Selected topics in solid state physics 2

Part 2

Alexander Shnirman

on sabbatical leave from Karlsruhe Institute of Technology, Karlsruhe, Germany

(Dated: November 10, 2021)

I. JOSEPHSON JUNCTION

A. Elements of BCS theory

Our purpose now is to recall a bit of BCS theory in order to understand better the Josephson effect.

1. *BCS Hamiltonian*

Everything is done in the grand canonical ensemble. The grand canonical partition function

$$Z_\Omega = \sum_{n,N} e^{-\beta(E_{n,N}-\mu N)} \tag{1}$$

shows that at $T=0$ one has to minimize $H_G = H - \mu N$ and at $T>0$ one has to minimize $\Omega = \langle H\rangle - TS - \mu N$.

One considers attraction between electrons due to the longitudinal acoustic phonons. The Hamiltonian reads

$$H_G = \sum_{k,\sigma} (\epsilon_k - \mu) c^\dagger_{k,\sigma}\, c_{k,\sigma} - \frac{1}{2}\frac{g}{V} \sum_{k_1,\sigma_1,k_2,\sigma_2,q} c^\dagger_{k_1+q,\sigma_1}\, c^\dagger_{k_2-q,\sigma_2}\, c_{k_2,\sigma_2}\, c_{k_1,\sigma_1} \tag{2}$$

where the interaction term works only if the energy transfer $\epsilon_{k_1+q} - \epsilon_{k_1}$ is smaller than the Debye energy $\hbar\omega_D$. One can also see (Fig. 1) that under this restriction the phase space available for the interaction is maximal if $\vec{K} \equiv \vec{k}_1 + \vec{k}_2 \approx 0$. Thus, one introduces a reduced

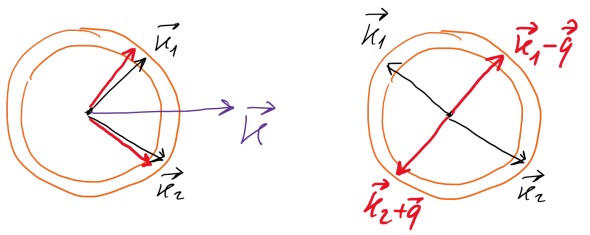

FIG. 1: For $\vec{K} \approx 0$ the phase space available for interaction is much bigger.

BSC Hamiltonian. The reduced Hamiltonian is the one in which $k_1 = -k_2$ and $\sigma_1 = -\sigma_2$:

$$H_{\rm BCS} = \sum_{k,\sigma} (\epsilon_k - \mu) c^\dagger_{k,\sigma}\, c_{k,\sigma} - \frac{1}{2}\frac{g}{V} \sum_{k,q,\sigma} c^\dagger_{k+q,\sigma}\, c^\dagger_{-k-q,-\sigma}\, c_{-k,-\sigma}\, c_{k,\sigma}\ . \tag{3}$$

Renaming $k' = k + q$ we obtain

$$H_{\rm BCS} = \sum_{k,\sigma} (\epsilon_k - \mu) c^\dagger_{k,\sigma} c_{k,\sigma} - \frac{1}{2}\frac{g}{V} \sum_{k,k',\sigma} c^\dagger_{k',\sigma} c^\dagger_{-k',-\sigma} c_{-k,-\sigma} c_{k,\sigma} \ , \tag{4}$$

or

$$H_{\rm BCS} = \sum_{k,\sigma} (\epsilon_k - \mu) c^\dagger_{k,\sigma} c_{k,\sigma} - \frac{g}{V} \sum_{k,k'} c^\dagger_{k',\uparrow} c^\dagger_{-k',\downarrow} c_{-k,\downarrow} c_{k,\uparrow} \ , \tag{5}$$

Also the condition on k and k' gets simplified. We just demand that

$$\mu - \hbar\omega_D < \epsilon_k, \epsilon_{k'} < \mu + \hbar\omega_D \ . \tag{6}$$

Although the Hamiltonian conserves the number of particles, BCS (J. Bardeen, L. Cooper, and R. Schrieffer, 1957) constructed a trial wave function which is a superposition of different numbers of particles:

$$|BCS\rangle = \prod_k (u_k + v_k c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow})\, |0\rangle \ . \tag{7}$$

with the purpose to use u_k and v_k as variational parameters and minimize $\langle BCS|\, H_G \,|BCS\rangle$. We will not pursue this original strategy here, but rather present the (completely equivalent) mean-field approach.

2. *Mean field*

We adopt the mean field approximation for the BCS Hamiltonian.

$$H_{\rm BCS} \ = \ \sum_{k,\sigma} (\epsilon_k - \mu) c^\dagger_{k,\sigma} c_{k,\sigma} - \frac{g}{V} \sum_{k,k'} c^\dagger_{k',\uparrow} c^\dagger_{-k',\downarrow} c_{-k,\downarrow} c_{k,\uparrow} \ . \tag{8}$$

Note that in the interaction the terms with $k = k'$ are absent, since the matrix element of the electron-phonon interaction is proportional to the momentum transfer $q = k - k'$. Thus the only averages we can extract in the interaction term are $\langle c_{-k,\downarrow} c_{k,\uparrow}\rangle$ and $\langle c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow}\rangle$. Why such averages are at all possible will be discussed later.

We denote for brevity $A = c_{-k,\downarrow} c_{k,\uparrow}$ and $B = c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow}$. We use

$$AB = \langle A\rangle \langle B\rangle + \langle A\rangle (B - \langle B\rangle) + (A - \langle A\rangle) \langle B\rangle + (A - \langle A\rangle)(B - \langle B\rangle)$$

and neglect the last term. Then we obtain

$$AB \approx A \langle B\rangle + \langle A\rangle B - \langle A\rangle \langle B\rangle \ .$$

The mean field Hamiltonian reads

$$\begin{aligned} H^{\rm MF}_{\rm BCS} &= \sum_{k,\sigma}(\epsilon_k-\mu)c^\dagger_{k,\sigma}\,c_{k,\sigma} + \frac{g}{V}\sum_{k,k'}\langle c^\dagger_{k',\uparrow}\,c^\dagger_{-k',\downarrow}\rangle\,\langle c_{-k,\downarrow}\,c_{k,\uparrow}\rangle \\ &- \frac{g}{V}\sum_{k,k'}\langle c^\dagger_{k',\uparrow}\,c^\dagger_{-k',\downarrow}\rangle\,c_{-k,\downarrow}\,c_{k,\uparrow} - \frac{g}{V}\sum_{k,k'}c^\dagger_{k',\uparrow}\,c^\dagger_{-k',\downarrow}\,\langle c_{-k,\downarrow}\,c_{k,\uparrow}\rangle \\ &= \sum_{k,\sigma}\xi_k c^\dagger_{k,\sigma}\,c_{k,\sigma} - \sum_k \Delta^*\,c_{-k,\downarrow}\,c_{k,\uparrow} - \sum_k \Delta\,c^\dagger_{k,\uparrow}\,c^\dagger_{-k,\downarrow} + V\frac{\Delta^2}{g}\ , \end{aligned} \tag{9}$$

where $\Delta \equiv \frac{g}{V}\sum_k\langle c_{-k,\downarrow}\,c_{k,\uparrow}\rangle$ and $\Delta^* \equiv \frac{g}{V}\sum_k\langle c^\dagger_{k,\uparrow}\,c^\dagger_{-k,\downarrow}\rangle$ is the superconducting order parameter.

3. Nambu formalism

We rewrite the mean-field Hamiltonian in a matrix form:

$$H^{\rm MF}_{\rm BCS} = \sum_k \begin{pmatrix} c^\dagger_{k,\uparrow} & c_{-k,\downarrow}\end{pmatrix}\begin{pmatrix}\xi_k & -\Delta \\ -\Delta^* & 0\end{pmatrix}\begin{pmatrix} c_{k,\uparrow} \\ c^\dagger_{-k,\downarrow}\end{pmatrix} + \sum_k \xi_k c^\dagger_{k,\downarrow}\,c_{k,\downarrow} + V\frac{\Delta^2}{g} \tag{10}$$

Next we rewrite $\sum_k \xi_k c^\dagger_{k,\downarrow}\,c_{k,\downarrow} = \sum_k \xi_k(1-c_{k,\downarrow}\,c^\dagger_{k,\downarrow}) = \sum_k \xi_k(1-c_{-k,\downarrow}\,c^\dagger_{-k,\downarrow})$. This gives

$$H^{\rm MF}_{\rm BCS} = \sum_k \begin{pmatrix} c^\dagger_{k,\uparrow} & c_{-k,\downarrow}\end{pmatrix}\begin{pmatrix}\xi_k & -\Delta \\ -\Delta^* & -\xi_k\end{pmatrix}\begin{pmatrix} c_{k,\uparrow} \\ c^\dagger_{-k,\downarrow}\end{pmatrix} + \sum_k \xi_k + V\frac{\Delta^2}{g} \tag{11}$$

