§3 Superconductivity

3.1 Origin of the attractive interaction

external density $\delta\rho$

screening charge ρ_{ind}

Dynamics of ions

$\rho_{tot} = \rho_{ind} + \delta\rho$ ~~$\int_\varepsilon$~~ $\frac{\delta\rho}{\varepsilon} = \rho_{tot}$ $\varepsilon = \frac{\delta\rho}{\rho_{tot}}$

$\rho_{ind} = \rho_{e,ind} + \rho_{i,ind}$

Poisson eq. $\nabla^2 V = -\frac{1}{\varepsilon_0}(\delta\rho + \rho_{i,ind} + \rho_e)$

Equation of motion for ions in presence of electric field

$\vec{E} = -\nabla V$

n ← density of atoms

$M\vec{V}\cdot\frac{d\vec{j}_i}{dt} = n Z e^2 \vec{V}\cdot\vec{E}$ equation of motion

$\partial_t^2 \rho_i + \partial_t \vec{V}\cdot\vec{j}_i = 0 \Rightarrow \partial_t \vec{V}\cdot\vec{j} = -\partial_t^2\rho$

"small motion approximation" $M\,\partial_t j_i = n Z e^2 E$

$M\partial_t^2\rho_i + nZe^2\vec{V}\cdot(-\vec{V}\varphi) = 0$

$\Rightarrow \partial_t^2\rho_i = \frac{nZe^2}{M}\Delta V$

$\Rightarrow \omega^2\rho_i(q,\omega) = \omega_i^2\underbrace{[\rho_i + \rho_e + \delta\rho]}_{\rho_{tot}}$

$\omega_i^2 = \frac{nZe^2}{\varepsilon_0 M}$

Next need ρ_{ind} for an external $\delta\rho$

density response gives

$$\delta\rho_{ind} = \Pi_0 V_{tot}$$

$$= \Pi_0 \rho U(q) \rho_{tot}$$

$$\left(= \Pi V_{ext} \right.$$
$$\left. = \Pi U(q) \delta\rho \right)$$

Need ρ_{ind} as function of ρ_{tot}

$$\rho_{ind} = \Pi_0 U(q) \rho_{tot}$$

$$\Rightarrow \quad \rho_{ind} = \frac{\omega_p^2}{\omega^2} \rho_{tot}$$

$$\Rightarrow \quad \rho_{ind} + \rho_{ind} = \left(\frac{\omega_p^2}{\omega^2} + \Pi_0 U(q) \right) \rho_{tot}$$

$$\Rightarrow \quad \rho_{ind} = \left[\frac{\omega_p^2}{\omega^2} + \Pi_0 U(q) \right] \left(\rho_{ind} + \delta\rho \right)$$

$$\varepsilon = \frac{\delta\rho}{\rho_{ind} + \delta\rho} \quad \text{just reminder}$$

$$\Rightarrow \quad \rho_{ind} \left[1 - \frac{\omega_p^2}{\omega^2} - \Pi_0 U(q) \right] = \left[\frac{\omega_p^2}{\omega^2} + \Pi_0 U(q) \right] \delta\rho$$

$$\Rightarrow \quad \Rightarrow \left(\rho_{ind} + \delta\rho \right) \left[1 - \frac{\omega_p^2}{\omega^2} - \Pi_0 U(q) \right] = \delta\rho = \left[\frac{\omega_p^2}{\omega^2} + \Pi_0 V + 1 \right] \rho_{tot}$$

$$\Rightarrow \quad \varepsilon = \frac{\rho_{ind}}{\rho_{ind} + \rho} = \frac{1}{1 - \frac{\omega_i^2}{\omega^2} - \Pi_0 U(q)}$$

$$= \frac{1}{\varepsilon}$$

$$U(q) = \frac{e^2}{\varepsilon_0 q^2}$$

$$\Rightarrow \quad \varepsilon = 1 - \frac{\omega_i^2}{\omega^2} + \frac{\rho_i e^2}{\varepsilon_0 q^2}$$

$$= \frac{\omega^2 q^2 + q^2 \omega_i^2 + q^2/\lambda^2 \omega^2}{\omega^2 q^2}$$

$$\boxed{\varepsilon(q,\omega) = \frac{\omega^2\left(\frac{1}{\lambda^2} + q^2\right) - \omega_i^2 q^2}{\omega^2 q^2}}$$

spontaneous modes of vibration for $\rho_{ind} = 0$ or $\varepsilon = 0$

$$\Rightarrow \quad \omega_q^2 = \omega_i^2 \frac{q^2}{\frac{1}{\lambda^2} + q^2}$$

$\Rightarrow$ for small q we find $\omega_q \xrightarrow{\omega} \omega_i \lambda q$

gives realistic estimate for sound velocity in a metal if z is close to the valency of the metal.

In terms of ω_q, we can rewrite

$$\frac{1}{\varepsilon} = \frac{\omega^2 q^2}{\omega^2\left(q^2 + \frac{1}{\lambda^2}\right) - \omega_i^2 q^2}$$

$=$

Check again the decomposition using the exact plasmon frequency $\omega_q^2 = \omega_i^2 \dfrac{q^2}{\frac{1}{\Lambda^2} + q^2}$

$$\frac{1}{\varepsilon(q,\omega)} = \frac{q^2}{q^2+\Lambda^{-2}}\left[1 + \frac{\omega_q^2}{\omega^2 - \omega_q^2}\right]$$

$$= \frac{q^2}{q^2+\Lambda_1^{-2}}\left[\frac{\omega^2 - \omega_q^2 + q^2}{\omega^2 - \omega_q^2}\right.$$

$$= \frac{q^2\omega^2}{q^2+\Lambda^{-2}\left(\omega^2 - \dfrac{\omega_i^2 q^2}{\frac{1}{\Lambda^2}+q^2}\right)}$$

