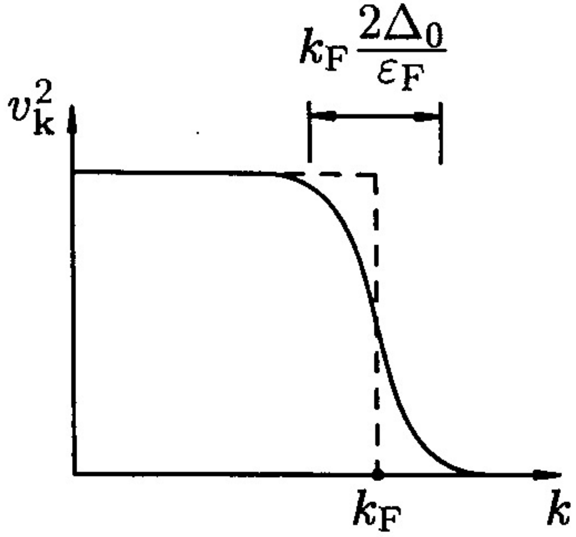
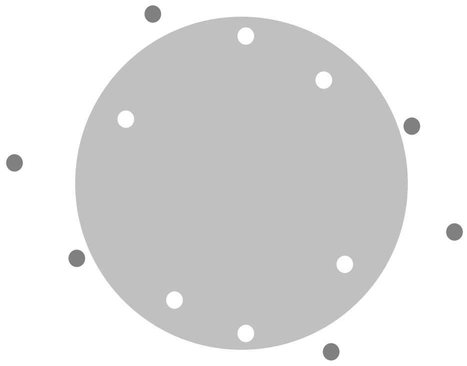
Superconductivity
Lecture 6





Introduction in BCS theory

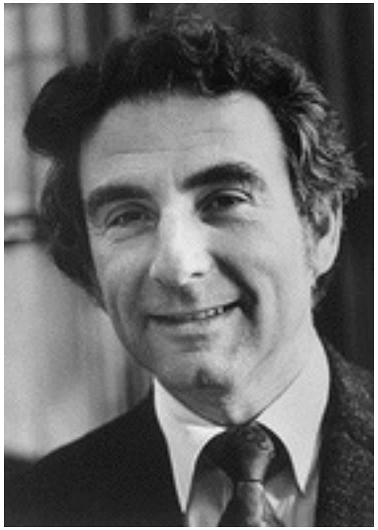
- Basic idea: Cooper pairs
- Electron-phonon interaction
- Ground state of a superconductor
- Energy gap
- Ground-state energy

BCS = Bardin-Cooper-Schrieffer

The Nobel Prize in Physics 1972
„for their jointly developed theory of superconductivity“

original paper: 1957

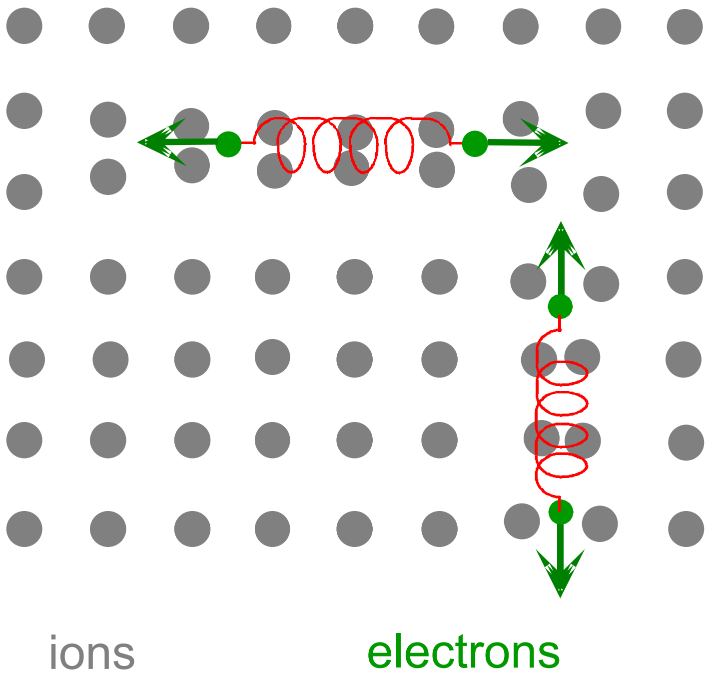
John Bardeen



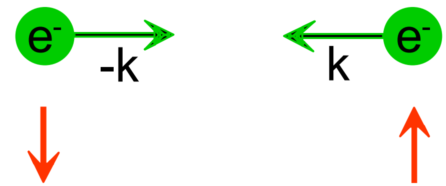
Leon Neil Cooper

John Robert Schrieffer

Basic idea: Cooper pairs



Cooper pair



spin singlet

angular momentum 0 (s-state)