The eigenvalues of the matrix $\begin{pmatrix}\xi_k & -\Delta \\ -\Delta^* & -\xi_k\end{pmatrix}$ read $\pm E_k$, where $E_k = \sqrt{|\Delta|^2+\xi_k^2}$. For simplicity let us, first, assume that Δ is real, i.e., $\Delta = \Delta^*$. Below we will lift this restriction. For the eigenvectors we get

$$\begin{pmatrix}\xi_k & -\Delta \\ -\Delta & -\xi_k\end{pmatrix}\begin{pmatrix} u_k \\ -v_k\end{pmatrix} = E_k\begin{pmatrix} u_k \\ -v_k\end{pmatrix} \tag{12}$$

and

$$\begin{pmatrix}\xi_k & -\Delta \\ -\Delta & -\xi_k\end{pmatrix}\begin{pmatrix} v_k \\ u_k\end{pmatrix} = -E_k\begin{pmatrix} v_k \\ u_k\end{pmatrix} \tag{13}$$

It is easy to find

$$v_k = \sqrt{\frac{1}{2}-\frac{\xi_k}{2E_k}} \tag{14}$$

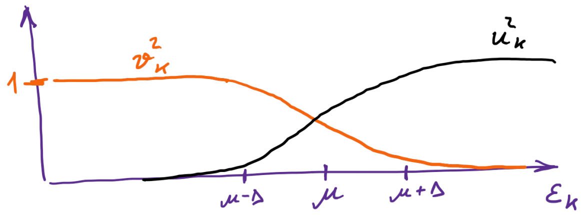

FIG. 2: Functions v_k^2 and v_k^2.

$$u_k = \sqrt{\frac{1}{2} + \frac{\xi_k}{2E_k}} \ . \tag{15}$$

These functions are shown in Fig. 2. Thus, if Δ is real, the functions v_k and u_k are also real and positive.

We use the matrix of eigenvectors to diagonalize the Hamiltonian:

$$U^\dagger \begin{pmatrix} \xi_k & -\Delta \\ -\Delta & -\xi_k \end{pmatrix} U = \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} \ , \tag{16}$$

where

$$U \equiv \begin{pmatrix} u_k & v_k \\ -v_k & u_k \end{pmatrix} \tag{17}$$

We obtain

$$H_{\rm BCS}^{\rm MF} = \sum_k \begin{pmatrix} c_{k,\uparrow}^\dagger & c_{-k,\downarrow} \end{pmatrix} UU^\dagger \begin{pmatrix} \xi_k & -\Delta \\ -\Delta & -\xi_k \end{pmatrix} UU^\dagger \begin{pmatrix} c_{k,\uparrow} \\ c_{-k,\downarrow}^\dagger \end{pmatrix} + \sum_k \xi_k + V\frac{\Delta^2}{g} \tag{18}$$

We use the diagonalization (16) and introduce the Bogoliubov transformation written in the matrix form as

$$\begin{pmatrix} \alpha_{k,\uparrow} \\ \alpha_{-k,\downarrow}^\dagger \end{pmatrix} = U^\dagger \begin{pmatrix} c_{k,\uparrow} \\ c_{-k,\downarrow}^\dagger \end{pmatrix} = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix} \begin{pmatrix} c_{k,\uparrow} \\ c_{-k,\downarrow}^\dagger \end{pmatrix} \tag{19}$$

to obtain

$$H_{\rm BCS}^{\rm MF} = \sum_k \begin{pmatrix} \alpha_{k,\uparrow}^\dagger & \alpha_{-k,\downarrow} \end{pmatrix} \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} \begin{pmatrix} \alpha_{k,\uparrow} \\ \alpha_{-k,\downarrow}^\dagger \end{pmatrix} + \sum_k \xi_k + V\frac{\Delta^2}{g} \tag{20}$$

Using again the commutation relations for the α operators we obtain

$$H_{\rm BCS}^{\rm MF} = \sum_{k,\sigma} E_k \alpha_{k,\sigma}^\dagger \alpha_{k,\sigma} + \sum_k (\xi_k - E_k) + V\frac{\Delta^2}{g} \ . \tag{21}$$

4. 4X4 Nambu formalism

In the 2X2 Nambu formalism presented above we have explicitly broken the symmetry between spin up and spin down. There is a way to do the same without breaking the symmetry. Introduce a 4-spinor $\begin{pmatrix} c_{k,\uparrow} & c_{k,\downarrow} & c^\dagger_{-k,\downarrow} & -c^\dagger_{-k,\uparrow} \end{pmatrix}$. Then

$$H^{\rm MF}_{\rm BCS} = \sum_k \begin{pmatrix} c^\dagger_{k,\uparrow} & c^\dagger_{k,\downarrow} & c_{-k,\downarrow} & -c_{-k,\uparrow} \end{pmatrix} \begin{pmatrix} \xi_k & 0 & -\Delta & 0 \\ 0 & \xi_k & 0 & 0 \\ -\Delta & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} c_{k,\uparrow} \\ c_{k,\downarrow} \\ c^\dagger_{-k,\downarrow} \\ -c^\dagger_{-k,\uparrow} \end{pmatrix} + V\frac{\Delta^2}{g} . \tag{22}$$

One observes, however, that there is a redundancy here and we can rewrite

$$H^{\rm MF}_{\rm BCS} = \sum_k \begin{pmatrix} c^\dagger_{k,\uparrow} & c^\dagger_{k,\downarrow} & c_{-k,\downarrow} & -c_{-k,\uparrow} \end{pmatrix} \begin{pmatrix} \xi_k & 0 & -\Delta/2 & 0 \\ 0 & \xi_k & 0 & -\Delta/2 \\ -\Delta/2 & 0 & 0 & 0 \\ 0 & -\Delta/2 & 0 & 0 \end{pmatrix} \begin{pmatrix} c_{k,\uparrow} \\ c_{k,\downarrow} \\ c^\dagger_{-k,\downarrow} \\ -c^\dagger_{-k,\uparrow} \end{pmatrix} + V\frac{\Delta^2}{g} . \tag{23}$$

Also the kinetic energy can be written in a more symmetric form

$$H^{\rm MF}_{\rm BCS} = \frac{1}{2}\sum_k \begin{pmatrix} c^\dagger_{k,\uparrow} & c^\dagger_{k,\downarrow} & c_{-k,\downarrow} & -c_{-k,\uparrow} \end{pmatrix} \begin{pmatrix} \xi_k & 0 & -\Delta & 0 \\ 0 & \xi_k & 0 & -\Delta \\ -\Delta & 0 & -\xi_k & 0 \\ 0 & -\Delta & 0 & -\xi_k \end{pmatrix} \begin{pmatrix} c_{k,\uparrow} \\ c_{k,\downarrow} \\ c^\dagger_{-k,\downarrow} \\ -c^\dagger_{-k,\uparrow} \end{pmatrix} + \sum_k \xi_k + V\frac{\Delta^2}{g} . \tag{24}$$

Of course the 4×4 matrix factorizes to two 2×2 matrices considered above. In this sense we did not achieve anything new. Yet, for superconductors with spin-orbit interaction or for systems like graphen or surfaces of topological insulators, the single-particle hamiltonian h_k is usually not diagonal. Then, the reduction to 2×2 representation is not possible and the 4×4 BdG matrix (for s-wave order parameter) looks like

$$\begin{pmatrix} h_k & -\Delta\sigma_0 \\ -\Delta^*\sigma_0 & -\sigma_y h^*_k \sigma_y \end{pmatrix}$$

.

5. Order parameter, phase

Thus far Δ was real. We could however introduce a complex order parameter $\Delta = |\Delta|e^{i\phi}$. It is easy to see that in the Nambu formalism described above this could be compensated by replacing $v_k \to v_k^* \equiv |v_k|e^{-i\phi}$ (so that $v_k = |v_k|e^{i\phi}$) and keeping u_k real. We still have

$$|v_k| = \sqrt{\frac{1}{2} - \frac{\xi_k}{2E_k}} \tag{25}$$

$$|u_k| = \sqrt{\frac{1}{2} + \frac{\xi_k}{2E_k}} \ . \tag{26}$$

That is the eigenvectors are now given by

$$\begin{pmatrix} \xi_k & -\Delta \\ -\Delta^* & -\xi_k \end{pmatrix} \begin{pmatrix} u_k \\ -v_k^* \end{pmatrix} = E_k \begin{pmatrix} u_k \\ -v_k^* \end{pmatrix} \tag{27}$$

and

$$\begin{pmatrix} \xi_k & -\Delta \\ -\Delta^* & -\xi_k \end{pmatrix} \begin{pmatrix} v_k^* \\ u_k \end{pmatrix} = -E_k \begin{pmatrix} v_k^* \\ u_k \end{pmatrix} \tag{28}$$

Introduction of the phase corresponds to a different BCS ground state:

$$|BCS(\phi)\rangle = \prod_k (|u_k| + e^{i\phi}|v_k| c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow}) \, |0\rangle \ . \tag{29}$$

Exercise: check that

$$|BCS(N)\rangle = \int_0^{2\pi} \frac{d\phi}{2\pi} \, |BCS(\phi)\rangle \, e^{-iN\phi} \tag{30}$$

gives a state with a fixed number of electrons N. Further details in Section III A.

