Mean-field description of Superconducting state

We consider $T=0$ limit

$$\hat{H} = \int \left[-\psi^+_\alpha \frac{\nabla^2}{2m} \psi_\alpha + \frac{\lambda}{2} \psi^+_\alpha \psi^+_\beta \psi_\beta \psi_\alpha \right] d^3 r$$

Let us derive the Eqs. of motion for ψ-operators (Home task)

$$\left(i\frac{\partial}{\partial t} + \frac{\nabla^2}{2m} \right) \psi_\alpha - \lambda \left(\psi^+_\gamma \psi_\gamma \right) \psi_\alpha = 0$$

$$\left(i\frac{\partial}{\partial t} - \frac{\nabla^2}{2m} \right) \psi^+_\alpha + \lambda \psi^+_\alpha \left(\psi^+_\gamma \psi_\gamma \right) = 0$$

Then we can obtain an Equation for the Green's function

$$G_{\alpha\beta}(x, x') = -i \langle T \psi_\alpha(x) \psi^+_\beta(x') \rangle$$

$$\left(i\frac{\partial}{\partial t} + \frac{\nabla^2}{2m} \right) G_{\alpha\beta}(x, x') + i\lambda \langle T \psi^+_\gamma \psi_\gamma \psi_\alpha(x) \psi^+_\beta(x') \rangle = \delta(x - x')$$

$$\langle T \psi^+_\gamma \psi_\gamma \psi_\alpha(x) \psi^+_\beta(x') \rangle = -\langle T \psi_\gamma \psi^+_\gamma \rangle \langle T \psi_\alpha(x) \psi^+_\beta(x') \rangle +$$

$$+ \langle T \psi_\alpha(x) \psi^+_\gamma(x) \rangle \langle T \psi_\gamma(x) \psi^+_\beta(x') \rangle + \underbrace{\langle T \psi^+_\gamma \psi^+_\beta(x') \rangle \langle \psi_\gamma \psi_\alpha \rangle}_{\text{anomalous averages}} +$$

+ vertex corrections

The presence of anomalous averages is the consequence of the non-trivial ground state. It consists of the superposition of states with different particle number.

$$i F_{\alpha\beta}(x, x') = + \langle T \psi_\alpha(x) \psi_\beta(x') \rangle$$

$$i F^+_{\alpha\beta}(x, x') = + \langle T \psi^+_\alpha(x) \psi^+_\beta(x') \rangle$$

$\Delta(r) = -i\lambda F_{\alpha\beta}(+0) = \lambda \langle \psi_\alpha(x) \psi_\beta(x) \rangle$ is called the order parameter or gap function

The reconstruction of a ground state is described by the presence of order parameter.

Symmetry properties of the order parameter

The permutation of field operators yields

$$iF_{\beta\alpha}(x',x) = +\langle T\psi_\beta(x')\psi_\alpha(x)\rangle = -\langle T\psi_\alpha(x)\psi_\beta(x')\rangle = -iF_{\alpha\beta}(x,x')$$

Anomalous function is antisymmetric by all indices.

Thus for the order parameter we get

$$\Delta_{\alpha\beta}(X) = -\Delta_{\beta\alpha}(X) = \Delta\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \Delta\, i\sigma_y$$

Hence $\quad F_{\alpha\beta}(x_1 x_2) = F(x_1 x_2)\, i\sigma_y$

Sometimes F has components which do not appear in Δ: $F(t=0)=0$. These components correspond to odd-freq. pairing

The physical meaning of the $F(x,x)$ is the wave function of Cooper pairs. Althoug $\Delta \sim F(x,x)$ but Δ is not the wave function since it contains the coupling λ.

When $\lambda = 0$ the Cooper pairs can penetrate from the region with $\lambda \neq 0$. This is proximity effect.

The spin structure of Cooper pair

The spin basis $\quad F, G \sim \begin{pmatrix} \uparrow\uparrow & \uparrow\downarrow \\ \downarrow\uparrow & \downarrow\downarrow \end{pmatrix}$ Hence $\psi \sim (\uparrow\downarrow - \downarrow\uparrow)$ is a singlet state

Gorkov equations

$$\begin{cases} \left(i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} + \mu\right) G(x_1 x_2) + \Delta(x_1) F^+(x_1 x_2) = \delta(x_1 - x_2) \\ \left(i\frac{\partial}{\partial t_1} - \frac{\nabla_1^2}{2m} - \mu\right) F^+(x_1 x_2) + \Delta^*(x_1) G(x_1 x_2) = 0 \end{cases}$$

similarly for the functions $\quad \bar{G}(x_1 x_2) = +i\langle T\psi^+(x_1)\psi(x_2)\rangle$

$$F^+ = \langle T\psi^+(x_1)\psi^+(x_2)\rangle$$

$$\begin{cases} -\left(i\frac{\partial}{\partial t_1} - \frac{\nabla_1^2}{2m} - \mu\right)\bar{G}(x_1 x_2) + \Delta^*(x_1) F(x_1 x_2) = \delta(x_1 - x_2) \\ \left(i\frac{\partial}{\partial t_1} - \frac{\nabla_1^2}{2m} - \mu\right) F(x_1 x_2) + \Delta(x_1)\bar{G}(x_1 x_2) = 0 \end{cases}$$