attractive interaction electron-phonon

coherence length ~ 100 nm

>> atom spacing

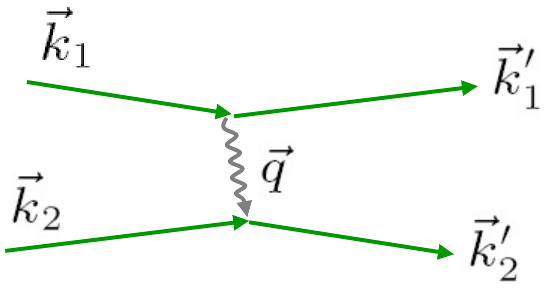
order parameter $\Delta = \Delta_0 e^{i\varphi}$

The physical mechanism of superconductivity became clear only 46 years after this phenomenon was discovered.

Electron-phonon interaction

The first indication of the relation to phonons was obtained with the discovery of the isotope effect

$$T_c M^a = \mathrm{const}$$
$$a \sim 0.5$$



$\hbar\omega_{\vec{q}}$ phonon energy

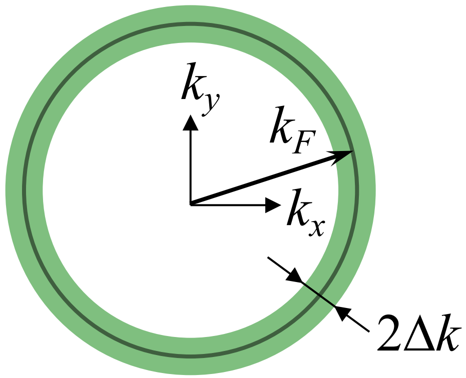
electron–electron interaction via emission and subsequent absorption of a phonon of momentum $\hbar\vec{q}$

$$\vec{k}_1 = \vec{k}_1' + \vec{q} \quad \Rightarrow \quad \vec{k}_1 + \vec{k}_2 = \vec{k}_1' + \vec{k}_2'$$

Scattering from state $\vec{k}_1$ to the state $\vec{k}_1'$ gives rise to local oscillations of electron density of frequency $\omega = (\overline{\varepsilon}_{\vec{k}1} - \overline{\varepsilon}_{\vec{k}1'})/\hbar$, where $\omega < \omega_{\mathrm{D}}$ (Debye frequecy).

To enable an electron to go from the state $\vec{k}_1$ to the state $\vec{k}_1'$, the latter must be free (Pauli principle) that is possible only in the vicinity of the Fermi surface.

Phonon-mediated interaction between electrons



Fermi sphere

In the BSC model, only those electrons are mutually attracted which occupy the states within a narrow $2\Delta k$ layer near the Fermi surface.

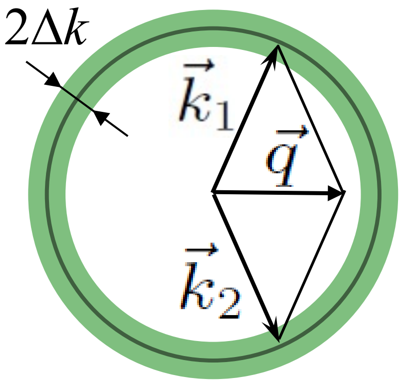
$$\frac{\Delta k}{k_\mathrm{F}} \sim \frac{\hbar\omega_\mathrm{D}}{\varepsilon_\mathrm{F}}\,, \quad \varepsilon_\mathrm{F} = \frac{\hbar^2 k_\mathrm{F}^2}{2m}\,.$$