It is easy to see that the operator $A^\dagger = e^{-i\phi}$ increases the number of Cooper pairs by one

$$A^\dagger \, |BCS(N)\rangle = \int_0^{2\pi} \frac{d\phi}{2\pi} \, |BCS(\phi)\rangle \, e^{-i(N+1)\phi} = |BCS(N+1)\rangle \ . \tag{31}$$

We have seen that the excitations above the BCS ground state have an energy gap Δ. Thus, if $T \ll \Delta$ no excitations are possible. The only degree of freedom left is the pair of conjugate variables N, ϕ with commutation relations $[N, e^{-i\phi}] = e^{-i\phi}$. Indeed the ground state energy is independent of ϕ. This degree of freedom is, of course, non-existent if the number of particles is fixed. Thus a phase of an isolated piece of a superconductor is quantum mechanically smeared between 0 and 2π and no dynamics of the degree of freedom N, ϕ is possible. However in a bulk superconductor the phase can be space dependent $\phi(\vec{r})$. One can still add a constant phase to $\phi(\vec{r}) + \phi_0$ without changing the state. More precisely the phase ϕ_0 is smeared if the total number of particles is fixed. However the difference of phases, i.e., the phase gradient can be well defined and corresponds to a super-current.

We have to consider the gauge invariance. The usual gauge transformation reads

$$\vec{A} \rightarrow \vec{A} + \vec{\nabla}\chi \ , \tag{32}$$

$$\Psi \rightarrow \Psi e^{\frac{ie}{\hbar c}\chi} \ , \tag{33}$$

where Ψ is the electron wave function (field). Comparing with (29) we see that adding phase ϕ corresponds to a transformation $c^{\dagger}_{k,\sigma} \rightarrow e^{i\phi/2} c^{\dagger}_{k,\sigma}$. This we identify

$$\frac{\phi}{2} = -\frac{e}{\hbar c}\chi \ . \tag{34}$$

Thus

$$\vec{A} \rightarrow \vec{A} - \frac{\hbar c}{2e}\vec{\nabla}\phi \tag{35}$$

We postulate here the gauge invariant form of the London equation

$$\vec{j}_s = -\frac{e^2 n_s}{mc}\left(\vec{A} - \frac{\hbar c}{2e}\vec{\nabla}\phi\right) \ , \tag{36}$$

where n_s is the density of superconducting electrons. At $T = 0$ all electrons are superconducting, thus $n_s = n$. We do not derive this relation here, but we do so later for the tunneling current between two superconductors with a phase difference between them.

6. *Flux quantization*

In the bulk of a superconductor, where $\vec{j}_s = 0$, we obtain

$$\vec{A} - \frac{\hbar c}{2e}\vec{\nabla}\phi = 0 \tag{37}$$

$$\oint \vec{A} d\vec{l} = \frac{\hbar c}{2e}\oint \vec{\nabla}\phi d\vec{l} = \frac{\hbar c}{2e} 2\pi n = \frac{hc}{2e} n = n\Phi_0 \tag{38}$$

This quantization is very important for, e.g., a ring geometry. If the ring is thick enough (thicker than λ_L) the total magnetic flux threading the ring is quantized.

7. Number and phase again

We analyze once again the quasiparticle annihilation operators introduced in Eq. (19). Taking into account the 4×4 generalization we can write

$$\alpha_{k,\uparrow} = |u_k| c_{k,\uparrow} - e^{i\phi} |v_k| c^\dagger_{-k,\downarrow} \ , \tag{39}$$

and

$$\alpha_{k,\downarrow} = |u_k| c_{k,\downarrow} + e^{i\phi} |v_k| c^\dagger_{-k,\uparrow} \ . \tag{40}$$

The difference in sign is because of the minus in the 4-spinor $\begin{pmatrix} c_{k,\uparrow} & c_{k,\downarrow} & c^\dagger_{-k,\downarrow} & -c^\dagger_{-k,\uparrow} \end{pmatrix}$. The short form reads

$$\alpha_{k,\sigma} = |u_k| c_{k,\sigma} - \sigma e^{i\phi} |v_k| c^\dagger_{-k,-\sigma} \ . \tag{41}$$

The factors $e^{i\phi}$ in (39) and (40) can be given a very important interpretation. On the first sight the operators $\alpha^\dagger_{k,\sigma} = |u_k| c^\dagger_{k,\sigma} - \sigma e^{-i\phi} |v_k| c_{-k,-\sigma}$ acting on a state with a given number of particles M creates a superposition of a state with $M+1$ particles and a state with $M-1$ particles. However, this is not so. Let us recall the role of the operator $e^{-i\phi}$. From the analysis after Eq. (29) we can conclude that the operator $e^{-i\phi}$ increases the number of Cooper pairs in the condensate by one. Thus the proper interpretation should read

$$\alpha^\dagger_{k,\sigma} = |u_k| c^\dagger_{k,\sigma} - \sigma S^\dagger |v_k| c_{-k,-\sigma} \ , \tag{42}$$

where $S^\dagger = e^{-i\phi}$ creates an extra Cooper pair in the condensate. This way the operator $\alpha^\dagger_{k,\sigma}$ adds a single electron to the system and creates a quasi-particle excitation. Of course one can also define another operator

$$\tilde{\alpha}^\dagger_{k,\sigma} = S \alpha^\dagger_{k,\sigma} = S |u_k| c^\dagger_{k,\sigma} - \sigma |v_k| c_{-k,-\sigma} \ . \tag{43}$$

This operator removes one electron from the system and creates a quasi-particle excitation. The operators S were already present in the original paper by Josephson [1] and are discussed in the book by Tinkham.

In what follows we will stick to the operators $\alpha_{k,\sigma}$ and not $\tilde{\alpha}_{k,\sigma}$. The inverse Bogoliubov transformation then reads

$$c_{k,\sigma} = |u_k| \alpha_{k,\sigma} + \sigma S |v_k| \alpha^\dagger_{-k,-\sigma} \ . \tag{44}$$

B. Josephson effect

We consider now a tunnel junction between two superconductors with different phases ϕ_L and ϕ_R. The Hamiltonian reads

$$H = H_{BCS,L} + H_{BCS,R} + H_T \ , \tag{45}$$

where the tunnelling Hamiltonian reads

$$H_T = \sum_{k_1,k_2,\sigma} T \left[R^\dagger_{k_1,\sigma} L_{k_2,\sigma} + L^\dagger_{k_2,\sigma} R_{k_1,\sigma} \right] \ . \tag{46}$$

Here $R_{k,\sigma} \equiv c^{(R)}_{k,\sigma}$ is the annihilation operator of an electron in the right superconductor. Two important things: 1) microscopically the electrons and not the quasiparticles tunnel; 2) tunnelling conserves spin.

1. *Original consideration by Josephson*

Josephson [1] used (55) and calculated the tunneling current. The current operator is given by time derivative of the number of particles in the right lead $N_R = \sum_{k,\sigma} R^\dagger_{k,\sigma} R_{k,\sigma}$

$$I = -e\dot{N}_R = -\frac{ie}{\hbar}[H_T, N_R] = \frac{ie}{\hbar} \sum_{k_1,k_2,\sigma} T \left[R^\dagger_{k_1,\sigma} L_{k_2,\sigma} - L^\dagger_{k_2,\sigma} R_{k_1,\sigma} \right] \ . \tag{47}$$

The first order time-dependent perturbation theory gives for the density matrix of the system in the interaction representation

$$\rho(t) = U(t)\rho_0 U^\dagger(t) \ , \tag{48}$$

where

$$U(t) \equiv T e^{-i\int_{-\infty}^{t} dt' H_T(t')} \ . \tag{49}$$

Alternatively, one can go to the Heisenberg picture, keeping the initial density matrix ρ_0 and calculating the Heisenberg current operator

$$I_H(t) = U^\dagger(t) I(t) U(t) \ , \tag{50}$$

where $I(t)$ stands for the current operator in the interaction representation. This gives (expanding the operators U and $U^\dagger$ to the first order

$$I_H(t) = I(t) - i\int_{-\infty}^{t} dt' \left[I(t), H_T(t') \right] \ . \tag{51}$$

Substituting (46) and (47) we would obtain several combinations of operators R and L. Some of these combinations are of the type $R^\dagger L L^\dagger R$. The others are of the type $R^\dagger L R^\dagger L$. Usually, e.g., in the non-superconducting case, the combination of the type $R^\dagger L R^\dagger L$ would give zero upon averaging with the density matrix ρ_0. However here we have, first, to go to the quasiparticle basis, in which the BCS ground state is simple. Using the Bogoliubov transformation

$$L_{k,\sigma} = |u_k|\alpha_{k,\sigma} + \sigma S_L |v_k| \alpha^\dagger_{-k,-\sigma} \ , \tag{52}$$

$$R_{k,\sigma} = |u_k|\beta_{k,\sigma} + \sigma S_R |v_k| \beta^\dagger_{-k,-\sigma} \ , \tag{53}$$

we observe that the combination $R^\dagger L R^\dagger L$ would contain terms of the type

$$S_R^\dagger |v|\beta|u|\alpha|u|\beta^\dagger S_L |v|\alpha^\dagger \sim |v||u||u||v|\, \beta\alpha\beta^\dagger\alpha^\dagger\, S_R^\dagger\, S_L \ . \tag{54}$$

In the BCS ground state the combination $\beta\alpha\beta^\dagger\alpha^\dagger$ averages to a non-zero value. The combination $S_R^\dagger\, S_L$ describes the transfer of one Cooper pair from left to right. If the left and the right phases are determined (broken $U(1)$ symmetry), $S_R^\dagger\, S_L$ becomes a number. The contributions of this type form the Josephson current.