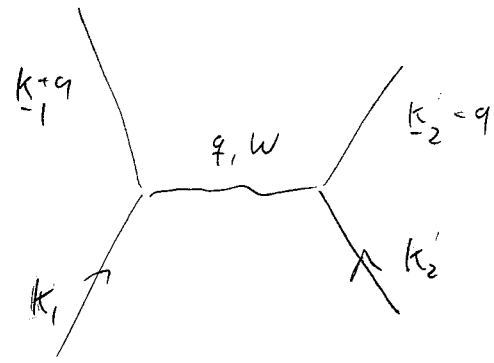
$$= \frac{q^2\omega^2}{\left(q^2+\Lambda^{-2}\right)\omega^2 - \omega_i^2 q^2}$$

$$U_{eff} = \frac{U(q)}{\varepsilon(q,\omega)} = \frac{e^2}{\varepsilon_0 q^2} \cdot \frac{q^2+\Lambda^{-2}}{\omega^2}\left[1 + \frac{\omega_q^2}{\omega^2 - \omega_q^2}\right]$$

$$U_{eff}(q) = \frac{e^2}{\varepsilon_0\left(q^2+\Lambda^{-2}\right)}\left[1 + \frac{\omega_q^2}{\omega^2 - \omega_q^2}\right]$$

is attractive for $|\omega| < \omega_q$

Interpretation of $V(q,\omega)$



For q on the order of k_F, we find $\omega_q \simeq \omega_i \simeq \omega_D$

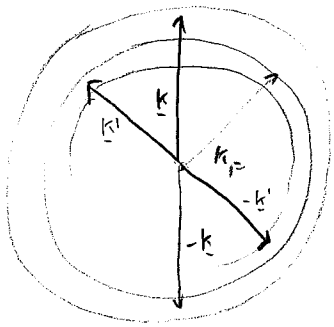
(Einstein model of phonons)

Interpret ω as the energy transf. for attractive interaction $\Rightarrow \left(|\xi_{k+q} - \xi_k|/\hbar\right) \leq \hbar\omega_D$

and consider two electrons with zero center of mass momentum, i.e. $\underline{k}' = -\underline{k}$

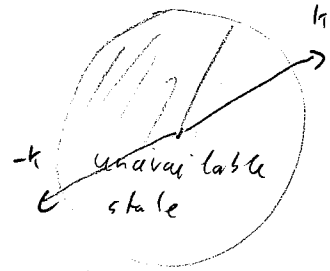
In order to make calculation feasible, we consider the following model interaction (setting $\underline{k}_1 = \underline{k}$, $\underline{k}_2 = -\underline{k}$, $\underline{k}_1 + q = \underline{k}'$, $\underline{k}_2 - q = -\underline{k}'$)

$$V_{kk'} = \begin{cases} -\frac{V}{\Omega} & \text{if } |\xi_k| \leq \hbar\omega_D, \ |\xi_{k'}| \leq \hbar\omega_D \\ 0 & \text{otherwise} \end{cases}$$



3.2 Cooper Pairs

Remark – the existence of bound states in ~~not~~ weakly attractive potentials: in 1d/2d for any potential strength a (logarithmically) bound state exists, in 3d a minimum potential strength is needed. This is different in the presence of a Fermi surface



Ansatz for wave function $\Psi(\underline{r}_1, \underline{r}_2) = e^{i \underline{Q} \cdot \frac{\underline{r}_1 + \underline{r}_2}{2}} \varphi(\underline{r}_1 - \underline{r}_2) \chi_{\text{singlet}}$

χ_{singlet} is antisymmetric $\Rightarrow$ $\varphi(\underline{r} - \underline{r}')$ is symmetric

Fourier representation $\varphi(\underline{r} - \underline{r}') = \sum_{\underline{k}} g(\underline{k}) e^{i \underline{k} \cdot (\underline{r} - \underline{r}')}$

two-electron Schrödinger equation

$$-\frac{\hbar^2}{2m} \left(\nabla_1^2 + \nabla_2^2 \right) \Psi(\underline{r}_1, \underline{r}_2) + V(|\underline{r}_1 - \underline{r}_2|) \Psi = \left(E + \frac{\hbar^2 K_F^2}{m} \right) \Psi$$

$$\Rightarrow \frac{\hbar^2}{m} k^2 g(\underline{k}) + \sum_{\underline{k}'} g(\underline{k}') V_{\underline{k}\underline{k}'} = (E + 2E_F) g(\underline{k}) \quad (*)$$

$$V_{\underline{k}\underline{k}'} = \frac{1}{\Omega} \int V(\underline{r}) e^{i (\underline{k} - \underline{k}') \cdot \underline{r}} \, d\underline{r}$$

For our model interaction $\sum_{\underline{k}'}$ extends over $\underline{k}'$ such that

$$E_F < \frac{\hbar^2 k'^2}{2m} \leq E_F + \hbar\omega_D$$

Introduce $G' = -\frac{V}{\Omega} \sum_{\underline{k}'} g(\underline{k}')$ (independent of $\underline{k}'$)

$\Rightarrow$ (*) becomes $\left(-\frac{\hbar^2 k^2}{m} + E + 2E_F\right) g(k) = G'$

$$\Rightarrow g(\underline{k}) = \frac{G'}{1 - \frac{\hbar^2 k^2}{m} + E + 2E_F}$$

This gives rise to the self-consistency condition

$$1 = \frac{V}{\Omega} \sum_{\underline{k}'} \frac{1}{\frac{\hbar^2 \underline{k}'^2}{2m} - E - 2E_F}$$

We now set $\xi' = \frac{\hbar^2 \underline{k}'^2}{2m} - E_F$ and use

$\frac{1}{\Omega} \sum_{\underline{k}'} \rightarrow \int d\xi' \rho_F$, the condition becomes

$$1 = V \int_0^{\hbar\omega_D} \rho_F \frac{1}{2\xi' - E} d\xi'$$

$$= \frac{1}{2} V \rho_F \int_0^{\hbar\omega_D} \frac{1}{\xi' - E/2} d\xi'$$

$E < 0$ for bound state $|E| \ll \hbar\omega_D$ for weak interaction

$$= \frac{1}{2} V \rho_F \left[\ln\left|\hbar\omega_D - \frac{E}{2}\right| - \ln\left|-\frac{E}{2}\right| \right] = \frac{1}{2} V \rho_F \ln \frac{E - 2\hbar\omega_D}{E}$$

$$1 \approx \frac{1}{2} V g_F \ln \frac{2\hbar\omega_D}{-E}$$

$$\Rightarrow \quad \frac{2\hbar\omega_D}{-E} = e^{\frac{2}{V g_F}}$$

$$\boxed{E = -2\hbar\omega_D \, e^{-\frac{2}{V g_F}}}$$

3.3 Many-particle ground state and elementary excitations

A natural generalization of the pair wave function $\varphi(\underline{r}_1 - \underline{r}_2)$ to N electrons is

$$\Phi_N(\underline{r}_1, \underline{r}_2, \ldots, \underline{r}_N) = \varphi(\underline{r}_1 - \underline{r}_2)\, \varphi(\underline{r}_3 - \underline{r}_4) \ldots \varphi(\underline{r}_{N-1} - \underline{r}_N)$$

Remarks: i) Φ_N can only be constructed for an even number N of electrons. For odd N, one electron would need to be placed in a separate state. However for $N \sim 10^{23}$ this will only give rise to effects of order $\frac{1}{N}$ and will be unimportant.

ii) for electron spins, we select singlet states for each pair

iii) Φ_N must be anti-symmetrized

$$\Phi_N = A\, \varphi(\underline{r}_1 - \underline{r}_2)\, \chi_{\text{singlet},12} \ldots \varphi(\underline{r}_{N-1} - \underline{r}_N)\, \chi_{\text{singlet},N-1\,N}$$

Although we can explicitly write down ψ_N, it would be rather difficult to do actual calculations with it.