Matrix element of the electron interaction

$$V_{\vec{k}\vec{k}'} = \begin{cases} -V, & |\bar{\varepsilon}_{\vec{k}} - \varepsilon_\mathrm{F}| \le \hbar\omega_\mathrm{D}, \quad |\bar{\varepsilon}_{\vec{k}'} - \varepsilon_\mathrm{F}| \le \hbar\omega_\mathrm{D}, \\ 0, & |\bar{\varepsilon}_{\vec{k}} - \varepsilon_\mathrm{F}| > \hbar\omega_\mathrm{D}, \quad |\bar{\varepsilon}_{\vec{k}'} - \varepsilon_\mathrm{F}| > \hbar\omega_\mathrm{D}. \end{cases}$$

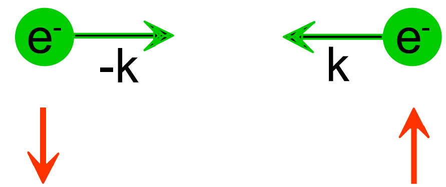
Interacting electrons

Assume $T = 0$

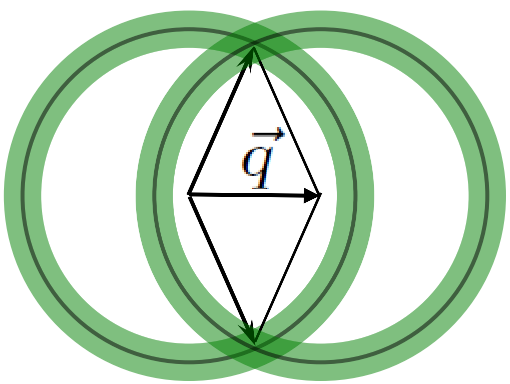


$$\vec{k}_1 + \vec{k}_2 = \vec{k}_1' + \vec{k}_2'$$

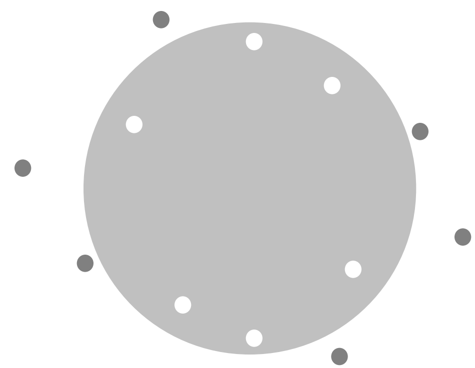
$$\vec{k}_1 + \vec{k}_2 = \vec{q}$$



Maximum number of interacting electrons for $q = 0$



All states within a band of width $\sim 2\hbar\omega_{\mathrm{D}}$ near the Fermi surface will contribute to the reduction of the average energy.



lowest energy state

Ground state of a superconductor

$v_{\vec{k}}^2$ is the probability that the state $(\vec{k}, \ -\vec{k})$ is occupied.

$u_{\vec{k}}^2 = 1 - v_{\vec{k}}^2$ is the probability that the state $(\vec{k}, \ -\vec{k})$ is free.

The amplitude of the state with all states $(\vec{k}, \ -\vec{k})$ occupied and all states $(\vec{k}', \ -\vec{k}')$ free is

$$a_n = \left[v_{\vec{k}}^2 (1 - v_{\vec{k}'}^2) \right]^{1/2}$$

The amplitude of the state with all states $(\vec{k}, \ -\vec{k})$ free and all states $(\vec{k}', \ -\vec{k}')$ occupied is

$$a_m = v_{\vec{k}'} u_{\vec{k}} \ .$$

We can write the total energy of a superconductor as

$$E_{\mathrm{s}} = \sum_{\vec{k}} 2\varepsilon_{\vec{k}} v_{\vec{k}}^2 + \sum_{\vec{k},\vec{k}'} V_{\vec{k}\vec{k}'} v_{\vec{k}'} u_{\vec{k}} v_{\vec{k}} u_{\vec{k}'} \ .$$

Total energy

$$E_s = \sum_{\vec{k}} 2\varepsilon_{\vec{k}} v_{\vec{k}}^2 + \sum_{\vec{k}.\vec{k}'} V_{\vec{k}\vec{k}'} v_{\vec{k}'} u_{\vec{k}} v_{\vec{k}} u_{\vec{k}'}$$