2. *Calculation with gauge transformation*

A gauge transformation $L_{k,\sigma} \to e^{i\phi_L/2} L_{k,\sigma}$ and $R_{k,\sigma} \to e^{i\phi_R/2} R_{k,\sigma}$ "removes" the phases from the respective BCS wave functions (making v_k, u_k, and Δ real) and renders the tunneling Hamiltonian

$$H_T = \sum_{k_1,k_2,\sigma} T \left[R^\dagger_{k_1,\sigma} L_{k_2,\sigma} e^{-i\phi/2} + L^\dagger_{k_2,\sigma} R_{k_1,\sigma} e^{i\phi/2} \right] \ , \tag{55}$$

where $\phi \equiv \phi_R - \phi_L$. Note the similarity with the Full Counting Statistics.

We consider here a time-independent phase difference ϕ. The current operator is given by time derivative of the number of particles in the right lead $N_R = \sum_{k,\sigma} R^\dagger_{k,\sigma} R_{k,\sigma}$

$$I = -e\dot{N}_R = -\frac{ie}{\hbar}[H_T, N_R] = \frac{ie}{\hbar} \sum_{k_1,k_2,\sigma} T \left[R^\dagger_{k_1,\sigma} L_{k_2,\sigma} e^{-i\phi/2} - L^\dagger_{k_2,\sigma} R_{k_1,\sigma} e^{i\phi/2} \right] \ . \tag{56}$$

The first order time-dependent perturbation theory gives for the density matrix of the system in the interaction representation

$$\rho(t) = T e^{-i\int_{-\infty}^t dt' H_T(t')} \rho_0 \tilde{T} e^{i\int_{-\infty}^t dt' H_T(t')} \approx -i \int_{-\infty}^t dt' [H_T(t'), \rho_0] \ . \tag{57}$$

For the expectation value of the current this gives

$$\begin{aligned}\langle I(t)\rangle &= \mathrm{Tr}\{\rho(t)I(t)\} = -i\int_{-\infty}^{t} dt'\,\mathrm{Tr}\left\{[H_T(t'),\rho_0]I(t)\right\} = -i\int_{-\infty}^{t} dt'\,\mathrm{Tr}\left\{[I(t),H_T(t')]\,\rho_0\right\}\\ &= -i\int_{-\infty}^{t} dt'\,\langle[I(t),H_T(t')]\rangle_0\ . \end{aligned} \tag{58}$$

In particular, at zero temperature $\langle\ldots\rangle_0$ corresponds to averaging over BCS states on both superconductors. We obtain

$$[I(t),H_T(t')] = \frac{ie}{\hbar}T^2\sum_{k_1,k_2,\sigma,q_1,q_2,\gamma}$$
$$\left[\left(R^\dagger_{k_1,\sigma}(t)L_{k_2,\sigma}(t)e^{-i\phi/2} - L^\dagger_{k_2,\sigma}(t)R_{k_1,\sigma}(t)e^{i\phi/2}\right),\left(R^\dagger_{q_1,\gamma}(t')L_{q_2,\gamma}(t')e^{-i\phi/2} + L^\dagger_{q_2,\gamma}(t')R_{q_1,\gamma}(t')e^{i\phi/2}\right)\right] \tag{59}$$

To get Josephson current we collect only the terms in which the phase ϕ does not disappear. The other terms contribute only if ϕ is time-dependent. We, thus, are left with

$$[I(t),H_T(t')] = \ldots + \frac{ie}{\hbar}T^2\sum_{k_1,k_2,\sigma,q_1,q_2,\gamma}$$
$$e^{-i\phi}\left[\left(R^\dagger_{k_1,\sigma}(t)L_{k_2,\sigma}(t)\right),\left(R^\dagger_{q_1,\gamma}(t')L_{q_2,\gamma}(t')\right)\right] - e^{i\phi}\left[\left(L^\dagger_{k_2,\sigma}(t)R_{k_1,\sigma}(t)\right),\left(L^\dagger_{q_2,\gamma}(t')R_{q_1,\gamma}(t')\right)\right]\ , \tag{60}$$

where ... stands for omitted terms.

Upon averaging we obtain

$$\langle[I(t),H_T(t')]\rangle_0 = \ldots - \frac{ie}{\hbar}T^2\sum_{k_1,k_2,\sigma}\Big[$$
$$e^{-i\phi}\left\{\langle R^\dagger_{k_1,\sigma}(t)R^\dagger_{-k_1,-\sigma}(t')\rangle_0\langle L_{k_2,\sigma}(t)L_{-k_2,-\sigma}(t')\rangle_0 - \langle R^\dagger_{k_1,\sigma}(t')R^\dagger_{-k_1,-\sigma}(t)\rangle_0\langle L_{k_2,\sigma}(t')L_{-k_2,-\sigma}(t)\rangle_0\right\}$$
$$-e^{i\phi}\left\{\langle L^\dagger_{k_2,\sigma}(t)L^\dagger_{-k_2,-\sigma}(t')\rangle_0\langle R_{k_1,\sigma}(t)R_{-k_1,-\sigma}(t')\rangle_0 - \langle L^\dagger_{k_2,\sigma}(t')L^\dagger_{-k_2,-\sigma}(t)\rangle_0\langle R_{k_1,\sigma}(t')R_{-k_1,-\sigma}(t)\rangle_0\right\}$$
$$\Big]\ . \tag{61}$$

At zero temperature we use

$$\begin{aligned}&\langle c^\dagger_{k,\sigma}(t_1)\,c^\dagger_{-k,-\sigma}(t_2)\rangle_0 = \langle BCS|\,c^\dagger_{k,\sigma}(t_1)\,c^\dagger_{-k,-\sigma}(t_2)\,|BCS\rangle\\ &= \langle BCS|\left(u_k\alpha^\dagger_{k,\sigma}(t_1) + \sigma v_k\alpha_{-k,-\sigma}(t_1)\right)\left(u_k\alpha^\dagger_{-k,-\sigma}(t_2) - \sigma v_k\alpha_{k,\sigma}(t_2)\right)|BCS\rangle\\ &= \sigma v_k u_k e^{-iE_k(t_1-t_2)}\ ,\end{aligned} \tag{62}$$

and

$$
\begin{aligned}
&\langle BCS|\, c_{k,\sigma}(t_1)\, c_{-k,-\sigma}(t_2)\, |BCS\rangle \\
&= \langle BCS| \left(u_k \alpha_{k,\sigma}(t_1) + \sigma v_k \alpha^{\dagger}_{-k,-\sigma}(t_1)\right) \left(u_k \alpha_{-k,-\sigma}(t_2) - \sigma v_k \alpha^{\dagger}_{k,\sigma}(t_2)\right) |BCS\rangle \\
&= -\sigma v_k u_k e^{-iE_k(t_1-t_2)} \ , \qquad (63)
\end{aligned}
$$

After some algebra we obtain (from the anomalous correlators, the rest gives zero)

$$
\begin{aligned}
\langle I(t)\rangle = &- 2eT^2 e^{-i\phi} \int_{-\infty}^{t} dt' \sum_{k_1,k_2} v_{k_1} u_{k_1} v_{k_2} u_{k_2} \left[e^{-i(E_{k_1}+E_{k_2})(t-t')} - e^{i(E_{k_1}+E_{k_2})(t-t')}\right] \\
&+ 2eT^2 e^{i\phi} \int_{-\infty}^{t} dt' \sum_{k_1,k_2} v_{k_1} u_{k_1} v_{k_2} u_{k_2} \left[e^{-i(E_{k_1}+E_{k_2})(t-t')} - e^{i(E_{k_1}+E_{k_2})(t-t')}\right] \\
&= 8eT^2 \sin(\phi) \sum_{k_1,k_2} \frac{v_{k_1} u_{k_1} v_{k_2} u_{k_2}}{E_{k_1}+E_{k_2}} = 2eT^2 \sin(\phi) \sum_{k_1,k_2} \frac{\Delta^2}{E_{k_1} E_{k_2} (E_{k_1}+E_{k_2})} \\
&= 2\pi^2 T^2 \nu^2 e \Delta \hbar^{-1} \sin(\phi) = I_c \sin(\phi) \ , \qquad (64)
\end{aligned}
$$

where the Josephson critical current is given by

$$
I_c = \frac{g_T e \Delta}{4\hbar} = \frac{\pi \Delta}{2eR_T} \ , \qquad (65)
$$

where $g_T = 2 \times 4\pi^2 T^2 \nu^2$ is the dimensionless conductance of the tunnel junction (factor 2 accounts for spin), while the tunnel resistance is given by $R_T = \frac{h}{e^2} \frac{1}{g_T}$. This is the famous Ambegaokar-Baratoff relation [2] (see also erratum [3]). At finite temperature the relation reads (no derivation is provided, see Ref. [3]):

$$
I_c = \frac{\pi \Delta(T)}{2eR_T} \tanh\left(\frac{\beta \Delta(T)}{2}\right) \ , \qquad (66)
$$

where $\Delta(T)$ is the temperature dependent gap.