Computations become considerably easier in a second quantized notation, which automatically takes care of antisymmetrization. In momentum space, the pair two-particle paired state can be represented as

$$\sum_k g(k)\, a^+_{k\uparrow}\, a^+_{-k\downarrow} |0\rangle$$

Similarly, we can write down an N-particle state as

$$|\psi_N\rangle = \sum_{k_1} \cdots \sum_{k_{N/2}} g(k_1) \cdots g(k_{N/2})\, a^+_{k_1\uparrow} a^+_{-k_1\downarrow} \cdots a^+_{k_{N/2}\uparrow} a^+_{-k_{N/2}\downarrow} |0\rangle$$

This is still quite difficult to deal with. We consider instead a product over all ~~occupied~~ states

$$|\tilde{\psi}\rangle = \frac{1}{N} \prod_k \left(1 + g_k\, a^+_{k\uparrow} a^+_{-k\downarrow}\right)|0\rangle$$

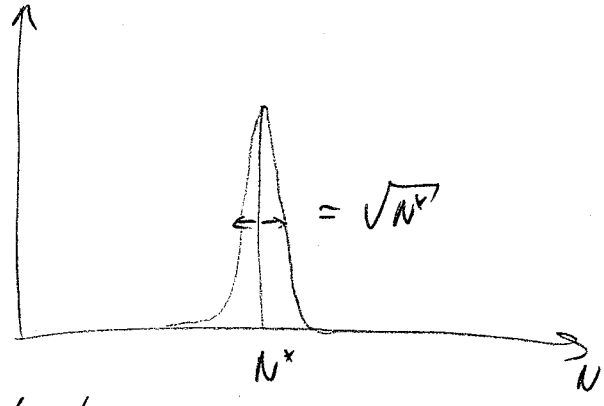
One sees that $|\psi_N\rangle$ is the part of $|\tilde{\psi}\rangle$ which has exactly N creation operators acting on the vacuum. We now incorporate the normalization factor into the wavefunction as $|\tilde{\psi}\rangle = \prod_k \left(u_k + v_k\, a^+_{k\uparrow} a^+_{-k\downarrow}\right)|0\rangle$

with $\frac{v_k}{u_k} = g_k$, $u_k^2 + v_k^2 = 1$

$|\tilde{\varphi}\rangle$ was introduced by Bardeen, Cooper, Schrieffer in 1957, it is much simpler than $|\varphi_N\rangle$

Claim: for large N, all calculations can be performed on $|\tilde{\varphi}\rangle$ rather than φ_N. To prove this, we look at the expansion $|\tilde{\varphi}\rangle = \sum_N \lambda_N |\varphi_N\rangle$ with $\sum_N |\lambda_N|^2 = 1$ for normalization. When choosing g_k, u_k, and v_k real, then the λ_N are real as well. We will later see that this restriction is unimportant

For large N, the form of λ_N is



The maximum can be obtained by calculating the average number of particles in the state

$$N^* = \langle N \rangle = \sum_k 2v_k^2 = \frac{\Omega}{(2\pi)^3} \int dk\, 2v_k^2$$

The variance is given by $\langle N^2 \rangle - \langle N \rangle^2$

(variance of Bernoulli distribution is $p(1-p)$)

$$\langle N^2\rangle - \langle N\rangle^2 = \sum_k 4 v_k^2 u_k^2 = \frac{\Omega}{(2\pi)^3}\int d^3k\, 4 v_k^2 u_k^2$$

$\Rightarrow$ $\langle N^2\rangle - \langle N\rangle^2$ is proportional to Ω, therefore the N $\Rightarrow$ the standard deviation (= half-width of the curve $|\Lambda_N|$) is of order $\sqrt{N^2}$ $\Rightarrow$ relative fluctuations in the particle number are $O\left(\frac{1}{\sqrt{N^2}}\right)$, very small.

Correspondence between matrix elements of an arbitrary operator $\hat{F}$ taken between $|\varphi_N\rangle$ or $|\tilde{\varphi}\rangle$

$$\langle\tilde{\varphi}|\hat{F}|\tilde{\varphi}\rangle = \sum_{N,N'} \Lambda_N^* \Lambda_{N'} \langle\varphi_N|\hat{F}|\varphi_{N'}\rangle$$

If $\hat{F}$ conserves the number of particles, then

$$\langle\tilde{\varphi}|\hat{F}|\tilde{\varphi}\rangle = \sum_N |\Lambda_N|^2 \langle\varphi_N|\hat{F}|\varphi_N\rangle$$

If the matrix element $\langle\varphi_N|\hat{F}|\varphi_{N'}\rangle$ varies slowly with N, we can replace it by its value at the peak $\langle\varphi_{N^*}|\hat{F}|\varphi_{N^*}\rangle$, and with $\sum_N |\Lambda_N|^2 = 1$ we obtain $\langle\tilde{\varphi}|\hat{F}|\tilde{\varphi}\rangle = \langle\varphi_{N^*}|\hat{F}|\varphi_{N^*}\rangle$

Similarly, if $\hat{F}|\varphi_N\rangle \propto |\varphi_{N+p}\rangle$, then

$$\langle \tilde{\varphi}|F|\tilde{\varphi}\rangle = \sum_N \lambda^*_{N+p}\lambda_N \langle \varphi_{N+p}|\hat{F}|\varphi_N\rangle$$

$$= \sum_N |\lambda_N|^2 \langle \varphi_{N+p}|F|\varphi_N\rangle$$

$$\cong \langle \varphi_{N'+p}|F|\varphi_{N'}\rangle$$

Calculation of the energy

Let $\hat{H} = \hat{H}_0 + \hat{H}_{int}$ be the Hamiltonian of the interacting electron system. We now want to determine the parameters $\{u_k, v_k\}$ in $|\tilde{\varphi}\rangle$ such that the grand canonical energy

$$\langle \tilde{\varphi}|\hat{H}|\tilde{\varphi}\rangle - E_F\langle \tilde{\varphi}|\hat{N}|\tilde{\varphi}\rangle \text{ is minimized.}$$

Here, the Fermi energy E_F enters as a Lagrange multiplier.