The kinetic energy of an electron measured from the Fermi level

$$\varepsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m} - \frac{\hbar^2 k_F^2}{2m} = \overline{\varepsilon}_{\vec{k}} - \varepsilon_F \ .$$

The mean potential energy of electron interaction with the matrix element $V_{\vec{k}\vec{k}'}$

Let us search for a minimum of the total energy E_s versus $v_{\vec{k}}^2$.

$$\frac{\partial E_s}{\partial v_{\vec{k}}^2} = 0 \quad \Rightarrow \quad 2\varepsilon_{\vec{k}} - V \frac{1 - 2v_{\vec{k}}^2}{v_{\vec{k}} u_{\vec{k}}} \sum_{\vec{k}'}{}' v_{\vec{k}'} u_{\vec{k}'} = 0$$

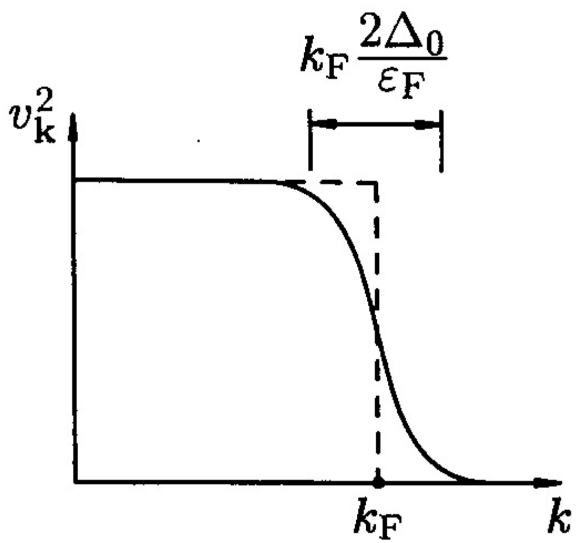
$$\Rightarrow \quad \frac{v_{\vec{k}} u_{\vec{k}}}{1 - 2v_{\vec{k}}^2} = \frac{\Delta_0}{2\varepsilon_{\vec{k}}}$$, where $$\Delta_0 = V \sum_{\vec{k}}{}' v_{\vec{k}} u_{\vec{k}} \ .$$

Electron distribution in the ground state

Using $u_{\vec{k}}^2 = 1 - v_{\vec{k}}^2$ we get a quadratic equation $v_{\vec{k}}^4 - v_{\vec{k}}^2 + \frac{\Delta_0^2}{4E_{\vec{k}}^2} = 0$,

where $E_{\vec{k}} = \sqrt{\varepsilon_{\vec{k}}^2 + \Delta_0^2}$. Since at $\vec{k} \to 0$ we have $v_{\vec{k}}^2 \to 1$ and $\varepsilon_{\vec{k}} \to -E_{\vec{k}}$

$$\Rightarrow \quad v_{\vec{k}}^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_{\vec{k}}}{E_{\vec{k}}}\right) \quad \text{and} \quad u_{\vec{k}}^2 = \frac{1}{2}\left(1 + \frac{\varepsilon_{\vec{k}}}{E_{\vec{k}}}\right) .$$



Thus, even at $T=0$, the ground state corresponds to the „smeared“ electron distribution around the Fermi energy !

Calculation of Δ_0

$$\Delta_0 = V \sum_{\vec{k}}{}' v_{\vec{k}} u_{\vec{k}} = V \sum_{\vec{k}}{}' \left[\frac{1}{2}\left(1 - \frac{\varepsilon_{\vec{k}}}{E_{\vec{k}}}\right) \frac{1}{2}\left(1 + \frac{\varepsilon_{\vec{k}}}{E_{\vec{k}}}\right)\right]^{1/2} =$$

$$= \frac{V}{2} \sum_{\vec{k}}{}' \left(\frac{E_{\vec{k}}^2 - \varepsilon_{\vec{k}}^2}{E_{\vec{k}}^2}\right)^{1/2} = \frac{V\Delta_0}{2} \sum_{\vec{k}}{}' \left(\varepsilon_{\vec{k}}^2 + \Delta_0^2\right)^{-1/2} .$$

