v_k$) with sound velocity $c = \sqrt{n_0 g / m}$ . At high $k$ (i.e., $\varepsilon_k >> n_0 g$) the spectrum is quadratic and the excitations are single-particle excitations ($u_k \approx 1$, $v_k \approx 0$) with energy $\varepsilon_k$.

# IC. Elementary Excitations and Superfluidity

For finite $g$ the model gives the spectrum $E_k$ shown in the figure below. The Landau critical velocity is finite and equal to the speed of sound. The depression of the density of states of elementary excitations due to the repulsive interaction turns a BEC into a superfluid.

$$\alpha_k^+ = u_k a_k^+ + v_k a_{-k}$$




In this model the low $k$ excitations correspond to Goldstone modes that arise because of the breaking of a continuous symmetry (see p. 14). Lattice vibrations in solids and spin waves in magnetic systems arise for similar reasons. Though a major improvement over Hartree-Fock the Bogoliubov theory does not predict the existence of rotons expected to arise in the presence of strong interactions, as in He-II.

# ID. Condensate Depletion

Interactions reduce the condensate fraction $n_0/n$ in the one-particle state $\varphi_0$. This effect can be calculated from

$$\hat{N} = \sum_k a_k^+ a_k = \hat{N}_0 + \sum_{k \neq 0} a_k^+ a_k$$

and rewriting $a_k^+$ and $a_k$ in terms of $\alpha_k^+$ and $\alpha_k$ of the Bogoliubov transformation

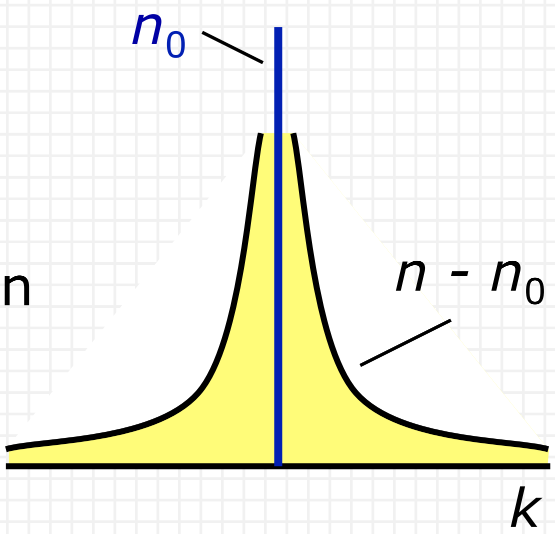
$$a_k^+ = u_k \alpha_k^+ - v_k \alpha_{-k} \qquad a_k = u_k \alpha_k - v_k \alpha_{-k}^+$$

In the product $a_k^+ a_k$ the term $v_k^2 \alpha_{-k} \alpha_{-k}^+ = v_k^2 \alpha_{-k}^+ \alpha_{-k} + v_k^2$ leads to a correction in $\hat{N}$ even in the absence of thermal excitations. Thus, in the ground state

$$\frac{N}{V} = \frac{<\hat{N}>}{V} = \frac{N_0}{V} + \frac{1}{V} \sum_{k \neq 0} v_k^2 \text{ , or } \quad \boxed{n = n_0 + \frac{1}{3\pi^2} \left( \frac{mc}{\hbar} \right)^3}$$

The condensate fraction $n_0/n$ is thus less than unity unless the speed of sound $c \rightarrow 0$. In atomic gases $n_0/n$ is above 90%, whereas in He-II it is of the order of or less than 10%.

Single-particle momentum distribution




Note that $n_0$ should not be confused with $n_s$ in the two-fluid model or in the Ginzburg-Landau model. In particular, the superfluid current density is given by $n_s v_s$ and not by $n_0 v_s$. The particles $N - N_0$ should not be thought of as being in excited incoherent states. They are bound up in a coherent ground state wavefunction along with $N_0$ and are thus "dragged" with $N_0$ to produce the total superfluid current at $T$ = 0K (see, e.g., Waldram §2.2 and §9.4).

# II. Connection to Ginzburg-Landau Model
## IIA. Order Parameter $\psi_s(r)$

In the absence of interactions all particles condense in the same single-particle state

$$\varphi_s(r) = \frac{e^{is\cdot r}}{\sqrt{V}}$$

where $s$ is non-zero if the BEC carries a current. The many-particle state for fixed particle number $N$ is

$$|\Psi_s\rangle = \varphi_s(r_1)\ldots\varphi_s(r_N)$$

More generally we assume $|\Psi_s\rangle$ can be approximated by a trial many-body state satisfying

$$\hat{\psi}(r)|\Psi_s\rangle = \psi_s(r)|\Psi_s\rangle$$

i.e., we assume that $|\Psi_s\rangle$ is a coherent state. Recall that a coherent state is an eigenstate of the annihilation operator, so that the latter can essentially be replaced by a c-number.