The system can be written in a matrix form in the Gorkov-Nambu space

$$\hat{G}(x_1, x_2) = \begin{pmatrix} G(x_1, x_2) & F(x_1, x_2) \\ -F^+(x_1, x_2) & \bar{G}(x_1, x_2) \end{pmatrix}$$

$$\hat{G}^{-1} = i\tau_3 \frac{\partial}{\partial t} - \hat{H}$$

$$\hat{H} = \begin{pmatrix} -\frac{\nabla^2}{2m} - \mu & +\Delta \\ -\Delta^* & -\frac{\nabla^2}{2m} - \mu \end{pmatrix}$$

$$G_0^{-1} G = \hat{I}\, \delta(x_1 - x_2)$$

Gauge invariance

Suppose that we multiply all wave functions by the same phase factor $e^{i\varphi}$, then field operators transform like $\psi \to \psi e^{i\varphi}$. It is easy to see that the normal propagators are invariant with respect to the $U(1)$ transform $iG = \langle T\psi\psi^+\rangle$. On the other hand the anomalous part is not $iF = \langle T\psi\psi\rangle \to e^{2i\varphi}\langle T\psi\psi\rangle$

This corresponds to the nature of superconducting transition which breaks $U(1)$ symmetry. When the phase φ does not depend on coordinates this is global $U(1)$ transform. What if $\varphi = \varphi(x)$? – the local transform? Gorkov Eqs. should be gauge-invariant, hence we have covariant derivative

$$\hat{H} = \begin{pmatrix} -\frac{1}{2m}\left(\nabla - \frac{ie}{c}A\right)^2 - \mu & +\Delta \\ -\Delta^* & -\frac{1}{2m}\left(\nabla + \frac{ie}{c}A\right)^2 - \mu \end{pmatrix}$$

Quasiparticle spectrum

The poles of GF determine the spectrum of quasiparticles

Let us switch to the frequency representation

$$G(x_1, x_2) = G(r_1, r_2) e^{-i\varepsilon(t_1 - t_2)}$$

Then $\quad G^{-1} = \tau_3 \varepsilon - \hat{H}$

Bogolubov - de Gennes equations.

- Solving the Gorkov equations we find the GF which poles determine the quasiparticle spectrum in a superconductor. It is quite instructive to formulate the spectral problem in terms of the quasiparticle wave functions

- Let us consider the following two-component wave function

$$\varphi = \begin{pmatrix} u \\ +v \end{pmatrix}, \quad \begin{cases} H_0 u + \Delta v = \varepsilon u \\ +H_0^* v + \Delta^* u = \varepsilon v \end{cases}, \quad \text{where } \hat{H}_0 = -\frac{1}{2m}\left(\nabla - \frac{ie}{2c}A\right)^2$$

We can determine the GF for this system of two coupled differential equations. Consider the set of eigenfunctions
1) $\sum_n \varphi_n(r_1)\varphi_n^+(r_2) = \delta(r_1-r_2)$ $\int(\varphi_i^+ \varphi_n)\,dr = \delta_{ni}$

$$G(r_1 r_2) = \sum_n \frac{\tau_3 \varphi_n(r_1)\varphi_n^+(r_2)}{\varepsilon - \varepsilon_n}, \quad \text{where } \varphi_n^+ = (u_n^+, v_n^+) \quad \varphi_n = \begin{pmatrix} u_n \\ +v_n \end{pmatrix}$$

so that
$$\varphi_n(r_1)\varphi_n^+(r_2) = \begin{pmatrix} u_n(r_1)u_n^*(r_2) & +u_n(r_1)v_n^*(r_2) \\ +v_n(r_1)u_n^*(r_2) & v_n(r_1)v_n^*(r_2) \end{pmatrix}$$

Then
$$\hat{H}(r_1)\varphi_n(r_1)\varphi_n^+(r_2) = \begin{pmatrix} H_0 & +\Delta \\ -\Delta^* & +H_0^* \end{pmatrix}\begin{pmatrix} u_n(r_1)u_n^*(r_2) & u_n(r_1)v_n^*(r_2) \\ v_n(r_1)u_n^*(r_2) & v_n(r_1)v_n^*(r_2) \end{pmatrix} =$$

$$= \begin{pmatrix} \left(H_0(r_1)u_n(r_1) + \Delta(r_1)v_n(r_1)\right)u_n^*(r_2) & \left(H_0(r_1)u_n(r_1) + \Delta(r_1)v_n(r_1)\right)v_n^*(r_2) \\ \left(+H_0^* v_n(r_1) - \Delta^* u_n(r_1)\right)u_n^*(r_2) & \left(+H_0^*(r_1)v_n(r_1) + \Delta^*(r_1)u_n(r_1)\right)v_n^*(r_2) \end{pmatrix} =$$

$$= \begin{pmatrix} \varepsilon_n u_n(r_1)u_n^*(r_2) & +\varepsilon_n u_n(r_1)v_n^*(r_2) \\ -\varepsilon_n v_n(r_1)u_n^*(r_2) & -\varepsilon_n v_n(r_1)v_n^*(r_2) \end{pmatrix} = \varepsilon_n \tau_3 \, \varphi_n(r_1)\varphi_n^+(r_2)$$

$$\left(\varepsilon\tau_3 - H(r_1)\right) G(r_1, r_2) = \sum_n \varphi_n(r_1)\varphi_n^+(r_2) = \delta(r_1 - r_2)$$

This equation coincides with Gorkov eqs.