- contribution of the kinetic term $H_0 = \sum_{k,\sigma} \xi_k a^+_{k\sigma} a_{k\sigma}$

  with $\xi_k = \frac{\hbar^2 k^2}{2m} - E_F$

  In the state $|\tilde{\varphi}\rangle$, the probability of finding the state k occupied is $v_k^2 = \langle \tilde{\varphi}|\hat{n}_{k\sigma}|\tilde{\varphi}\rangle = \sum_{k,\sigma} v_k^2 \xi_k$

- contribution of the interaction term

$$H_{int} = \frac{1}{2} \sum_{\substack{\underline{k}\underline{k}'\underline{q} \\ \sigma\sigma'}} V(\underline{k}+\underline{q}, \underline{k}'-\underline{q} | \underline{k}\,\underline{k}') \hat{a}^{\dagger}_{\underline{k}+\underline{q},\sigma} \hat{a}^{\dagger}_{\underline{k}'-\underline{q},\sigma'} \hat{a}_{\underline{k}'\sigma'} \hat{a}_{\underline{k}\sigma}$$

There are three types of terms contributing to $\langle \bar{q} | H_{int} | \bar{q} \rangle$

i) diagonal terms $V(\underline{k}\,\underline{k}' | \underline{k}\,\underline{k}')$

ii) exchange terms $V(\underline{k}', \underline{k} | \underline{k}, \underline{k}')$

iii) terms describing the transition of a pair from the state $(\underline{k}\uparrow, -\underline{k}\downarrow)$ to the state $(\underline{\ell}\uparrow, -\underline{\ell}\downarrow)$,
$V(\underline{\ell}, -\underline{\ell} | \underline{k} - \underline{k}) = V_{k\ell}$

The contributions i) and ii) are already present in a normal metal and can be incorporated into ξ_k (Hartree-Fock approximation with mean-field $\langle \hat{a}^{\dagger}_{k\sigma} \hat{a}_{k\sigma} \rangle = n_k$)
The relevant contribution to superconductivity comes from iii)
We denote components of the wave function with the pair state $(\underline{k}\uparrow, -\underline{k}\downarrow)$ occupied or unoccupied by $\varphi_{\underline{k}1}$ and $\varphi_{\underline{k}0}$ $\Rightarrow \bar{\varphi} = v_{\underline{k}} \varphi_{\underline{k}1} + u_{\underline{k}} \varphi_{\underline{k}0}$

Similarly, we can decompose $\bar{\varphi}$ into four components describing the occupancy of two different pair states $(\underline{k}\uparrow, -\underline{k}\downarrow)$ and $(\underline{\ell}\uparrow, -\underline{\ell}\downarrow)$

$$\bar{\varphi} = v_k v_\ell \varphi_{\underline{k}1,\underline{\ell}1} + v_k u_\ell \varphi_{\underline{k}1,\underline{\ell}0} + u_k v_k \varphi_{\underline{k}0,\underline{\ell}1} + u_k u_\ell \varphi_{\underline{k}0\underline{\ell}0}$$

The scattering of a pair from state $(\underline{k}\uparrow, -\underline{k}\downarrow)$ to state $(\underline{\ell}\uparrow, -\underline{\ell}\downarrow)$ contributes an interaction energy

$$u_{\underline{k}} v_{\underline{\ell}} \langle \varphi_{\underline{k}\uparrow \underline{\ell}\downarrow} | \hat{H}_{int} | \varphi_{\underline{k}\downarrow \underline{\ell}\uparrow} \rangle v_{\underline{k}} u_{\underline{\ell}} = v_{\underline{k}} u_{\underline{k}} v_{\underline{\ell}} u_{\underline{\ell}} V_{\underline{k}\underline{\ell}}$$

$$\Rightarrow \langle \tilde{\varphi} | \hat{H} - E_F \hat{N} | \tilde{\varphi} \rangle = 2 \sum_{\underline{k}} \xi_{\underline{k}} v_{\underline{k}}^2 + \sum_{\underline{k},\underline{\ell}} V_{\underline{k}\underline{\ell}} u_{\underline{k}} v_{\underline{k}} u_{\underline{\ell}} v_{\underline{\ell}} \quad (*)$$

In order to minimize while taking into account the normalization condition $u_{\underline{k}}^2 + v_{\underline{k}}^2 = 1$, we parametrize

$$u_{\underline{k}} = \sin\theta_{\underline{k}}, \quad v_{\underline{k}} = \cos\theta_{\underline{k}}$$

$$\Rightarrow \langle \tilde{\varphi} | \hat{H} - E_F \hat{N} | \tilde{\varphi} \rangle = 2 \sum_{\underline{k}} \xi_{\underline{k}} \cos^2\theta_{\underline{k}} + \frac{1}{4} \sum_{\underline{k},\underline{\ell}} \sin 2\theta_{\underline{k}} \times \sin 2\theta_{\underline{\ell}} V_{\underline{k}\underline{\ell}}$$

The minimization equations are

$$0 = \frac{\partial}{\partial \theta_{\underline{k}}} \langle \tilde{\varphi} | \hat{H} - E_F \hat{N} | \tilde{\varphi} \rangle$$

$$\sin\alpha\cos\alpha = \tfrac{1}{2}\sin 2\alpha$$
$$\cos^2\alpha - \sin^2\alpha = \cos 2\alpha$$

$$= -2 \xi_{\underline{k}} \sin 2\theta_{\underline{k}} + \sum_{\underline{\ell}} \cos 2\theta_{\underline{k}} \sin 2\theta_{\underline{\ell}} V_{\underline{k}\underline{\ell}}$$

$$\Rightarrow \xi_{\underline{k}} \tan 2\theta_{\underline{k}} = \frac{1}{2} \sum_{\underline{\ell}} V_{\underline{k}\underline{\ell}} \sin 2\theta_{\underline{\ell}}$$

We now define $\Delta_{\underline{k}} = -\sum_{\underline{\ell}} V_{\underline{k}\underline{\ell}} u_{\underline{\ell}} v_{\underline{\ell}}$, $\varepsilon_{\underline{k}} = \sqrt{\xi_{\underline{k}}^2 + \Delta_{\underline{k}}^2}$