The eigenvalue, $\psi_s(r)$, of $\hat{\psi}(r)$ for this many-body state, represents the macroscopic wave-function or the order parameter in the Ginzburg-Landau model; $\psi_s(r)$ reduces to the single-particle state $\varphi_s(r)$ only in the absence of interactions.

The reasons for choosing a coherent state for the trial wavefunction are that

- it gives the correct state in the absence of interactions;
- it involves a superposition of states of different number of particles as is appropriate for a grand canonical ensemble;
- and it allows us to evaluate the Hamiltonian in a straightforward way since the operators $\hat{\psi}^+(r)$ and $\hat{\psi}(r)$ reduce to the *c*-numbers $\psi_s^*(r)$ and $\psi_s(r)$ at each *r*.

Recall that even a crude trial wavefunction can produce accurate energies. We look for internal consistency of the theory and consistency with experiment.

# IIB. Ginzburg-Landau Free Energy

To obtain the Ginzburg-Landau model we evaluate a free energy for the superfluid defined as

$$F_S = \langle \Psi_S \,|\, \hat{H} - \mu\hat{N} \,|\, \Psi_S \rangle$$

From the relations between ($\psi(r)$, $\psi^+(r)$) and ($a_k$, $a_k^+$) we easily confirm that for $\varepsilon_k = \hbar^2 k^2 / 2m$ the Hamiltonian can be written as

$$\hat{H} = \sum_k \frac{\hbar^2 k^2}{2m} a_k^+ a_k + \frac{g}{2V} \sum_{kk'q} a_{k+q}^+ a_{k'-q}^+ a_{k'} a_k$$

$$= \int dr \left[ \frac{\hbar^2}{2m} \left| \nabla \hat{\psi}(r) \right|^2 + \frac{g}{2} \hat{\psi}^+(r) \hat{\psi}^+(r) \hat{\psi}(r) \hat{\psi}(r) \right]$$

The kinetic energy factor $|\nabla \hat{\psi}|^2$ is equivalent to $-\hat{\psi}^+ \nabla^2 \hat{\psi}$ via integration by parts as in lecture 2.

Using the fact that $|\Psi_s\rangle$ is a coherent state, we then find

$$F_S = E_S - \mu N = \int dr \left( -\mu \, |\psi_S|^2 + \frac{\hbar^2}{2m} |\nabla \psi_S|^2 + \frac{g}{2} |\psi_S|^4 \right)$$

where $\mu$ is the chemical potential equal to *ng* in the Hatree-Fock approximation. The integrand is essentially the Ginzburg-Landau free energy density as a function of the order parameter $\psi_s(r)$ (at $T$->0K). This provides a connection between the macroscopic parameters of the Ginzburg-Landau and the microscopic parameters of the underlying Hamiltonian, i.e., in this model the Ginzburg-Landau parameters defined in the first lecture are

$\alpha = -ng$, $m = m$ and $\beta = g$.

Finally, the dynamics of the order parameter may be described as in the Gross-Pitaevskii theory (going beyond Hatree-Fock) by

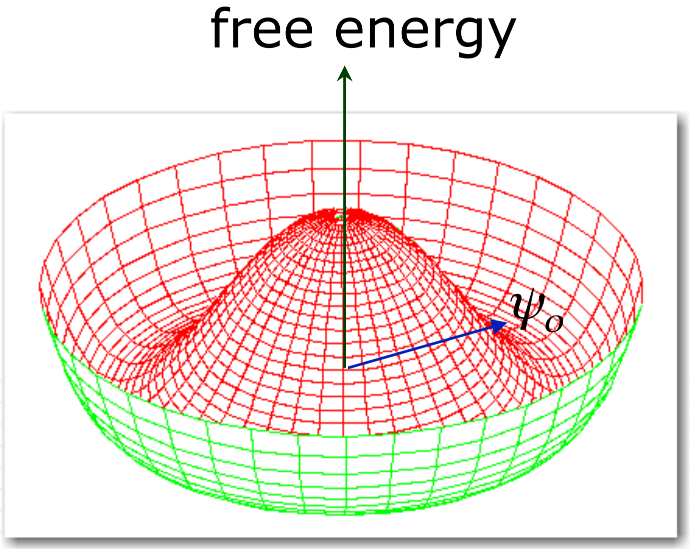
$$-(\hbar^2 / 2m)\nabla^2 \psi_s + g\left|\psi_s\right|^2 \psi_s = i\hbar\dot{\psi}_s$$

(Pethick & Smith ch. 7)

This predicts that small oscillations $\delta\psi_s$ about the equilibrium state $\psi_0$ , i.e., Goldstone modes at small *k*, correspond to the low-lying excitations in the Bogoliubov theory.

# Goldstone and Higgs Modes

Goldstone modes correspond to fluctuations of the order parameter transverse to the equilibrium $\psi_o$ in the complex plane, and are gapless as *k* goes to 0. Higgs modes correspond to fluctuations parallel to $\psi_o$ and have an energy gap in their spectrum. The Goldstone modes for a superfluid are collisionless sound waves as obtained in the Bogoliubov theory.




Broken U(1) symmetry