CONTRIBUTION TO THE THEORY OF TUNNELING IN SUPERCONDUCTORS

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A kinetic approach is proposed to the theory of the tunnel effect in superconductors, making it possible to develop a theory for the nonstationary Josephson current. Conditions are considered under which the nonstationary current arises, and a physical interpretation of the effect is presented.

THE theory of the tunnel effect in superconductors was constructed on the basis of the microscopic theory of superconductivity[1,2] in many recent papers.[3-8] The starting point of these investigations is an approach based on the use of a model described by a so-called tunnel Hamiltonian. This model was proposed first in explicit form in the paper of Cohen, Falicov, and Phillips.[3] The use of this approach has made it possible not only to describe theoretically several singularities of tunneling already discovered experimentally in superconductors, but also to predict (see [4]) new interesting effects, subsequently observed in experiments:[9] 1) stationary current at zero voltage on the junction, and 2) oscillations of the current at nonzero voltage (we shall henceforth refer to them as the "first" and "second" Josephson effects).

However, a convincing theory of the Josephson alternating current is still missing. First, the microscopic analysis given in [4-8] is utterly unsuitable in the case of alternating voltage on the barrier, which is precisely realized in the experiment. The physical nature of the effect remains unclear. Ambegaokar and Baratoff[5] even expressed doubts whether the main premise of the theory of the existence of a coherent phase different between the superconductors remains in force at nonzero voltage.

The purpose of this article is to construct a new theoretical scheme, based on the use of a kinetic approach, which would permit a general analysis of the effect and its physical interpretation. Considerable attention will be paid to the question of the occurrence of a coherent phase difference. We note that the problem of justifying the model itself was discussed by Prange.[10]

The tunnel Hamiltonian is of the form

$$H = H_1 + H_2 + T. \tag{1}$$

Here H_1 and H_2 are the Hamiltonian of the first and second (left and right) superconductors, and T is an operator describing the transitions of the electrons through the dielectric layer separating the superconductors. In terms of the creation and annihilation operators of the "left" and "right" electrons, the operator T is written

$$T = \sum_{kq\sigma} (T_{kq} a_{k\sigma}^+ a_{q\sigma} + T_{kq}^* a_{q\sigma}^+ a_{k\sigma}). \tag{2}$$

The index k pertains here to the left single-particle states, q to the right, σ is the spin variable, and T_{kq} is the matrix element determining the electron tunneling probability.

For the Hamiltonian of any of the superconductors, for example H_1, we assume the usual approximation of superconductivity theory:

$$H_1 = \sum_{k\sigma} \varepsilon_k a_{k\sigma}^+ a_{k\sigma} - \frac{g_1}{2V} \sum_{kk'\sigma} a_{k\sigma}^+ a_{-k,\,-\sigma}^+ a_{-k'-\sigma} a_{k'\sigma}. \tag{3}$$

Here ϵ_k is the kinetic energy of the electron, g_1 is the coupling constant (pertaining to the first superconductor), and V is the volume. We use units in which Planck's constant is $\hbar = 1$.

The influence of the tunneling operator T will be taken into account by perturbation theory. We must take into consideration here the fact that in the thermodynamic limit $V \to \infty$ the static equilibrium state of the superconductor is degenerate in the phase,[11] which can be fixed arbitrarily, since it drops out from the expressions for the observed mean values. Inclusion of the operator T lifts partially the degeneracy with respect to the phases φ_1 and φ_2 of the first and second superconductors, since the operator T has a lower symmetry than the zeroth-approximation Hamiltonian $H_1 + H_2$, and conserves only the total number of particles $N = N_1 + N_2$, but not N_1 and N_2 separately. For this reason, the observed mean values turned out to be in general dependent on the phase difference $\varphi = \varphi_1 - \varphi_2$. Taking the foregoing into account, we conclude that for a correct choice of the zeroth approximation it is necessary to use a representation with fixed phases, but not particle numbers N_1 and N_2. It will be shown below that the phase difference will enter in the expression for the current, and therefore to "prepare" the states with fixed φ it is necessary to connect the system under consideration in an electric circuit with a definite emf, resistance, etc.

