Microscopic theory of superconductivity

- Superfluidity
- Phonon attraction
- Cooper pairs
- BCS theory
- Energy gap
- Correlation length
- Type-I and type-II superconductors

Superfluidity

Liquid Helium-4: at low temperature flows with zero viscosity

Relative to the liquid (velocity ***v***): viscosity means creation of quasiparticles

Momentum ***p***; energy $\varepsilon(\vec{p})$

Relative to the ground: momentum $\vec{P}' = \vec{P} + M\vec{v}$

energy $E' = E + \vec{P}\vec{v} + Mv^2/2$

M – mass of the liquid

Energy change associated with the creation of a quasiparticle:

$$\Delta E = \varepsilon(\vec{p}) + \vec{p}\vec{v}$$

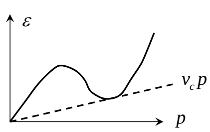
If it is positive, superfluid (no viscosity)

$$v < v_c = \min(\varepsilon(p)/p)$$

Superfluidity

Helium-4

(bosons)



Fermi-system: Elementary excitations are electron-hole pairs
Energy: may be arbitrarily small
Momentum: can be finite

No superfluidity!

May be electrons are bound in pairs and behave like Helium atoms.
Difficulty: Why do not they repel each other then?

Electron-phonon interaction again

One electron emits a phonon, another one absorbs this phonon:
Mechanism for electron-electron interaction!!

Initial state: electron #1 with $\vec{p}_1$ and electron #2 with $\vec{p}_2$

Intermediate state: electron #1 with $\vec{p}_1 - \hbar\vec{k}$, electron #2 with $\vec{p}_2$
phonon with $\vec{k}$

Final state: electron #1 with $\vec{p}_1 - \hbar\vec{k}$ and electron #2 with $\vec{p}_2 + \hbar\vec{k}$

$$\varepsilon(\vec{p}_1) + \varepsilon(\vec{p}_2) = \varepsilon(\vec{p}_1 - \hbar\vec{k}) + \varepsilon(\vec{p}_2 + \hbar\vec{k})$$

-same energy of initial and final states

Second-order perturbation theory: $\Delta E_i = \sum_\nu \frac{|M_{i\nu}|^2}{E_i - E_\nu}$

$$\Delta E_{1\vec{p}_1} = \frac{|V_{\vec{k}}|^2}{\varepsilon(\vec{p}_1) - \varepsilon(\vec{p}_1 - \hbar\vec{k}) - \hbar\omega(\vec{k})} = \frac{\lambda}{gV}\frac{\hbar\omega(\vec{k})}{\varepsilon(\vec{p}_1) - \varepsilon(\vec{p}_1 - \hbar\vec{k}) - \hbar\omega(\vec{k})}$$

Electron-phonon interaction again

Another process contributing: electron absorbs a phonon with ***-k***

Initial state: electron #1 with $\vec{p}_1$ and electron #2 with $\vec{p}_2$

Intermediate state: electron #1 with $\vec{p}_1$, electron #2 with $\vec{p}_2 + \hbar\vec{k}$
phonon with $-\vec{k}$

Final state: electron #1 with $\vec{p}_1 - \hbar\vec{k}$ and electron #2 with $\vec{p}_2 + \hbar\vec{k}$

$$\varepsilon(\vec{p}_1) + \varepsilon(\vec{p}_2) = \varepsilon(\vec{p}_1 - \hbar\vec{k}) + \varepsilon(\vec{p}_2 + \hbar\vec{k})$$

-same energy of initial and final states

Second-order perturbation theory: $\Delta E_i = \sum_\nu \frac{|M_{i\nu}|^2}{E_i - E_\nu}$

$$\Delta E_{2\vec{p}_1} = \frac{|V_{\vec{k}}|^2}{\varepsilon(\vec{p}_2) - \varepsilon(\vec{p}_2 + \hbar\vec{k}) - \hbar\omega(\vec{k})} = -\frac{\lambda}{gV}\frac{\hbar\omega(\vec{k})}{\varepsilon(\vec{p}_1) - \varepsilon(\vec{p}_1 - \hbar\vec{k}) + \hbar\omega(\vec{k})}$$

Phonon attraction

Summing up:

$$\Delta E_{\vec{p}_1} = \Delta E_{1\vec{p}_1} + \Delta E_{2\vec{p}_1} = \frac{2\lambda}{gV}\frac{\left[\hbar\omega(\vec{k})\right]^2}{\left[\varepsilon(\vec{p}_1) - \varepsilon(\vec{p}_1 - \hbar\vec{k})\right]^2 - \left[\hbar\omega(\vec{k})\right]^2}$$

For $\varepsilon(\vec{p}_1) - \varepsilon(\vec{p}_1 - \hbar\vec{k}) \ll \hbar\omega(\vec{k})$ $\quad \Delta E = -\frac{2\lambda}{gV}$

Corresponds to attracting point-like interaction!!