Thus we have obtained the first Josephson relation $I = I_c \sin\phi$. We have introduced the variable ϕ as the difference of two phases $\phi = \phi_R - \phi_L$. The gauge invariant definition reads

$$
\phi = \phi_R - \phi_L - \frac{2e}{\hbar c} \int_L^R \vec{A} d\vec{l} \ . \qquad (67)
$$

As a shortest way to the second Josephson relation we assume that an electric field exists in the junction and that it is only due to the time-dependence of $\vec{A}$. Then we obtain

$$
\dot{\phi} = -\frac{2e}{\hbar c} \int_L^R \left[\frac{\partial}{\partial t} \vec{A}\right] d\vec{l} = \frac{2e}{\hbar} \int_L^R \vec{E} d\vec{l} = -\frac{2e}{\hbar} V \ , \qquad (68)
$$

where V is the voltage. Here we all the time treated e as the charge of the electron, i.e., $e < 0$. Usually one uses e as a positive quantity. Then

$$\dot{\phi} = \frac{2eV}{\hbar} \ . \tag{69}$$

An alternative way to derive this is to start with a difference of (time-dependent) chemical potentials

$$H = H_L + H_R - eV_L(t) \sum_{k,\sigma} L^\dagger_{k,\sigma} L_{k,\sigma} - eV_R(t) \sum_{k,\sigma} R^\dagger_{k,\sigma} R_{k,\sigma} + H_T \ , \tag{70}$$

where $V_{L/R}$ are the applied electro-chemical potentials (in addition to the constant chemical potential μ, which is included in H_L and H_R). A transformation with

$$U = e^{\frac{e}{\hbar}\hat{N}_L \int^t V_L(t')dt'} \, e^{\frac{e}{\hbar}\hat{N}_R \int^t V_R(t')dt'} \tag{71}$$

In the new Hamiltonian

$$\tilde{H} = i\dot{U}U^{-1} + UHU^{-1} \ . \tag{72}$$

the terms with V_L and V_R are cancelled and instead the electronic operators are replaced by, e.g,

$$L \to ULU^{-1} = Le^{i\phi_L/2} \ , \tag{73}$$

where $\phi_L = const. - \frac{2e}{\hbar} \int^t V_L(t')dt'$ and, thus, $\dot{\phi} = \dot{\phi}_R - \dot{\phi}_L = -\frac{2e}{\hbar}V$.

C. Macroscopic quantum phenomena

1. *Resistively shunted Josephson junction (RSJ) circuit*

Consider a circuit of parallelly connected Josephson junction and a shunt resistor R. A Josephson junction is simultaneously a capacitor. An external current I_{ex} is applied. The Kirchhoff rules lead to the ecquation

$$I_c \sin\phi + \frac{V}{R} + \dot{Q} = I_{ex} \ . \tag{74}$$

As $Q = CV$ and $V = \frac{\hbar}{2e}\dot{\phi}$. Thus we obtain

$$I_c \sin\phi + \frac{\hbar}{2eR}\,\dot{\phi} + \frac{\hbar C}{2e}\,\ddot{\phi} = I_{ex} \ . \tag{75}$$

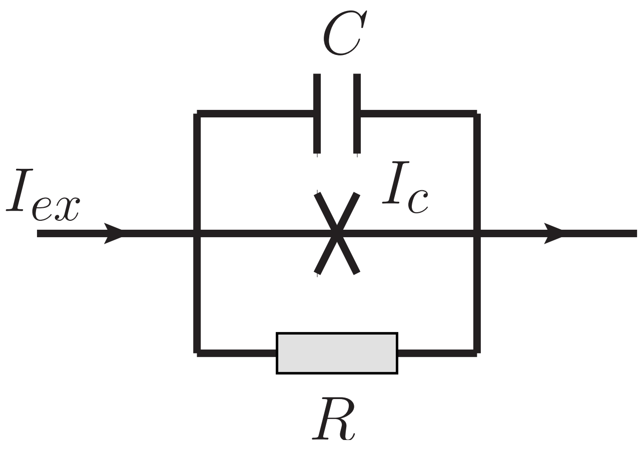

FIG. 3: RSJ Circuit.

It is very convenient to measure the phase in units of magnetic flux, so that $V = \frac{1}{c}\dot{\Phi}$ (in SI units $V = \dot{\Phi}$):

$$\Phi = \frac{c\hbar}{2e}\,\phi = \frac{\Phi_0}{2\pi}\,\phi \quad , \quad \phi = 2\pi\frac{\Phi}{\Phi_0} \ . \tag{76}$$

Then the Kirchhoff equation reads

$$I_c \sin\left(2\pi\frac{\Phi}{\Phi_0}\right) + \frac{\dot{\Phi}}{cR} + \frac{C\ddot{\Phi}}{c} = I_{ex} \ , \tag{77}$$

or in SI units

$$I_c \sin\left(2\pi\frac{\Phi}{\Phi_0}\right) + \frac{\dot{\Phi}}{R} + C\ddot{\Phi} = I_{ex} \ . \tag{78}$$

There are two regimes. In case $I_{ex} < I_c$ there exists a stationary solution $\phi = \arcsin(I_{ex}/I_c)$. All the current flows through the Josephson contact as a super-current. Indeed $V \propto \dot{\phi} = 0$. At $I_{ex} > I_c$ at least part of the current must flow through the resistor. Thus a voltage develops and the phase starts to ”run”.

2. *Particle in a washboard potential*

The equation of motion (78) can be considered as an equation of motion of a particle with the coordinate $x = \Phi$. We must identify the capacitance with the mass, $m = C$, the inverse resistance with the friction coefficient $\gamma = R^{-1}$. Then we have

$$m\ddot{x} = -\gamma\dot{x} - \frac{\partial U}{\partial x} \ , \tag{79}$$

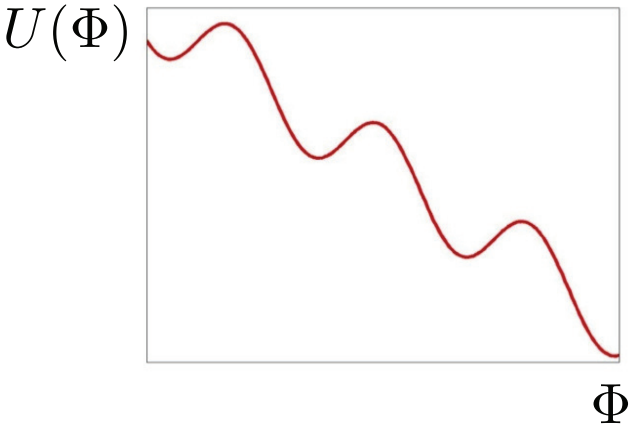

FIG. 4: Washboard potential.

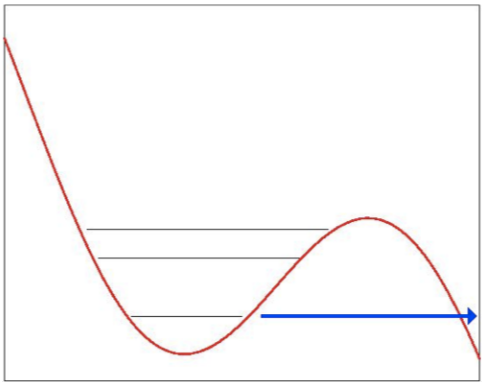

FIG. 5: Macroscopic Quantum Tunneling (MQT).

where for the potential we obtain

$$U(\Phi) = -E_J \cos\left(2\pi \frac{\Phi}{\Phi_0}\right) - I_{ex}\Phi \ , \tag{80}$$

where

$$E_J \equiv \frac{I_c \Phi_0}{2\pi} = \frac{\hbar I_c}{2e} \tag{81}$$

is called the Josephson energy. The potential energy $U(\Phi)$ has a form of a washboard and is called a washboard potential. In Fig. 4 the case $I_{ex} < I_c$ is shown. In this case the potential has minima and, thus, classically stationary solutions are possible.

When the external current is close to the critical value a situation shown in Fig. 5 emerges. If we allow ourselves to think of this situation quantum mechanically, then we would conclude that only a few quantum levels should remain in the potential well. Moreover a tunneling process out of the well should become possible. This tunneling process was named Macro-

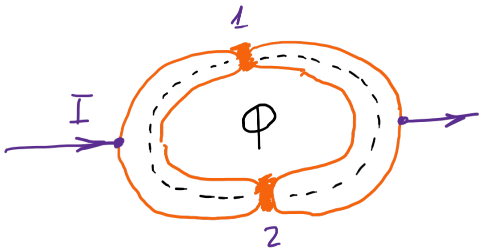

FIG. 6: dc-SQUID. The superconducting parts assumed thicker that λ_L. The dashed line is deep in the superconducting parts so that the superconducting velocity there vanishes. This is used for the discussion of the flux dependence.

scopic Quantum Tunneling because in the 80-s and the 90-s many researchers doubted the fact one can apply quantum mechanics to the dynamics of the "macroscopic" variable Φ. It was also argued that a macroscopic variable is necessarily coupled to a dissipative bath which would hinder the tunneling. Out these discussions the famous Caldeira-Leggett model emerged [4, 5].