We can solve the BdG system which resembles the Schroedinger equation but with non-diagonal order parameter potential.

<u>Symmetry</u>. BdG eq. has symmetry
$$\varepsilon \to -\varepsilon, \quad u \to -v^*, \quad v \to u^*$$

The solution of Gorkov's equation is not uniquely defined

Indeed formaly if $G(r_1, r_2, \varepsilon)$ is a solution we can add (5)

$\hat{G} = G + \sum d_n \delta(\varepsilon - \varepsilon_n)\, \tau_3 \varphi_n(r_1) \varphi_n^+(r_2)$ is also a solution

Indeed

$$(\varepsilon\tau_3 - H)\tilde{G} = (\varepsilon\tau_3 - H)G + \underbrace{\sum d_n (\varepsilon - \varepsilon_n)\delta(\varepsilon - \varepsilon_n)\varphi_n(r_1)\varphi_n^+(r_2)}_{=0}$$

Adding different δ-functional terms we can change the analytical properties of the GF.

For example, retarded and advanced functions are

$$G^{R(A)} = \sum_n \frac{\tau_3 \varphi_n(r_1) \varphi_n^+(r_2)}{\varepsilon - \varepsilon_n \pm i\delta}$$

Causal:

$$T=0 \quad G = \sum_n \frac{\tau_3 \varphi_n(r_1) \varphi_n^+(r_2)}{\varepsilon - \varepsilon_n + i\delta\, \mathrm{sgn}\, \varepsilon}$$

It becomes more tricky at finite temperatures because we do not know yet the analytical properties of the Causal GF at $T \neq 0$. That is we do not know what coefficient d_n should be chosen.

At finite temperatures d_n contain information about the equilibrium population of quasiparticle states.

It is possible to avoid this problem by using analytical continuation of the spectral functions $G^{R,A}$ into the complex plane and introducing the so-called temperature GF or Matsubara GF. In the time domain it means that we introduce the imaginary time using the so-called Wick rotation

Properties of BdG equations.

1. Physical meaning of components u, v

Consider the field operator

Bogolubov transform

$$\gamma_{n\uparrow} = \int d^3r \left(u_n^*(r)\,\psi_\uparrow(r) - v_n^*(r)\,\psi_\downarrow^+(r) \right)$$

$$\gamma_{n\downarrow}^+ = \int d^3r \left(u_n(r)\,\psi_\downarrow^+(r) + v_n(r)\,\psi_\uparrow(r) \right)$$

They satisfy fermi algebra

$$\{\gamma_{n,\alpha}\, \gamma_{n,\beta}\} = 0$$

$$\{\gamma_{n\alpha}, \gamma_{n'\beta}^+\} = \delta_{\alpha\beta}\, \delta_{nn'}$$

Bogolubov transform diagonalizes mean-field Ham-n

$$H = H_0 + \int \left(\Delta(r)\, \psi_\uparrow^+ \psi_\downarrow^+ + h.c. \right) d^3r$$

They describe fermionic quasiparticles in superconductors sometimes they are called bogolons

From the definition one can see that they consist of superposition of electron and hole. Hence they have charge different from electrons

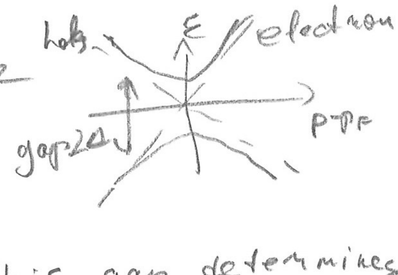
$$Q_n^* = e\left(\overline{|u_n|^2} - \overline{|v_n|^2} \right)$$

But spin is the same

$$S_n^* = \frac{1}{2}\left(\overline{|u_n|^2} + \overline{|v_n|^2} \right) = \frac{1}{2}$$

2. Consider the homogeneous case $\Delta(r) = \text{const}$

$$\begin{cases} (\xi_p - \varepsilon)\, u + \Delta v = 0 \\ -(\xi_p + \varepsilon)\, v + \Delta u = 0 \end{cases} \Rightarrow \varepsilon^2 = \xi_p^2 + \Delta^2$$



There are no quasiparticles with $|\varepsilon| < \Delta$. This gap determines superconducting properties, because the electrons can flow without scattering.

3. Andreev reflection