$\Rightarrow$ we find $\tan 2\theta_{\underline{k}} = -\frac{\Delta_{\underline{k}}}{2\xi_{\underline{k}}}$

$$2u_{\underline{k}} v_{\underline{k}} = \sin 2\theta_{\underline{k}} = \frac{-\tan 2\theta_{\underline{k}}}{\sqrt{1+\tan^2 2\theta_{\underline{k}}}} = \frac{\Delta_{\underline{k}}}{\varepsilon_{\underline{k}}}$$

$$v_{\underline{k}}^2 - u_{\underline{k}}^2 = \cos 2\theta_{\underline{k}} = -\frac{\xi_{\underline{k}}}{\varepsilon_{\underline{k}}}$$

The choice of sign in the last equation is such that for large positive $\xi_{\underline{k}}$, $u_{\underline{k}} = 1$, $v_{\underline{k}} = 0$, such that the total number of electrons $\sum_{\underline{k}} v_{\underline{k}}^2$ converges.

Using the above results, we obtain the equation for Δ

$$\Delta_{\underline{k}} = -\sum_{\underline{\ell}} V_{\underline{k}\,\underline{\ell}} \frac{\Delta_{\underline{\ell}}}{2\sqrt{\xi_{\underline{\ell}}^2 + \Delta_{\underline{\ell}}^2}}$$

The equation has a trivial solution $\Delta_k = 0$, $\tan 2\theta_k = 0$

$$\cos 2\theta_k = -\operatorname{sign} \xi_k \Rightarrow \theta_k = \begin{cases} 0 & \xi_k < 0 \\ \frac{\pi}{2} & \xi_k > 0 \end{cases}$$

$$\Rightarrow v_k = \cos\theta_k = \begin{cases} 1 & \xi_k < 0 \\ 0 & \xi_k > 0 \end{cases}$$

The associated wave function is simply $|\Psi_0\rangle = \prod_{|\underline{k}|<k_F} \hat{a}^\dagger_{\underline{k}\uparrow} \hat{a}^\dagger_{-\underline{k}\downarrow} |0\rangle$, a slater determinant formed from all states with an energy less than $E_F = \frac{\hbar^2 k_F^2}{2m}$, the ground state of a non-interacting electron gas

To find a non-trivial solution, we again consider the simplified interaction

$$V_{\underline{k}\underline{\ell}} = \begin{cases} -\frac{V}{\Omega} & \text{if } |\xi_{\underline{k}}|, |\xi_{\underline{\ell}}| \leq \hbar\omega_D \\ 0 & \text{otherwise} \end{cases}$$

with a positive constant V ("BCS-interaction")

Then, $\Delta_{\underline{k}} = 0$ for $|\xi_{\underline{k}}| > \hbar\omega_D$

$\Delta_{\underline{k}} = \Delta$ (independent of $\underline{k}$) for $|\xi_{\underline{k}}| < \hbar\omega_D$

Using $\frac{1}{\Omega}\sum_{\underline{\ell}} = \int \frac{d^3\ell}{(2\pi)^3} \approx \rho_F \int d\xi$, we obtain

$$\Delta = \rho_F V \int_{-\hbar\omega_D}^{\hbar\omega_D} d\xi \, \frac{\Delta}{2\sqrt{\xi^2+\Delta^2}}$$

$$\Rightarrow \frac{1}{\rho_F V} = \int_0^{\hbar\omega_D} \frac{d\xi}{\sqrt{\xi^2+\Delta^2}} = \int_0^{\hbar\omega_D/\Delta} \frac{dx}{\sqrt{x^2+1}} = \sinh^{-1}\left(\frac{\hbar\omega_D}{\Delta}\right)$$

$$\Rightarrow \Delta = \frac{\hbar\omega_D}{\sinh\frac{1}{\rho_F V}} \quad ; \text{ since typically } \hbar\omega_D \approx 300\,K \; \Delta \approx 10\,K \text{ we are in the weak coupling regime } V\rho_F \ll 1$$

$$\Rightarrow \sinh\frac{1}{\rho_F V} \gg 1 \Rightarrow \sinh\frac{1}{\rho_F V} \approx \frac{1}{2} e^{\frac{1}{\rho_F V}}$$

$$\Rightarrow \Delta \cong 2\hbar\omega_D \, e^{-\frac{1}{\rho_F V}} \quad \text{We will see later that}$$

Δ is the energy gap for excitations (corresponds to breaking up a Cooper pair, i.e. Δ is approximately the

binding energy of a Cooper pair). In addition, in a homework problem you will show that $\Delta = 1.75\, k_B T_c$, i.e. Δ also determines the critical (transition) temperature.

We can now compute the kinetic and potential energies:

$$\langle \tilde{\Psi} | \hat{H} - E_F \hat{N} | \tilde{\Psi} \rangle = 2 \sum_{\underline{k}} \xi_{\underline{k}} v_{\underline{k}}^2 + \sum_{\underline{k},\underline{\ell}} V_{\underline{k}\underline{\ell}}\, u_{\underline{k}} v_{\underline{k}} u_{\underline{\ell}} v_{\underline{\ell}}$$

Use now $v_k^2 = \frac{1}{2}\left(1 - \frac{\xi_k}{\varepsilon_k}\right)$

$$u_k v_k = \frac{\Delta_k}{2\varepsilon_k}$$

$$\Rightarrow \langle \tilde{\Psi} | \hat{H} - E_F \hat{N} | \tilde{\Psi} \rangle = \sum_{\underline{k}} \left(\xi_{\underline{k}} - \frac{\xi_{\underline{k}}^2}{\varepsilon_{\underline{k}}} \right) + \sum_{\underline{k},\ell} V_{\underline{k}\ell} \frac{\Delta_{\underline{k}}}{2\varepsilon_{\underline{k}}} \frac{\Delta_\ell}{2\varepsilon_\ell}$$

$$= \sum_{k} \left(\xi_k - \frac{\xi_k^2}{\varepsilon_k} \right) - \frac{\Omega}{V} \underbrace{\left(\sum_{k} V_{k\ell} \frac{\Delta_k}{2\varepsilon_k} \right)}_{\Delta} \underbrace{\left(\sum_{\ell} V_{k\ell} \frac{\Delta_\ell}{2\varepsilon_\ell} \right)}_{\Delta}$$