3. dc-SQUID

The simplest dc-SQUID (Superconducting QUantum Interference Device) is shown in Fig. 6. It consists of two Josephson junctions in a superconducting ring. The current bias is applied. The simplest case is when the superconducting parts of the ring are thick (thicker than the London penetration depth λ_L). Then along the dashed line in Fig. 6 the superconducting velocity vanishes. That is

$$\left(\vec{A} + \frac{\hbar c}{2e}\vec{\nabla}\phi\right) = 0 \tag{82}$$

along the dashed line (in the electrodes) but not in the junctions. Integrating along a closed contour we obtain for the total flux Φ:

$$\begin{aligned} \Phi &= \oint \vec{A}d\vec{l} = \int_{electrodes} \vec{A}d\vec{l} + \int_{junctions} \vec{A}d\vec{l} \\ &= -\frac{\Phi_0}{2\pi}\int_{electrodes} \vec{\nabla}\phi\, d\vec{l} + \int_{junctions} \vec{A}d\vec{l} \end{aligned} \tag{83}$$

The phase of the order parameter is single valued $(mod(2\pi))$. Therefore

$$\int_{electrodes} \vec{\nabla}\phi\, d\vec{l} + \Delta\phi_1 + \Delta\phi_2 = 0[mod(2\pi)]. \tag{84}$$

Here $\Delta\phi_1$ and $\Delta\phi_2$ are the phase drops counted according to the integration direction (later on the contour minus earlier on the contour). This gives

$$\frac{\Phi_0}{2\pi}\Delta\phi_1 + \int_{junction\ 1} \vec{A}d\vec{l} + \frac{\Phi_0}{2\pi}\Delta\phi_2 + \int_{junction\ 2} \vec{A}d\vec{l} = \Phi[mod(\Phi_0)] \ . \tag{85}$$

This can be written as

$$\phi_1 + \phi_2 = \frac{2\pi\Phi}{\Phi_0} \ , \tag{86}$$

where ϕ_1 and ϕ_2 are the gauge invariant phase drops on the junctions (counted in the direction of the contour). Here we use a clockwise contour in Fig. 6 and, thus, a positive magnetic flux ”goes into the picture”. Recalling the discussion on the signs of the phase drops at the end of Sec.**??** we obtain for the current (from left to right)

$$I = -I_c \sin\phi_1 + I_c \sin\phi_2 \ . \tag{87}$$

For simplicity we assume here that the two critical currents are equal.

Of course, we can now change the signs of ϕ_1 and ϕ_2 and get the commonly used

$$I = I_c \sin\phi_1 - I_c \sin\phi_2 \ . \tag{88}$$

This gives

$$I = 2I_c \sin\frac{\phi_1 - \phi_2}{2} \cdot \cos\frac{\phi_1 + \phi_2}{2} = 2I_c \cos\frac{\pi\Phi}{\Phi_0} \cdot \sin\frac{\phi_1 - \phi_2}{2} \tag{89}$$

The combination $(\phi_1 - \phi_2)/2$ is the effective phase drop in the SQUID considered as an effective Josephson junction. The effective critical current is given by

$$I_c^{SQUID} = 2I_c \left|\cos\frac{\pi\Phi}{\Phi_0}\right| \ . \tag{90}$$

4. Quantization

We write down the Lagrangian that would give the equation of motion (79 or 78). Clearly we cannot include the dissipative part in the Lagrange formalism. Thus we start from the limit $R \to \infty$. The Lagrangian reads

$$L = \frac{C\dot{\Phi}^2}{2} - U(\Phi) = \frac{C\dot{\Phi}^2}{2} + E_J \cos\left(2\pi\frac{\Phi}{\Phi_0}\right) + I_{ex}\Phi \ . \tag{91}$$

We transform to the Hamiltonian formalism and introduce the canonical momentum

$$Q \equiv \frac{\partial L}{\partial\dot{\Phi}} = C\dot{\Phi} \ . \tag{92}$$

The Hamiltonian reads

$$H = \frac{Q^2}{2C} + U(\Phi) = \frac{Q^2}{2C} - E_J \cos\left(2\pi\frac{\Phi}{\Phi_0}\right) - I_{ex}\Phi \ . \tag{93}$$

The canonical momentum corresponds to the charge on the capacitor (junction). The usual commutation relations should be applied

$$[\Phi, Q] = i\hbar \ . \tag{94}$$

In the Hamilton formalism it is inconvenient to have an unbounded from below potential. Thus we try to transform the term $-I_{ex}\Phi$ away. This can be achieved by the following canonical transformation

$$R = \exp\left[-\frac{i}{\hbar}Q_{ex}(t)\Phi\right] \ , \tag{95}$$

where $Q_{ex}(t) \equiv \int^t I_{ex}(t')dt'$. Indeed the new Hamiltonian reads

$$\tilde{H} = RHR^{-1} + i\hbar\dot{R}R^{-1} = \frac{(Q - Q_{ex}(t))^2}{2C} - E_J \cos\left(2\pi\frac{\Phi}{\Phi_0}\right) \ . \tag{96}$$

The price we pay is that the new Hamiltonian is time-dependent. The Hamiltonian (96) is very interesting. Let us investigate the operator

$$\cos\left(2\pi\frac{\Phi}{\Phi_0}\right) = \cos\left(\frac{2e}{\hbar}\Phi\right) = \frac{1}{2}\exp\left[\frac{i}{\hbar}2e\,\Phi\right] + h.c. \tag{97}$$

We have

$$\exp\left[\frac{i}{\hbar}2e\,\Phi\right]|Q\rangle = |Q + 2e\rangle \quad , \quad \exp\left[-\frac{i}{\hbar}2e\,\Phi\right]|Q\rangle = |Q - 2e\rangle \ . \tag{98}$$

Thus in this Hamiltonian only the states differing by an integer number of Cooper pairs get connected. The constant offset charge remains undetermined. This, however, can be absorbed into the bias charge Q_{ex}. Thus, we can restrict ourselves to the Hilbert space $|Q = 2em\rangle$.

5. *Josephson energy dominated regime*

In this regime $E_J \gg E_C$, where $E_C = \frac{(2e)^2}{2C}$ is the Cooper pair charging energy. Let us first neglect E_C completely, i.e., put $C = \infty$. Recall that C plays the role of the mass. Then the Hamiltonian reads $H = -E_J\cos\left(2\pi\frac{\Phi}{\Phi_0}\right)$. On one hand it is clear that the relevant state are

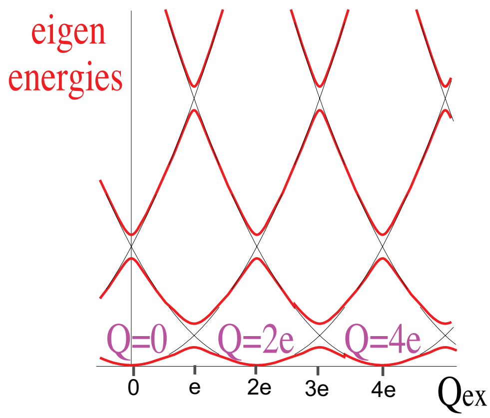

FIG. 7: Eigen levels in the coulomb blockade regime. Different parabolas correspond to different values of $Q = 2em$. The red lines represent the eigenlevels with the Josephson energy taken into account. The Josephson tunneling lifts the degeneracy between the charge states.

those with a given phase, i.e., $|\Phi\rangle$. On the other hand, in the discrete charge representation the Hamiltonian reads

$$H = -\frac{E_J}{2}\sum_m \left(|m+1\rangle\langle m| + |m\rangle\langle m+1|\right) \ . \tag{99}$$

The eigenstates of this tight-binding Hamiltonian are the Bloch waves $|k\rangle = \sum_m e^{ikm}|m\rangle$ with the wave vector k belonging to the first Brillouin zone $-\pi \le k \le \pi$. The eigenenergy reads $E_k = -E_J\cos(k)$. Thus we identify $k = \phi = \frac{2\pi\Phi}{\Phi_0}$.

6. Charging energy dominated regime

In this regime $E_J \ll E_C$. The main term in the Hamiltonian is the charging energy term

$$H_C = \frac{(Q - Q_{ex}(t))^2}{2C} = \frac{(2em - Q_{ex})^2}{2C} \ . \tag{100}$$

The eigenenergies corresponding to different values of m form parabolas as functions of Q_{ex} (see Fig. 7). The minima of the parabolas are at $Q_{ex} = 0, 2e, 4e, \ldots$. The Josephson tunneling term serves now as a perturbation $H_J = -E_J\cos\left(2\pi\frac{\Phi}{\Phi_0}\right)$. It lifts the degeneracies, e.g., at $Q_{ex} = e, 3e, 5e, \ldots$.