$$V_{ph} = -\frac{2\lambda}{g}\delta(\vec{r} - \vec{r}\,')$$

Phonon attraction

Electron-electron attraction: $V_{ph} = -\frac{2\lambda}{g}\delta(\vec{r}-\vec{r}\,')$

Compare this with Coulomb repulsion:

$$V_C = -\frac{e^2}{|\vec{r}-\vec{r}\,'|} \Rightarrow e^2 a_B^2 \delta(\vec{r}-\vec{r}\,')$$

$$g \sim mp_F/\hbar^3 \qquad a_B \sim \hbar^2/me^2$$

$$\frac{V_{ph}}{V_C} \sim \frac{\lambda}{ge^2a_B^2} \sim \frac{e^2\lambda}{\hbar v_F} \sim 1$$

Same order of magnitude

Attraction dominates > superconductivity
Repulsion dominates > no superconductivity

Cooper pairs

We found a (weak) electron-electron attraction, but it does not mean two electrons form a bound state (a pair).

Quantum mechanics: an electron in a shallow quantum well:
1D: always a bound state
2D and 3D: no bound state (only if the well is deep enough)

Now, we have not free electrons, but quasiparticles above the Fermi surface.

Two-particle Schrödinger equation:

$$\left[\hat{H}_1 + \hat{H}_2 + U(\vec{r}_1,\vec{r}_2)\right]\Psi(\vec{r}_1,\vec{r}_2) = E\Psi(\vec{r}_1,\vec{r}_2)$$

Ground state: total momentum and total spin of the pair equal zero

$$\Psi(\vec{r}_1,\vec{r}_2) = \sum_{\vec{p}} c_{\vec{p}} \psi_{\vec{p}\uparrow}(\vec{r}_1)\psi_{-\vec{p}\downarrow}(\vec{r}_2)$$

Cooper pairs

Back to Schrödinger equation:

$$2\xi_{\vec{p}}c_{\vec{p}} + \sum_{\vec{p}\,'} U_{\vec{p}\vec{p}\,'}c_{\vec{p}\,'} = Ec_{\vec{p}}$$

$$U_{\vec{p}\vec{p}\,'} = -U_0,\; p_F - \frac{\hbar\omega_D}{v_F} < p, p' < p_F + \frac{\hbar\omega_D}{v_F}$$

Solution: $E = -2\Delta$

$$c_{\vec{p}} = \frac{U_0}{2|\xi_{\vec{p}}+\Delta|}\sum_{p_F-\hbar\omega_D/v_F}^{p_F-\hbar\omega_D/v_F} c_{\vec{p}\,'} \Longrightarrow \frac{U_0 g(\varepsilon_F)}{2}\ln\left(\frac{\hbar\omega_D}{\Delta}\right) = 1$$

$$\Delta = \hbar\omega_D\exp(-2/g(\varepsilon_F)U_0) = \hbar\omega_D\exp(-4/\lambda)$$

No small parameter – non-perturbative calculation.

BCS Hamiltonian

$$\hat{H} = \sum_{\vec{p}\sigma}\xi_{\vec{p}}\hat{c}^\dagger_{\vec{p}\sigma}\hat{c}_{\vec{p}\sigma} - U_0\sum_{\vec{p}_1+\vec{p}_2=\vec{p}_1'+\vec{p}_2'}\hat{c}^\dagger_{\vec{p}_1'\uparrow}\hat{c}^\dagger_{\vec{p}_2'\downarrow}\hat{c}_{\vec{p}_2\downarrow}\hat{c}_{\vec{p}_1\uparrow}$$

Kinetic energy

Phonon attraction (only electrons with different spin interact)

What is the ground state corresponding to this Hamiltonian?
(Advanced quantum mechanics, Lecture 4)

$$\Psi = \prod_{\vec{p}}\left[u_{\vec{p}} + v_{\vec{p}}\hat{c}_{\vec{p}\uparrow}\hat{c}_{-\vec{p}\downarrow}\right] \qquad |u_{\vec{p}}|^2 + |v_{\vec{p}}|^2 = 1$$

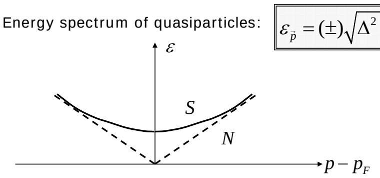
Normal state: *v=0*

Need to find *u* and *v* from the minimisation of energy (variational principle)

BCS theory

$$u_{\vec{p}} = \frac{1}{\sqrt{2}}\sqrt{1+\xi_{\vec{p}}/\varepsilon_{\vec{p}}},\; v_{\vec{p}} = \frac{1}{\sqrt{2}}\sqrt{1-\xi_{\vec{p}}/\varepsilon_{\vec{p}}}$$

Energy spectrum of quasiparticles: $\varepsilon_{\vec{p}} = (\pm)\sqrt{\Delta^2+\xi_{\vec{p}}^2}$

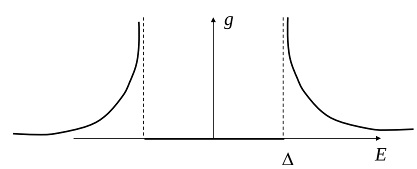


No quasiparticles with energy below *Δ*!