It is clear from the foregoing that inasmuch as the entire system as a whole (together with the classical elements) is not in equilibrium, we cannot assume beforehand that the subsystem made up of coupled superconductors will be in an equilibrium state. As will be made clear by the final result, equilibrium in the subsystem still remains possible in a certain range of the circuit parameters. In the general case, however, the calculation should be carried out with the aid of the nonstationary perturbation theory. Incidentally, direct application of perturbation theory, as was done for example in [5], seems to us inconvenient in view of the known difficulties with the secular terms. In our problem it is necessary to have an expansion which is valid not only in a time interval of the order of the reciprocal of the interaction energy, but over a much larger interval, in order to be able to take into account the possibility of time variation of the potential difference on the barrier. The use of the ordinary scheme of perturbation theory has made it possible to consider in [5] only the case of a constant potential difference, which is not realized in the experiment.

A new method of overcoming the foregoing difficulty is based on the ideas of N. N. Bogolyubov, of constructing kinetic equations, and is connected with a consideration of the characteristic time scales involved in the problem (see [12]). In our problem there are three such scales (in increasing order): the relaxation time τ_0 in each of the superconductors, the tunneling time τ, and the time of variation of the voltage on the barrier τ_D.

The main assumption which is usually made in the derivation of the kinetic equations is that during the synchronization time, the role of which in our case is played by the tunneling time τ, the nondiagonal elements of the single-particle density matrix become functionals of the diagonal elements. The assumption that $\tau_D \gg \tau$ is essential, for in the opposite case the rapid change in the chemical potentials would hinder the synchronization process.

The assumption that $\tau \gg \tau_0$, although not necessary for the construction of the kinetic equations, corresponds in our case to the experimental situation and greatly simplifies the calculation, since we are justified in assuming that the diagonal elements of the density matrix are given by the usual equilibrium expressions. Thus, local equilibrium exists in the system, i.e., the usual equilibrium relations are in force, but now the chemical potentials and the phase difference are slowly varying functions of the time and possibly of the coordinates.

Let us proceed to set up the kinetic equations. The diagonal elements of the density matrix $n_{k\sigma}(t) = \langle a_{k\sigma}^{+}(t)\, a_{k\sigma}(t)\rangle$ satisfy the equation

$$\frac{dn_{k\sigma}(t)}{dt} = 2\,\mathrm{Im}\sum_q T_{kq}\langle a_{k\sigma}{}^{+}(t)\, a_{q\sigma}(t)\rangle. \tag{4}$$

We now set up an equation for the "anomalous" mean—the quantity $A_{k\sigma}(t) = \langle a_{-k,\,-\sigma}(t) a_{k\sigma}(t)\rangle$—and take into consideration the fact that the expansions of the time derivatives begin with first-order quantities. We introduce also the operators

$$\tilde{a}_{k\sigma}(t) = e^{i\varphi_1/2}a_{k\sigma}(t), \quad \tilde{a}_{q\sigma}(t) = e^{i\varphi_2/2}a_{q\sigma}(t), \tag{5}$$

choosing the phases such that $\tilde{A}_{k\sigma}$ and $\tilde{A}_{q\sigma}$ are real. We put, by definition,

$$d\varphi_{1,2}/dt = 2\mu_{1,2}(t), \quad \xi_k = \varepsilon_k - \mu_1, \quad \xi_q = \varepsilon_q - \mu_2. \tag{6}$$

Then the equation for $A_{k\sigma}(t)$ in the lowest order will be

$$2\xi_k\tilde{A}_{k\sigma}(t) - |\Delta_{k\sigma}(t)|^2(1 - n_{k\sigma}(t) - n_{-k,\,-\sigma}(t)) = 0, \tag{7}$$

where

$$\Delta_{k\sigma} = \frac{g_1}{2V}\sum_{k'} A_{k'\sigma}(t). \tag{8}$$

Equation (7) reduces to an equation for the gap, if one identifies μ_1 with the "nonequilibrium" value of the chemical potential of the first superconductor.