Subtracting now the normal state energy $2 \sum_{|\underline{k}| < k_F} \xi_k$, we obtain for the condensation energy

$$\langle E \rangle_s - \langle E \rangle_n = \sum_{|\underline{k}| > k_F} \left(\xi_k - \frac{\xi_k^2}{E_k} \right) + \sum_{|\underline{k}| < k_F} \left(-\xi_k - \frac{\xi_k^2}{E_k} \right) - \frac{\Omega}{V} \Delta^2$$

$$= 2 \sum_{|k| > k_F} \left(\xi_{\underline{k}} - \frac{\xi_k^2}{E_k} \right) - \frac{\Omega}{V} \Delta^2$$

$$= 2\Omega \rho_F \int_0^{\hbar\omega_D} d\xi \left(\xi - \frac{\xi^2}{\sqrt{\xi^2 + \Delta^2}} \right) - \frac{\Omega}{V} \Delta^2$$

$$\Rightarrow \langle E\rangle_s - \langle E\rangle_n = 2\Omega\rho_F\left[\tfrac{1}{2}(\hbar\omega_D)^2 - \Delta^2\underbrace{\int_0^{\frac{\hbar\omega_D}{\Delta}} dy\,\frac{y^2}{\sqrt{y^2+1}}}_{\left[\frac{1}{2}y\sqrt{1+y^2}-\frac{1}{2}\sinh^{-1}y\right]_0^{\frac{\hbar\omega_D}{\Delta}}}\right] - \frac{\Omega}{V}\Delta^2$$

$$= \Omega\rho_F\Delta^2\left[\left(\frac{\hbar\omega_D}{\Delta}\right)^2 - \left(\frac{\hbar\omega_D}{\Delta}\right)^2\underbrace{\sqrt{\left(\frac{\Delta}{\hbar\omega_D}\right)^2+1}}_{\simeq 1+\frac{1}{2}\frac{\Delta^2}{(\hbar\omega_D)^2}} + \frac{1}{\rho_F V}\right] - \frac{\Omega}{V}\Delta^2$$

$$= \Omega\left[\frac{\Delta^2}{V} - \frac{1}{2}\rho_F\Delta^2\right] - \frac{\Omega}{V}\Delta^2$$

The leading term due to the attractive potential cancels, and we obtain $\langle E\rangle_s - \langle E\rangle_n = -\frac{1}{2}\Omega\rho_F\Delta^2$.

The condensed energy is lower by $\approx \frac{\Delta^2}{E_F}$ per electron (or $\frac{\Delta^2}{\hbar\omega_D}$ per "active" electron in the window $-\hbar\omega_D < \xi < \hbar\omega_D$).

It is this difference in energy which is measured experimentally, despite the fact that we do not know the normal state energy with this precision.

First excited states

In the ground state wave function we constructed, N particles are coupled in pairs. As an excitation, we now try to add one particle in the plane wave state $|\underline{m}\sigma\rangle$. We then obtain

a state

$$\varphi_{N+1,\underline{m}\alpha}(\underline{r}_1 \dots \underline{r}_{N+1}) = \hat{A}\, \varphi(\underline{r}_1 - \underline{r}_2)\, \varphi(\underline{r}_3 - \underline{r}_4) \dots \varphi(\underline{r}_{N-1} - \underline{r}_N) * \\ * e^{i\underline{m}\cdot\underline{r}_{N+1}} \chi_s(\alpha_1\alpha_2) \dots \chi_s(\alpha_{N-1}\alpha_N)\, \chi_{\alpha_{N+1}}$$

We again introduce a superposition of different particle numbers $|\tilde{\varphi}_{\underline{m}\alpha}\rangle = \sum_N \lambda_N |\varphi_{N+1,\underline{m}\alpha}\rangle$

By repeating our arguments for a second quantized version of $\tilde{\varphi}$, we arrive at

$$|\tilde{\varphi}_{\underline{m}\alpha}\rangle = \prod_{\underline{k}\neq\underline{m}} \left(u_{\underline{k}} + v_{\underline{k}}\, \hat{a}^+_{\underline{k}\uparrow}\, \hat{a}^+_{-\underline{k}\downarrow}\right) \hat{a}^+_{\underline{m}\alpha} |0\rangle$$

$|\tilde{\varphi}_{\underline{m}\alpha}\rangle$ is orthogonal to $|\tilde{\varphi}\rangle$. What is the energy of the the excited state $|\tilde{\varphi}_{\underline{m}\alpha}\rangle$? The kinetic energy is given by

$$\langle\tilde{\varphi}_{\underline{m}\alpha}|\hat{H}_{\cdot}|\tilde{\varphi}_{\underline{m}\alpha}\rangle = \langle\tilde{\varphi}|\hat{H}_{\cdot}|\tilde{\varphi}\rangle + \left(1 - 2v_{\underline{m}}^2\right)\xi_{\underline{m}}$$

↑ state $(\underline{m}\alpha)$ now occupied with prob. one

↑ previously, both $(\underline{m}\uparrow)$ and $(\underline{m}\downarrow)$ were occupied with prob. $v_{\underline{m}}^2$ each

Regarding the potential energy, we note that only transitions $(\underline{k}\alpha)(-\underline{k},-\alpha) \to (\underline{k}'\alpha)(-\underline{k}'-\alpha)$ with $\underline{k}\neq\underline{m}$ and $\underline{k}'\neq\underline{m}$ can contribute, as no pair can use the state $\underline{m}\alpha$

$$\Rightarrow \langle\tilde{\varphi}_{\underline{m}\alpha}|\hat{H}_{int}|\tilde{\varphi}_{\underline{m}\alpha}\rangle = \langle\tilde{\varphi}|\hat{H}_{int}|\tilde{\varphi}\rangle - 2\sum_{\underline{\ell}} V_{\underline{m}\underline{\ell}}\, u_{\underline{m}} v_{\underline{\ell}}\, u_{\underline{\ell}} v_{\underline{m}}$$