If a small enough external current is applied, $Q_{ex} = I_{ex}t$ the adiabatic theorem holds and the system remains in the ground state. Yet, one can see that between the degeneracies

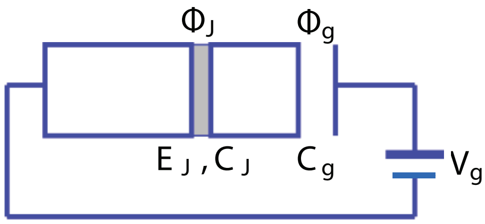

FIG. 8: Cooper Pair Box. The Josephson tunnel junction is characterized by the Josephson energy E_J and by the capacitance C_J. The superconducting island is controlled by the gate voltage V_g via the gate capacitance C_g. To derive the system's Lagrangian and Hamiltonian we introduce the phase drop on the Josephson junction Φ_J and the phase drop on the gate capacitor Φ_g.

at $Q_{ex} = e, 3e, 5e, \ldots$ the capacitance is charged and discharged and oscillating voltage $V = \partial E_0/\partial Q_{ex}$ appears. Here $E_0(Q_{ex})$ is the energy of the ground state. The Cooper pairs tunnel only at the degeneracy points. In between the Coulomb blockade prevents the Cooper pairs from tunneling because this would cost energy.

II. VARIOUS QUBITS

A. Charge qubit

We start by considering the so called Cooper pair box shown in Fig. 8. We derive the Hamiltonian starting from the Lagrangian

$$L = \frac{C_J \dot{\Phi}_J^2}{2} + \frac{C_g \dot{\Phi}_g^2}{2} - U_J(\Phi_J) \ , \tag{101}$$

where $U_J = -E_J \cos\left(2\pi \frac{\Phi_J}{\Phi_0}\right)$. The sum of all the phases along the loop must vanish and the phase on the voltage source is given by $const. + V_g t$. Thus we obtain

$$\dot{\Phi}_g = -\dot{\Phi}_J - V_g \tag{102}$$

and the Lagrangian in terms of the only generalized coordinate Φ_J reads

$$\begin{aligned} L &= \frac{C_J \dot{\Phi}_J^2}{2} + \frac{C_g(\dot{\Phi}_J + V_g)^2}{2} - U_J(\Phi_J) \\ &= \frac{(C_J + C_g)\dot{\Phi}_J^2}{2} + C_g \dot{\Phi}_J V_g - U_J(\Phi_J) + const. \ . \end{aligned} \tag{103}$$

The conjugated momentum (charge) reads

$$Q = \frac{\partial L}{\partial \dot{\Phi}_J} = (C_J + C_g)\dot{\Phi}_J + C_g V_g \ . \tag{104}$$

Since $C_J\dot{\Phi}_J$ is the charge on the Josephson junction capacitance while $C_g\dot{\Phi}_J + C_g V_g = -C_g\dot{\Phi}_g$ is minus the charge on the gate capacitance we conclude that $Q = 2em$ is the charge on the island (we disregard here the possibility to have an odd number of electrons on the island). We obtain

$$\dot{\Phi}_J = \frac{Q - C_g V_g}{C_J + C_g} \ . \tag{105}$$

The Hamiltonian reads

$$\begin{aligned} H = Q\,\dot{\Phi}_J - L \ &= \ \frac{(Q - C_g V_g)^2}{2(C_J + C_g)} + U_J(\Phi_J) \\ &= \ \frac{(Q - C_g V_g)^2}{2(C_J + C_g)} - E_J \cos\left(2\pi\,\frac{\Phi_J}{\Phi_0}\right) \ . \end{aligned} \tag{106}$$

This is exactly the Hamiltonian (96) with $Q_{ex} = C_g V_g$. The two level system is formed by the two lowest levels around $C_g V_g = e + 2eN$.

In Hamiltonian (106) the interplay of two energy scales determines the physical regime. These are 1) Josephson energy E_J; 2) Charging energy $E_C \equiv \frac{(2e)^2}{2(C_J+C_g)}$. In the simplest regime $E_J \ll E_C$ and for $Q_{ex} \sim e$ one can restrict the Hilbert space to two charge states with lowest charging energies $|\uparrow\rangle = |Q = 0\rangle$ and $|\downarrow\rangle = |Q = 2e\rangle$. In this Hilbert space we have

$$\cos\left(2\pi\,\frac{\Phi_J}{\Phi_0}\right) = \frac{1}{2}\,\sigma_x \ , \tag{107}$$

and

$$Q = e(1 - \sigma_z) \ . \tag{108}$$

Substituting these to (106) and disregarding constant energy shifts we obtain

$$H = -\frac{1}{2}\left(1 - \frac{Q_{ex}}{e}\right) E_C\,\sigma_z - \frac{1}{2}\,E_J\,\sigma_x \ . \tag{109}$$

Thus we obtain an effective spin-1/2 in a magnetic field whose z-component can be controlled by the gate voltage.

In Fig. 9 a charge qubit is shown in which the Josephson junction was replaced by a dc-SQUID. A straightforward derivation (assuming the geometrical inductance of the SQUID loop being vanishingly small) gives again the Hamiltonian (106) with $C_J \to 2C_J$ (just because there are two junctions instead of one) and

$$E_J \to 2E_J^{(0)} \cos\left(\frac{\pi\Phi_x}{\Phi_0}\right) \ . \tag{110}$$

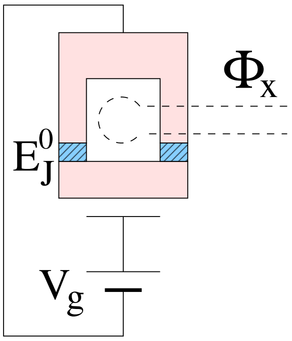

FIG. 9: Charge quit with controllable Josephson energy.

Here $E_J^{(0)}$ is the Josephson energy of a single junction. We assume the two junctions of the SQUID to be identical. Now we can control also the x-component of the effective magnetic field.

1. *Transmon*

A "Transmon" qubit is essentially a charge qubit shunted by a large capacitance in order to decrease the charging energy. The Hamiltonian can be written as

$$H = E_C(n - q_g)^2 - E_J \cos\phi \ , \tag{111}$$

where $q_g \equiv Q_g/2e = C_g V_g/2e$ is the dimensionless gate charge. The quantization is provided by the relation $e^{i\phi}|n\rangle = |n+1\rangle$. The system is controlled by the time-dependent $q_g(t)$. Due to the shunt capacitance one decreases the charging energy and reaches the regime $E_C < E_J$. In this case it is not sufficient to consider only two charge states.

B. Flux qubit

1. *RF-SQUID*

The simplest flux qubit is called RF-SQUID (Radio-Frequency-Superconducting-QUantum-Interference-Device) and is shown in Fig. 10 We recall the London equation $\vec{j}_s = -\frac{e^2 n_s}{mc}\left(\vec{A} - \frac{\hbar c}{2e}\vec{\nabla}\phi\right)$ and the fact that the super-current density $\vec{j}_s$ vanishes in the bulk of the superconductor. Thus assuming the ring in thick and integrating along the line which is in the middle of the ring (see Fig. 10) we obtain (we integrate clockwise along the dashed

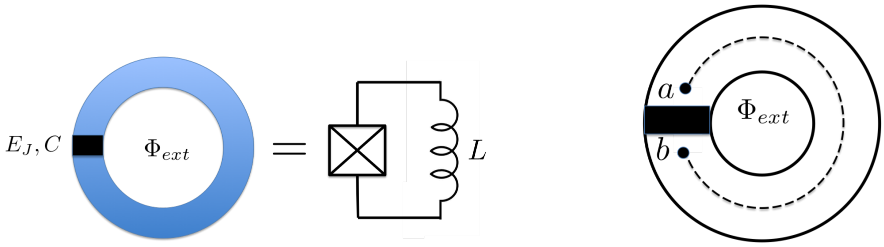

FIG. 10: RF-SQUID.

line)

$$0 = \int_a^b \left(\vec{A} - \frac{\hbar c}{2e}\vec{\nabla}\phi\right) d\vec{l} = \int_a^b \vec{A}d\vec{l} - \frac{\hbar c}{2e}(\phi_b - \phi_a) \ , \tag{112}$$

$$\frac{\hbar c}{2e}(\phi_b - \phi_a) = \int_a^b \vec{A}d\vec{l} \ . \tag{113}$$

$$\frac{\hbar c}{2e}(\phi_b - \phi_a) + \int_b^a \vec{A}d\vec{l} = \oint \vec{A}d\vec{l} = \Phi \ , \tag{114}$$

where Φ is the total flux through the ring. Thus the gauge invariant phase drop across the Josephson junction reads:

$$\Delta\phi = (\phi_a - \phi_b) - \frac{2e}{\hbar c}\int_b^a \vec{A}d\vec{l} = -\frac{2e}{\hbar c}\Phi = -2\pi\frac{\Phi}{\Phi_0} \ . \tag{115}$$

The Josephson energy can be written then as $-E_J \cos(\Delta\phi) = -E_J \cos(2\pi\Phi/\Phi_0)$. For the inductive energy we observe that the flux created by the current in the ring is given by $\Phi - \Phi_{ext}$. Thus the inductive energy reads $(\Phi - \Phi_{ext})^2/2L$. Finally the energy of the electric field reads $C\dot{\Phi}^2/2$. Thus, the Lagrangian of the system reads:

$$\mathcal{L} = \frac{C\dot{\Phi}^2}{2} - U(\Phi) \ , \tag{116}$$

where

$$U(\Phi) = \frac{(\Phi - \Phi_{ext})^2}{2L} - E_J \cos\left(\frac{2\pi\Phi}{\Phi_0}\right) \ . \tag{117}$$

At $\Phi_{ext} = \Phi_0/2$ we obtain a double-well potential.