Equation (4) takes the form

$$\frac{dn_{k\sigma}}{dt} = 2\,\mathrm{Im}\sum_q T_{kq}\langle \tilde{a}_{k\sigma}{}^{+}(t)\,\tilde{a}_{q\sigma}(t)\rangle$$
$$\times \exp\{i(\varphi_1(t) - \varphi_2(t))/2\}. \tag{9}$$

We must now find $\langle \tilde{a}_{k\sigma}^{+}\tilde{a}_{q\sigma}\rangle$ in the first order of perturbation theory. To this end it is convenient to carry out first the Bogolyubov canonical transformation and set up an equation for the mean values expressed in terms of the quasiparticle operators. In these equations it is necessary to discard all the quantities of higher order in T_{kq}, including the time derivatives and the derivatives with respect to the parameters of the canonical transformation.

As a result, the equations take the form

$$(id/dt + E_k - E_q)\langle \alpha_{k\sigma}^+(t)\,\alpha_{q\sigma}(t)\rangle$$
$$= T_{kq}^*(f_k - f_q)\{u_k u_q e^{-i\varphi/2} - v_k v_q e^{i\varphi/2}\}, \qquad (10)$$

$$(id/dt - E_k - E_q)\langle \alpha_{-k,-\sigma}(t)\,\alpha_{q\sigma}(t)\rangle$$
$$= T_{kq}^*(1 - f_k - f_q)\{v_k u_q e^{-i\varphi/2} + u_k v_q e^{i\varphi/2}\}, \qquad (11)$$

where

$$f = (e^{E/\theta} + 1)^{-1}, \quad E = \sqrt{\xi^2 + |\Delta|^2}. \qquad (12)$$

The solution of (11) and (12) must be subjected to the initial condition $F(-\infty) = 0$, where F is the sought function. In calculating the integrals making up the solution, we take into account the slow time variation of the chemical potentials and of the diagonal elements of the density matrix. Using relation (6), we obtain

$$\langle \alpha_{k\sigma}^+(t)\,\alpha_{q\sigma}(t)\rangle = T_{kq}^*(f_k - f_q)\left\{\frac{v_k v_q e^{i\varphi/2}}{E_q - E_k + eV - i\varepsilon} - \frac{u_k u_q e^{-i\varphi/2}}{E_q - E_k - eV - i\varepsilon}\right\}, \qquad (13)$$

$$\langle \alpha_{-k,-\sigma}(t)\,\alpha_{q\sigma}(t)\rangle = -\operatorname{sign}\sigma T_{kq}^*(1 - f_k - f_q) \times\left\{\frac{u_k v_q e^{i\varphi/2}}{E_k + E_q + eV - i\varepsilon} + \frac{v_k u_q e^{-i\varphi/2}}{E_k + E_q - eV - i\varepsilon}\right\}. \qquad (14)$$

The current through the barrier is determined in the usual manner

$$J = \langle dN_1/dt\rangle, \qquad N = \sum n_{k\sigma}. \qquad (15)$$

From this and on the basis of (9) we have ultimately

$$J = -\operatorname{Im} e^{i\varphi(t)} \sum_{kq} |T_{kq}|^2 \frac{|\Delta_k \Delta_q|}{E_k E_q}\Big\{(1 - f_k - f_q) \times\left(\frac{1}{E_k + E_q + eV - i\varepsilon} + \frac{1}{E_k + E_q - eV + i\varepsilon}\right) + (f_k - f_q)\left(\frac{1}{E_k - E_q + eV - i\varepsilon} + \frac{1}{E_k - E_q - eV + i\varepsilon}\right)\Big\} - \operatorname{Im}\sum_{kq}|T_{kq}|^2 \times\left\{\left(1 - \frac{\xi_k \xi_q}{E_k E_q}\right)\times(1 - f_k - f_q) \times\left(\frac{1}{E_k + E_q + eV + i\varepsilon} + \frac{1}{E_k + E_q - eV - i\varepsilon}\right) - \left(1 + \frac{\xi_k \xi_q}{E_k E_q}\right)(f_k - f_q)\left(\frac{1}{E_k - E_q + eV + i\varepsilon} + \frac{1}{E_k - E_q - eV - i\varepsilon}\right)\right\}. \qquad (16)$$

In the derivation of (16) we used the well known formulas for the coefficients of the canonical transformation, and made elementary simplifications.