The total energy becomes

$$\langle \tilde{\Phi}_{\underline{m}\alpha} | \hat{H} | \tilde{\Phi}_{\underline{m}\alpha} \rangle = E_0 + (1 - 2v_{\underline{m}}^2)\xi_{\underline{m}} + 2u_{\underline{m}} v_{\underline{m}} \Delta_{\underline{m}}$$

$$= E_0 + \frac{\xi_{\underline{m}}^2}{\varepsilon_{\underline{m}}} + \frac{\Delta_{\underline{m}}^2}{\varepsilon_{\underline{m}}}$$

$$= E_0 + \varepsilon_{\underline{m}} ,$$

where $v_{\underline{k}}^2 - u_{\underline{k}}^2 = -\frac{\xi_{\underline{k}}}{\varepsilon_{\underline{k}}}$, $2u_{\underline{k}} v_{\underline{k}} = \frac{\Delta_{\underline{k}}}{\varepsilon_{\underline{k}}}$, $\varepsilon_{\underline{k}} = \sqrt{\xi_{\underline{k}}^2 + \Delta_{\underline{k}}^2}$

was used. As E_0 is the energy of the ground state, the additional energy $\varepsilon_{\underline{m}} = \sqrt{\Delta_{\underline{m}}^2 + \xi_{\underline{m}}^2}$ is needed to add an extra particle in state $(\underline{m}\alpha)$. Even when $\xi_{\underline{m}} = 0$, $\varepsilon_{\underline{m}} = \Delta_{k_F} = \Delta$ is finite $\Rightarrow$ <u>the superconductor has an excitation gap Δ</u>

Next, we try to construct states with two excitations by using the function

$$|\Xi_{\underline{m}\alpha, \underline{n}\beta}\rangle = \prod_{\underline{k} \neq \underline{m}, \underline{n}} (u_{\underline{k}} + v_{\underline{k}} \hat{a}_{\underline{k}\uparrow}^{\dagger} \hat{a}_{-\underline{k}\downarrow}^{\dagger}) \hat{a}_{\underline{m}\alpha}^{\dagger} \hat{a}_{\underline{n}\beta}^{\dagger} |0\rangle$$

However, such states are not orthogonal to $|\tilde{\Phi}\rangle$ in general.

For example, $\langle \tilde{\Phi} | \Xi_{\underline{m}\uparrow, -\underline{m}\downarrow} \rangle = v_{\underline{m}} \neq 0$.

There are two options to avoid this difficulty.

(i) we could add to $|\Xi\rangle$ a component $\lambda |\tilde{\Phi}\rangle$ and choose λ

in such a way that the total state is orthogonal to $|\tilde{\Phi}\rangle$. The method was chosen originally by BCS, but is numerically rather tedious.

(ii) We reconsider the state $|\tilde{\Phi}_{m\alpha}\rangle$ for single excitations. We try to bring these excitations into the form

$$|\tilde{\Phi}_{i,m\alpha}\rangle = \hat{\gamma}^{+}_{m\alpha}\,|\tilde{\Phi}\rangle ,$$

where $\hat{\gamma}^{+}_{m\alpha}$ is the creation operator for one elementary excitation. We next need to find $\hat{\gamma}^{+}$ and $\hat{\gamma}$ such that

a) the $\hat{\gamma}_{m\alpha}$ and $\hat{\gamma}^{+}_{m'\beta}$ obey fermionic anti-commutation relations

and b) $\hat{\gamma}_{m\alpha}\,|\tilde{\Phi}\rangle = 0$, i.e. $|\tilde{\Phi}\rangle$ is the state with no excitations.

If a) and b) are satisfied, one sees that all states obtained by applying an arbitrary number of operators $\hat{\gamma}^{+}$ to $|\tilde{\Phi}\rangle$ are orthogonal to each other and the ground state $|\tilde{\Phi}\rangle$, and are properly normalized.

As a first step, we realize that $|\tilde{\Phi}_{i,m\alpha}\rangle = \frac{1}{u_m}\,\hat{a}^{+}_{m\alpha}\,|\tilde{\Phi}\rangle$ is normalized, but $\frac{1}{u_m}\,\hat{a}^{+}_{m\alpha}$ does not obey fermionic commutation relations. In a second attempt, we note that

$|\tilde{\Phi}_{m\downarrow}\rangle = \frac{1}{V_m} a_{m\uparrow} |\tilde{\Phi}\rangle$ is the same normalized state, but $\frac{1}{V_m} \hat{a}_{m,-\alpha}$ does not satisfy fermionic commutation relations either. We now try to define $\hat{\gamma}^{\dagger}_{m\alpha}$ as a linear combination of $\hat{a}^{\dagger}_{m\alpha}$ and $\hat{a}_{m,-\alpha}$. If we choose

$$\hat{\gamma}^{\dagger}_{m\uparrow} = u_m \hat{a}^{\dagger}_{m\uparrow} - v_m \hat{a}_{m\downarrow}$$

$$\hat{\gamma}^{\dagger}_{m\downarrow} = u_m \hat{a}^{\dagger}_{m\downarrow} + v_m \hat{a}_{m\uparrow}$$

we find that the fermionic commutation relations are satisfied. In addition,

$$\hat{\gamma}_{m\uparrow} |\tilde{\Phi}\rangle = \prod_{k \neq m} \left(u_k + v_k \hat{a}^{\dagger}_{k\uparrow} \hat{a}^{\dagger}_{k\downarrow}\right) \left(u_m \hat{a}_{m\uparrow} - v_m \hat{a}^{\dagger}_{m\downarrow}\right) \times \left(u_m + v_m \hat{a}^{\dagger}_{m\uparrow} \hat{a}^{\dagger}_{m\downarrow}\right) |0\rangle$$

$$= \prod_{k \neq m} \left(u_k + v_k \hat{a}^{\dagger}_{k\uparrow} \hat{a}^{\dagger}_{k\downarrow}\right) u_m v_m \left(\hat{a}^{\dagger}_{m\downarrow} - \hat{a}^{\dagger}_{m\downarrow}\right) |0\rangle$$

$$= 0$$

Here, we used that $\hat{a}_{m\alpha} |0\rangle = 0$, $\hat{a}_{m\alpha} a^{\dagger}_{m\alpha} |0\rangle = |0\rangle$, and the fermionic commutation relations.

Using $\hat{\gamma}$ and $\hat{\gamma}^{\dagger}$ operators enormously simplifies calculations. This method was introduced by Bogoliubov and Valatin in 1958.