C. 3-junction flux qubit

For a loop with three junction (a qubit proposed by J.E. Mooij, Fig 11) there are three gauge invariant phase drops across the three junctions (measured in units of flux), Φ_1, Φ_2,

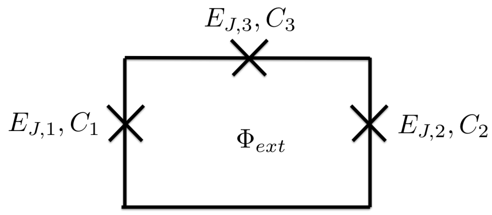

FIG. 11: 3-junction flux qubit. Proposed by J.E. Mooij et al.

Φ_3 and the argument similar to the provided for the RF-SQUIS gives

$$\Phi_1 + \Phi_2 + \Phi_3 = -\Phi \ , \tag{118}$$

where Φ is the total flux in the ring. Neglecting the geometric inductance of the ring we have $\Phi = \Phi_{ext}$. Thus we are left with two dynamical variables Φ_1 and Φ_2, whereas $\Phi_3 = -\Phi_{ext} - \Phi_1 - \Phi_2$. The Lagrangian reads

$$\mathcal{L} = K - U \ , \tag{119}$$

where

$$K = \frac{C_1\dot{\Phi}_1^2}{2} + \frac{C_2\dot{\Phi}_2^2}{2} + \frac{C_3(\dot{\Phi}_1 + \dot{\Phi}_2)^2}{2} \ , \tag{120}$$

and

$$U = -E_{J,1}\cos\left(\frac{2\pi\Phi_1}{\Phi_0}\right) - E_{J,2}\cos\left(\frac{2\pi\Phi_2}{\Phi_0}\right) - E_{J,3}\cos\left(\frac{2\pi(\Phi_1 + \Phi_2 + \Phi_{ext})}{\Phi_0}\right) \ . \tag{121}$$

An interesting regime arises for $E_{J,1} = E_{J,2}$ and $E_{J,3} = \alpha E_{J,1}$, where $\alpha \sim 0.7$.

D. Fluxonium

The Lagrangian is the same as that of an RF-SQUID

$$\mathcal{L} = \frac{C\dot{\Phi}^2}{2} - \frac{(\Phi - \Phi_{ext})^2}{2L} + E_J\cos\left(\frac{2\pi\Phi}{\Phi_0}\right) \ , \tag{122}$$

which gives the Hamiltonian

$$\mathcal{H} = \frac{Q^2}{2C} - \frac{(\Phi - \Phi_{ext})^2}{2L} + E_J\cos\left(\frac{2\pi\Phi}{\Phi_0}\right) \ . \tag{123}$$

III. BCS STATE WITH N COOPER PAIRS

A. BCS state with N Cooper pairs

Above we have introduced a BCS ground state with a phase ϕ:

$$|BCS(\phi)\rangle = \prod_k (u_k + e^{i\phi} v_k c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow})\,|0\rangle \quad . \tag{124}$$

(We now assume $v_k = |v_k|$ to be real and write the phase explicitly.) We have argued that state

$$|BCS(N)\rangle = \int_0^{2\pi} \frac{d\phi}{2\pi}\,|BCS(\phi)\rangle\, e^{-iN\phi} \tag{125}$$

gives a state with a fixed number of Cooper pairs N.

Here we try to see if the state $|BCS(N)\rangle$ corresponds to the same expectation value of the energy as the state $|BCS(\phi)\rangle$. First we discuss the normalization. Generalising Eqs. (**??**) we obtain

$$\begin{aligned}\langle BCS(\phi_2)|\,BCS(\phi_1)\rangle &= \langle 0|\prod_{k_2}(u_{k_2} + e^{-i\phi_2}\, v_{k_2} c_{-k_2,\downarrow} c_{k_2,\uparrow}) \prod_{k_1}(u_{k_1} + e^{i\phi_1}\, v_{k_1} c^\dagger_{k_1,\uparrow} c^\dagger_{-k_1,\downarrow})\,|0\rangle \\ &= \prod_k (u_k^2 + e^{i(\phi_1-\phi_2)}\, v_k^2) \ .\end{aligned} \tag{126}$$

Thus,

$$\begin{aligned}\langle BCS(N)|\,BCS(N)\rangle &= \int_0^{2\pi}\frac{d\phi_1}{2\pi}\int_0^{2\pi}\frac{d\phi_2}{2\pi}\, e^{-iN(\phi_1-\phi_2)}\,\langle BCS(\phi_2)|\,BCS(\phi_1)\rangle \\ &= \int_0^{2\pi}\frac{d\phi_1}{2\pi}\int_0^{2\pi}\frac{d\phi_2}{2\pi}\, e^{-iN(\phi_1-\phi_2)}\,\prod_k (u_k^2 + e^{i(\phi_1-\phi_2)}\, v_k^2) \\ &= \int_0^{2\pi}\frac{d\phi_1}{2\pi}\int_0^{2\pi}\frac{d\phi_2}{2\pi}\, e^{-iN(\phi_1-\phi_2)}\, e^{\sum_k \ln(u_k^2 + e^{i(\phi_1-\phi_2)}\, v_k^2)} \\ &= \int_0^{2\pi}\frac{d\phi_1}{2\pi}\int_0^{2\pi}\frac{d\phi_2}{2\pi}\, e^{-iN(\phi_1-\phi_2)}\, e^{\sum_k \ln(1+\left[e^{i(\phi_1-\phi_2)}-1\right]\, v_k^2)} \ .\end{aligned} \tag{127}$$

Assuming $N \gg 1$ we can use the stationary phase approximation and expand in $\phi_1 - \phi_2$. We obtain

$$\langle BCS(N)|\,BCS(N)\rangle = \int_0^{2\pi}\frac{d\phi_1}{2\pi}\int_0^{2\pi}\frac{d\phi_2}{2\pi}\, e^{-iN(\phi_1-\phi_2)}\, e^{\sum_k \left[i(\phi_1-\phi_2)v_k^2 - \frac{(\phi_1-\phi_2)^2}{2}\left(v_k^2 - v_k^4\right)\right]} \ . \tag{128}$$

We estimate $\sum_k v_k^2 \sim N(\mu)$, where $N(\mu)$ is (half) the number of electrons in a Fermi gas with chemical potential μ. Further,

$$A \equiv \sum_k (v_k^2 - v_k^4) = \sum_k \frac{1}{4} \frac{\Delta^2}{\Delta^2 + \xi_k^2} \approx \frac{\pi}{4} V \nu_0 \Delta \ , \tag{129}$$

where ν_0 is the density of states (per spin direction) at the Fermi surface and V is the volume. In sufficiently large systems $V\nu_0\Delta \gg 1$. (Moreover, if the system is so small that $V\nu_0\Delta < 1$, the superconductivity becomes impossible.) This gives

$$\begin{aligned} \langle BCS(N)|\, BCS(N)\rangle \ &= \int_0^{2\pi} \frac{d\phi_1}{2\pi} \int_0^{2\pi} \frac{d\phi_2}{2\pi}\, e^{-i(N-N(\mu))(\phi_1-\phi_2) - \frac{A(\phi_1-\phi_2)^2}{2}} \\ &\approx \frac{1}{\sqrt{2\pi A}} \exp\left[-\frac{(N-N(\mu))^2}{2A}\right] \end{aligned} \tag{130}$$

Thus, we see that if $|N - N(\mu)| \ll \sqrt{V\nu_0\Delta}$ the properly normalized state is

$$|BCS(N)\rangle_{\rm Norm} = (2\pi A)^{1/4} \int_0^{2\pi} \frac{d\phi}{2\pi}\, |BCS(\phi)\rangle\, e^{-iN\phi} \tag{131}$$

In conclusion, the projection of the BCS wave function on a state with a fixed number of particles works well if this number is sufficiently close to the one dictated by the chemical potential.

---

[1] B. D. Josephson, Physics Letters **1**, 251 (1962).

[2] V. Ambegaokar and A. Baratoff, Phys. Rev. Lett. **10**, 486 (1963).

[3] V. Ambegaokar and A. Baratoff, Phys. Rev. Lett. **11**, 104 (1963).

[4] A. O. Caldeira and A. J. Leggett, Phys. Rev. Lett. **46**, 211 (1981).

[5] A. O. Caldeira and A. J. Leggett, Annals of Physics **149**, 374 (1983).