Thus we get the equation for Δ_0 :

$$1 = \frac{V}{2} \sum_{\vec{k}}{}' \left(\varepsilon_{\vec{k}}^2 + \Delta_0^2\right)^{-1/2} .$$

Using $\sum_{\vec{k}}{}' \ldots = \int_{-\hbar\omega_D}^{\hbar\omega_D} \ldots N(\varepsilon)\, d\varepsilon$ with $N(\varepsilon)$ being the density of states

$$1 = \frac{N(0)\,V}{2} \int_{-\hbar\omega_D}^{\hbar\omega_D} \left(\varepsilon^2 + \Delta_0^2\right)^{-1/2} d\varepsilon = N(0)\,V \,\mathrm{arcsinh}\left(\frac{\hbar\omega_D}{\Delta_0}\right)$$

Value of Δ_0

From above equation we get

$$\frac{\hbar\omega_D}{\Delta_0} = \sinh\left(\frac{1}{N(0)\,V}\right) \quad .$$

For the majority of superconductors $N(0)\,V \leq 0.3$

and thus $\Delta_0 \simeq 2\hbar\omega_D \exp\left(-\frac{1}{N(0)\,V}\right) \quad .$

With $\hbar\omega_D \sim 100$ K we get an estimate $\Delta_0 \sim 4$ K.

Ground-state energy

Ground-state energy is $W = E_\mathrm{s} - E_\mathrm{n} = E_\mathrm{s} - \sum_{k<k_\mathrm{F}} 2\varepsilon_{\vec{k}}$.

$$W = \sum_{k<k_\mathrm{F}} 2\varepsilon_{\vec{k}}\,(v_{\vec{k}}^2 - 1) + \sum_{k>k_\mathrm{F}} 2\varepsilon_{\vec{k}} v_{\vec{k}}^2 - V \sum_{\vec{k}\,\vec{k}'}{}' v_{\vec{k}} u_{\vec{k}} v_{\vec{k}'} u_{\vec{k}'} =$$

$$= \sum_{k<k_\mathrm{F}} |\varepsilon_{\vec{k}}| \left(1 - \frac{|\varepsilon_{\vec{k}}|}{E_{\vec{k}}}\right) + \sum_{k>k_\mathrm{F}} \varepsilon_{\vec{k}} \left(1 - \frac{\varepsilon_{\vec{k}}}{E_{\vec{k}}}\right) - V \sum_{\vec{k}\,\vec{k}'}{}' v_{\vec{k}} u_{\vec{k}} v_{\vec{k}'} u_{\vec{k}'}$$

from definition of Δ_0 we have $\sum_{\vec{k}\,\vec{k}'}{}' v_{\vec{k}} u_{\vec{k}} v_{\vec{k}'} u_{\vec{k}'} = \frac{\Delta_0^2}{V^2}$.

$$W = 2 \sum_{k>k_\mathrm{F}} \varepsilon_{\vec{k}} \left(1 - \frac{\varepsilon_{\vec{k}}}{E_{\vec{k}}}\right) - \frac{\Delta_0^2}{V} = 2N(0) \int_0^{\hbar\omega_\mathrm{D}} \varepsilon \left(1 - \frac{\varepsilon}{\sqrt{\varepsilon^2 + \Delta_0^2}}\right) \mathrm{d}\varepsilon - \frac{\Delta_0^2}{V} .$$

Ground-state energy

Integration yields
$$W = N(0)\,\Delta_0^2 \left\{ \left(\frac{\hbar\omega_D}{\Delta_0}\right)^2 - \right.$$
$$\left. - \frac{\hbar\omega_D}{\Delta_0}\left[1 + \left(\frac{\hbar\omega_D}{\Delta_0}\right)^2\right]^{1/2} + \mathrm{arcsinh}\frac{\hbar\omega_D}{\Delta_0}\right\} - \frac{\Delta_0^2}{V}\,.$$

Knowing $\hbar\omega_D \gg \Delta_0$ we get finally $W = -\frac{1}{2}N(0)\,\Delta_0^2\,.$

The difference in energy between the superconducting and the normal state is negative, that is, the superconducting state is more favorable energetically.