Density of states

$$\varepsilon_{\vec{p}} = \sqrt{\Delta^2+\xi_{\vec{p}}^2}$$

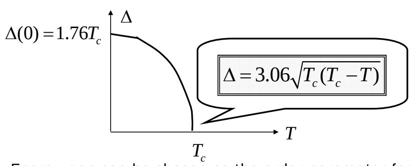
$$g(E) = \sum_{\vec{p}}\delta\left(E - \sqrt{\Delta^2+\xi_{\vec{p}}^2}\right) \propto \frac{\theta(E-\Delta)}{\sqrt{E-\Delta}}$$



Energy gap

$T_c = 1.4\hbar\omega_D U \exp(-2/(gU_0))$ - transition temperature

Energy spectrum of quasiparticles:



Energy gap can be chosen as the order parameter for the Landau description of the second order phase transition – *see next Lecture*.

Correlation length

What is a typical size of a Cooper pair?

$\delta p \sim \Delta / v$ ⟹ $\delta r \sim \hbar v / \Delta$

Example: $\Delta / k_B \sim T_c \sim 10K$, $v \sim 10^6 m/s$ ⟹ $\delta r \sim 10^{-6} m$

The "size" of a Cooper pair is much bigger than the distance between electrons: It does not make any sense.

It is better to talk about the correlation between electrons.

Correlation length: $\xi(T) \sim \hbar v / \Delta(T)$ Diverges at the transition point!

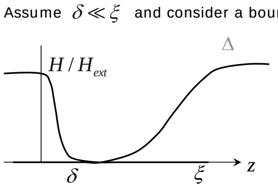
London equations: correspond to $\xi = 0$.

Pippard limit

Correlation length: $\xi(T) \sim \hbar v / \Delta(T)$ Both diverge as $1/\sqrt{T_c - T}$

Penetration depth: $\delta = \sqrt{mc^2/(4\pi n_S e^2)}$

Assume $\delta \ll \xi$ and consider a boundary between N and S



Region $\delta \ll z \ll \xi$

- no energy gap and no magnetic field

"Normal metal" with Meissner effect

$F_n - F_s = VH_c^2 / 8\pi$

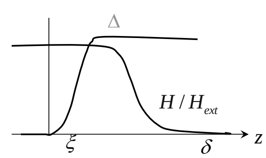
Positive boundary energy -> intermediate state

London limit

Assume now $\delta \gg \xi$

Region $\xi \ll z \ll \delta$ - both energy gap and magnetic field present.

"Superconductor" without Meissner effect



$F_n - F_s = VH_c^2 / 8\pi$

Negative boundary energy -> unusual behavior of a superconductor in an external field

Two types of superconductors

Type I: positive boundary energy $\delta \ll \xi$

Type II: negative boundary energy $\delta \gg \xi$

Criterion: $\kappa(T) = \delta(T) / \xi(T)$ -only weakly depends on temperature

$\kappa < 1/\sqrt{2}$ - type I

$\kappa > 1/\sqrt{2}$ - type II

Bogoliubov – de Gennes equations

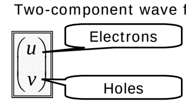
Mean-field treatment of BCS Hamiltonian

$$\hat{H} = \sum_{\vec{p}\sigma} \xi_{\vec{p}} \hat{c}^{\dagger}_{\vec{p}\sigma} \hat{c}_{\vec{p}\sigma} + \Delta \sum_{\vec{p}} \hat{c}^{\dagger}_{\vec{p}\uparrow} \hat{c}^{\dagger}_{-\vec{p}\downarrow} + \Delta^* \sum_{\vec{p}} \hat{c}_{\vec{p}\downarrow} \hat{c}_{-\vec{p}\uparrow}$$

It is quadratic: can be diagonalized

$\psi_{\vec{p}\uparrow} = u_{\vec{p}} \hat{c}_{\vec{p}\uparrow} + v_{\vec{p}} \hat{c}^{\dagger}_{-\vec{p}\downarrow}$ Not the same *u* and *v* as in BCS!!

Two-component wave function:



Bogoliubov – de Gennes equations

Minimizing the Hamiltonian:
Bogoliubov – de Gennes equations – Two-component generalization of Schrödinger equation

Best in the coordinate representation:

$$\hat{H}u + \Delta v = \varepsilon u$$
$$-\hat{H}v + \Delta^* v = \varepsilon v$$

Energy spectrum: same as BCS $\varepsilon_{\vec{p}} = \pm\sqrt{\Delta^2 + \xi_{\vec{p}}^2}$