Remarks: i) since $\hat{\gamma}^{+}_{\underline{k}\alpha} = u_k \hat{a}^{+}_{\underline{k}\alpha} - \mathrm{sign}(\alpha)\, \hat{a}_{-\underline{k}-\alpha}$,

the state $|\Psi_{N+1}, \underline{k}\alpha\rangle$ can be created either by adding an electron $|\underline{k}\alpha\rangle$ to the condensed state $|\Psi_N\rangle$ or by removing an electron $(-\underline{k}-\alpha)$ from the state $|\Psi_{N+2}\rangle$.

ii) addition of an electron in a state $\underline{k}$ can be achieved by tunneling through a thin oxide barrier between a normal metal and the superconductor. This allows to experimentally determine the energy gap Δ.

iii) Except from tunneling experiments, excited states are usually studied without changing the particle number N, for instance by application of infrared radiation. For even N, the first excited state now corresponds to the breaking of a pair, with an excitation energy $\varepsilon_k + \varepsilon_e$. Thus, the minimum excitation energy now is 2Δ. For odd N, there are two types of excitations: either a pair is broken as previously, or the state of the unpaired electron is changed. However, the absorption intensity for pair breaking is N times higher than that for exciting the unpaired electron. Thus, for $N \sim 10^{23}$ one always measures an absorption threshold at 2Δ.

iv) the addition of pairs $(\underline{k}\uparrow, -\underline{k}\downarrow)$ is possible <u>without an energy gap</u>. The probability amplitude

for obtaining the state $|\psi_{N+2}\rangle$ from $|\psi_N\rangle$ is given by $F_k = \langle \psi_{N+2} | a^+_{k\uparrow} a^+_{-k\downarrow} | \psi_N \rangle \equiv \langle \tilde{\psi} | a^+_{\underline{k}\uparrow} a^+_{-\underline{k}\downarrow} | \tilde{\psi} \rangle$

F_k is called condensation amplitude, and is used as the superconducting order parameter in a mean field theory (homework problem).

Case of two coupled superconductors

We consider two superconductors S and S' separated by an insulating layer. Tunneling of electrons through the barrier can be described by adding a small term $\hat{H}_T$ to the Hamiltonian $\hat{H}_{ss'}$ describing the two uncoupled superconductors.

$$\hat{H} = \hat{H}_{ss'} + \hat{H}_T$$

$$H_T = \sum_{\underline{k}\,\underline{\ell}} \left(a^+_{ks}\, a_{\ell s'}\, T_{\underline{k}\underline{\ell}} + a^+_{\ell s'}\, a_{ks}\, T^*_{\underline{k}\underline{\ell}} \right)$$

Here and in the following, we suppress the spin index. An eigenstate of $\hat{H}_{ss'}$ will be a product of eigenstates

$$|\psi_\nu\rangle = |\psi^{(s')}_{2(N-\nu)}\rangle \otimes |\psi^{(s)}_{2\nu}\rangle, \quad \hat{H}_{ss'} |\psi_\nu\rangle = E_\nu |\psi_\nu\rangle.$$

Here, the total number of electrons in the combined system

is fixed. Neglecting H_T for the moment, we find

$$E_{V+1} - E_V = 2\left(\bar{E}_F^{(S)} - \bar{E}_F^{(S')}\right).$$

If there is no voltage applied between S and S', then $E_F^{(S)} = E_F^{(S')}$ and the states $|\Psi_V\rangle$ are degenerate. The tunneling Hamiltonian H_T removes this degeneracy. Using 2nd order perturbation theory, one finds the following tunneling matrix element coupling the functions $|\Psi_V\rangle$ and $|\Psi_{V+1}\rangle$

$$J_c = \sum_{\substack{\underline{k},\underline{\ell} \\ \underline{k}',\underline{\ell}'}} \frac{\langle \Psi_{V+1}| T_{\underline{k}\underline{\ell}}\, \hat{a}^{\dagger}_{\underline{k}S}\, a_{\underline{\ell}S'} |J\rangle\langle J| T_{\underline{k}'\underline{\ell}'}\, \hat{a}^{\dagger}_{\underline{k}'S}\, \hat{a}_{\underline{\ell}'S}| \Psi_V\rangle}{E_V - E_J},$$

where $|J\rangle$ is an intermediate state with one extra electron on the S side and one extra hole on the S' side. The energy of such an intermediate state is $E_J = E_V + \xi_{\underline{k}'} + \xi_{\underline{\ell}'}$. The final state is composed of $(V+1)$ pairs, which can be achieved if $\underline{k} = -\underline{k}'$ and $\underline{\ell} = -\underline{\ell}'$. Using the symmetry relation $T_{-\underline{k}-\underline{\ell}} = T^{+}_{\underline{k}\underline{\ell}}$ (time-reversal symmetry), we find

$$J_c = -4 \sum_{\underline{k}\underline{\ell}} |T_{\underline{k}\underline{\ell}}|^2 \frac{u_{\underline{k}} v_{\underline{k}} u_{\underline{\ell}} v_{\underline{\ell}}}{\xi_{\underline{k}} + \xi_{\underline{\ell}}}$$

To second order in H_{T1} we can thus write

$$\hat{H} |\psi_v\rangle = E_v |\psi_v\rangle + J_0 \left(|\psi_{v+1}\rangle + |\psi_{v-1}\rangle \right)$$

This equation is in exact analogy to a tight-binding model for electrons hopping on a one-dimensional lattice, when identifying v with the lattice site index. Similar to the tight binding case, the eigenfunctions are a linear combination

$$|\psi_k\rangle = \sum_v |\psi_v\rangle e^{ikv}$$

where k is analogous to a wave vector. (We will see later that k actually describes the phase difference $\Delta\varphi$ between the superconductors).

The corresponding energy is

$$E(k) = E_v + 2J_0 \cos(k).$$

As the particle number $2v \approx 10^{23}$, its standard deviation $\Delta v \sim \sqrt{v} \sim 10^{11}$ is still large, and $\Delta k \sim \frac{1}{\Delta v}$ is small $\Rightarrow$ we can specify both v and k with excellent accuracy, and compute the velocity

at which such a wave packet moves

$$\frac{\hbar\, d\langle v\rangle}{dt} = \frac{\partial E(k)}{\partial k} = -2J_0 \sin k.$$

The time variation in $\langle v\rangle$ corresponds to a pair current tunneling through the junction

$$J = 2e\frac{d\langle v\rangle}{dt} = -4e\frac{J_0}{\hbar}\sin k \qquad (*)$$

If S and S' are attached to a current source, a current ($< 4eJ_0/\hbar$) can flow from S to S' under zero voltage! This is a first example that the condensed state has superfluid properties, an effect predicted by Josephson in 1961.

What happens when a voltage is applied between S and S'? We then find $E_{\nu+1} - E_\nu = 2eV$, analogous to a uniform electric field applied to a tight binding chain. The wave packet accelerates according to the force equation

$$\frac{d}{dt}\langle \hbar k\rangle = 2eV \qquad (**)$$

The equations (*) and (**) completely determine the behavior of the junction. For a constant voltage V,

an alternating current of frequency $\frac{2eV}{h}$ passes through the junction, which can be detected by virtue of the emitted microwave radiation.