In accord with the foregoing, the obtained current must be equated to the current in the external part of the circuit. For a circuit of the simplest form, consisting of a source of voltage $\mathscr{E}$ and an internal resistance R connected to the tunnel junction, we have

$$RJ(\varphi) = \mathscr{E} - V, \qquad (17)$$

and the barrier voltage V, according to (6), is

$$V = \frac{1}{2e}\frac{d\varphi}{dt}. \qquad (18)$$

In spite of the fact that from the point of view of the experimental situation Eq. (17) is highly idealized (in the real case, for example, it is necessary to take into account the magnetic field of the current), its consideration explains the main features of the phenomenon. It is clear, first, that the stationary values of the tunnel current are obtained only in the case when φ = const, i.e., V = 0. In this case $J(\varphi) = \mathscr{E}/R = J_S \sin\varphi$, where

$$J_s = 2\sum_{kq}|T_{kq}|^2 \frac{|\Delta_k\Delta_q|}{E_k E_q}\left(\frac{1 - f_k - f_q}{E_k + E_q} - \frac{f_k - f_q}{E_k - E_q}\right). \qquad (19)$$

Under these conditions, the tunnel junction offers no resistance to the current flowing through it (the first Josephson effect). It is obvious that stationary solutions are possible only for $\mathscr{E}/R \le J_S$. In the opposite case $V \neq 0$ and the current will be nonstationary (second Josephson effect).

We emphasize that, as is clear from (17) and (18), if the voltage on the junction differs from zero, it cannot be constant. For this reason, the formulation of the second Josephson effect usually encountered in the literature wherein it is regarded as consisting of current oscillations with frequency 2 eV at a constant voltage on the junction, seems incorrect to us.

It follows from (17) that in the case when a periodic solution is obtained, the amplitude of the potential oscillations is $\Delta V = 2J_S R$. If $\Delta V/\mathscr{E} = 2J_S/J_{c.s.} \ll 1$, where $J_{c.s.} = \mathscr{E}/R$ is the short-circuit current, we can neglect the time variation of V, putting $V \cong \mathscr{E}$, i.e., $\varphi = 2eVt + \varphi_0$. Thus, the case considered in [5] corresponds to neglecting the "self-action" effect.

We see from the developed approach that the occurrence of the alternating current is a consequence of including in the electric circuit an element with nonlinear dependence of the current on the voltage. We note that in this case we deal with a rather unique case of nonlinearity, when the current is determined at the given instant of time by the value of the voltage during all the preceding instants of time.

We emphasize that the physical nature of the alternating Josephson current is the same as that of the constant current: each of them is an ordinary superconducting current (of course, under conditions of weak superconductivity), flowing without dissipation of energy. Indeed, from (17) and (18) it is easy to see that $\overline{VJ} = 0$ (the bar denotes averaging with respect to time). The difference between them is that the constant Josephson current is in equilibrium, and the alternating one is not.

To construct a complete theory of the phenomena that occur during the tunneling, it is necessary to take into consideration the presence in the circuit of reactive elements and of the magnetic field, including the self-field of the current flowing through the junction. This will be done in a separate paper.

The term without the phase factor in (16) is a so-called quasiparticle current. As seen from (16), at zero temperature this term is missing when $eV < \Delta_1 + \Delta_2$. However, at voltages that exceed the threshold by an arbitrarily small amount, it reaches jumpwise a value equal to $\pi\sqrt{\Delta_1\Delta_2}/2eR_N$, where R_N is the resistance of the junction in the normal state. At temperatures different from zero, but much smaller than critical, and also for voltages much below the threshold, the quasiparticle current in the case of identical superconductors, is

$$\frac{V}{R_N}\frac{\Delta}{\theta}\ln\left|\frac{eV}{\Delta}\right| e^{-\Delta/\theta}. \qquad (20)$$

The estimate (20) obtained by us justifies the neglect of the quasiparticle current, as was done above in the consideration of the nonstationary effects.

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