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A.M. SHUTOVSKYI, A.V. SVIDZINSKYI, V.E. SAKHNYUK, O.YU. PASTUKH

Lesya Ukrainka Eastern European National University

(13, Volya Ave., Lutsk 43025, Ukraine; e-mail: arsen4sh@gmail.com)

MICROSCOPIC CALCULATION OF JOSEPHSON CURRENT IN TUNNEL JUNCTIONS WITH TWO-GAP SUPERCONDUCTORS

Quasiclassical equations of the one-gap superconductivity theory have been applied to superconductors with two energy gaps. Using the equations for Green's functions obtained in the t -representation, the Josephson current density through tunnel junctions with two-gap superconductors is calculated.

Keywords: quasiclassical equation, energy gap, Green's function, t -representation, current density, dielectric film, Josephson junction, two-gap superconductor, phase difference.

1. Introduction

The Josephson effect has been studied in plenty of works (see, e.g., reviews [1, 2]), including the current states in tunnel junctions of the superconductor-insulator-superconductor (SIS) type. In particular, in work [3], the non-stationary Josephson current was considered in the framework of the kinetic approach. The Josephson current at temperatures close to the critical one, T_c , was calculated in work [4] for pure superconductor electrodes and in works [5–7] for electrodes with non-magnetic impurities. The authors of works [8, 9] calculated the dependence of the current density on the phase difference across the tunnel SIS junction with regard for the unpairing effects, by using the asymptotic form obtained in the microscopic superconductivity theory for temperatures near T_c . However, all those works concerned only superconductors with a single energy gap.

A possibility for superconductors with two energy gaps to exist was considered as long ago as in works [10, 11]. But active researches in the domain of two-gap superconductivity were started after the discovery [12] of two energy gaps in the binary MgB₂ compound with the critical temperature $T_c = 39$ K, which is the highest one among superconductors with the phonon mechanism of electron pairing. The properties of MgB₂ were studied in works [13–18, 20, 21], where, in essence, the BCS theory for two-gap superconductors was developed.

In work [22], the dependence of the current density on the phase difference across a tunnel Josephson junction on the basis of MgB₂ was obtained in the framework of the Ginzburg–Landau phenomenological theory. In this work, we will carry on a microscopic calculation of the Josephson current in tunnel superconductor junctions including two-gap superconductors. The calculations are performed within the method of quasiclassical equations. This method was described in detail in monograph [23]. In the cited work, Gor'kov's equations for Green's functions were written in the so-called t -representation. The latter has already proven its efficiency in the one-gap theory of superconductivity. In other words, our aim is to extend the method of quasiclassical equations onto the case of superconductivity with two energy gaps.

2. Equations for Green's Functions

Let us write down the Hamiltonian for a system of free electrons in the field of complex sources of electron pairs [24]

$$\hat{H}_B = \sum_{l,\sigma} \int d\mathbf{r} \hat{\psi}_{l,\sigma}^+(\mathbf{r}) \hat{\xi} \hat{\psi}_{l,\sigma}(\mathbf{r}) - \left(\sum_{l,l'} g_{l,l'} \int d\mathbf{r} \Delta_{l'}(\mathbf{r}) \hat{\psi}_{l,\uparrow}^+(\mathbf{r}) \hat{\psi}_{l',\downarrow}^+(\mathbf{r}) + \text{h.c.} \right). \quad (1)$$

Since the superconductivity is assumed to have a two-gap origin, the band indices l and l' can acquire values of 1 and 2. The constants $g_{l,l'}$ describe the interaction

between the l -th and l' -th bands. In the case of magnetic field absence, we may write

$$\hat{\xi} = \frac{\hat{\mathbf{p}}^2}{2m} - \mu.$$

The complex functions $\Delta_l(\vec{r})$ in Eq. (1) are called the order parameters.

We seek for an expression for the current density in the framework of Green's function formalism. Green's functions are defined by the formulas

$$F_l(\mathbf{r}_1, \mathbf{r}_2; \tau_1, \tau_2) = \langle T_\tau \hat{\psi}_{l,\uparrow}^+(\mathbf{r}_1, \tau_1) \hat{\psi}_{l,\downarrow}^+(\mathbf{r}_2, \tau_2) \rangle,$$

$$G_l(\mathbf{r}_1, \mathbf{r}_2; \tau_1, \tau_2) = - \langle T_\tau \hat{\psi}_{l,\downarrow}(\mathbf{r}_1, \tau_1) \hat{\psi}_{l,\downarrow}^+(\mathbf{r}_2, \tau_2) \rangle.$$

They contain the so-called imaginary time τ , which varies from 0 to $1/T$. The creation and annihilation operators are taken in the Heisenberg representation. These Green's functions satisfy the closed system of Gor'kov's equations

$$\begin{aligned} & \left(\frac{\partial}{\partial \tau_1} + \hat{\xi}_1 \right) G_l(\mathbf{r}_1, \mathbf{r}_2; \tau_1, \tau_2) - \\ & - \sum_{l'} g_{l,l'} \Delta_{l'}(\mathbf{r}_1) F_l(\mathbf{r}_1, \mathbf{r}_2; \tau_1, \tau_2) = \\ & = -\delta(\tau_1 - \tau_2) \delta(\mathbf{r}_1 - \mathbf{r}_2), \end{aligned} \quad (2)$$

$$\begin{aligned} & \left(\frac{\partial}{\partial \tau_1} - \hat{\xi}_1 \right) F_l(\mathbf{r}_1, \mathbf{r}_2; \tau_1, \tau_2) - \\ & - \sum_{l'} g_{l,l'} \Delta_{l'}^*(\mathbf{r}_1) G_l(\mathbf{r}_1, \mathbf{r}_2; \tau_1, \tau_2) = 0. \end{aligned}$$

Since the order parameters do not depend on the variables τ_1 and τ_2 , Green's functions are characterized by the following properties:

$$F_l(\mathbf{r}_1, \mathbf{r}_2; \tau_1, \tau_2) = F_l(\mathbf{r}_1, \mathbf{r}_2; \tau_1 - \tau_2),$$

$$G_l(\mathbf{r}_1, \mathbf{r}_2; \tau_1, \tau_2) = G_l(\mathbf{r}_1, \mathbf{r}_2; \tau_1 - \tau_2).$$

By expanding these functions in the series in odd Matsubara frequencies $\omega_n = \pi T(2n + 1)$,

$$F_l(\mathbf{r}_1, \mathbf{r}_2; \tau_1 - \tau_2) = T \sum_{\omega_n} F_{l,\omega_n}(\mathbf{r}_1, \mathbf{r}_2) e^{-i\omega_n(\tau_1 - \tau_2)},$$

$$G_l(\mathbf{r}_1, \mathbf{r}_2; \tau_1 - \tau_2) = T \sum_{\omega_n} G_{l,\omega_n}(\mathbf{r}_1, \mathbf{r}_2) e^{-i\omega_n(\tau_1 - \tau_2)},$$

and substituting them into the system of Gor'kov's equations (2), we can obtain the following system of

equations:

$$\begin{aligned} & (i\omega_n - \hat{\xi}_1) G_{l,\omega_n}(\mathbf{r}_1, \mathbf{r}_2) + \\ & + \sum_{l'} g_{l,l'} \Delta_{l'}(\mathbf{r}_1) F_{l,\omega_n}(\mathbf{r}_1, \mathbf{r}_2) = \delta(\mathbf{r}_1 - \mathbf{r}_2), \end{aligned} \quad (3)$$

$$\begin{aligned} & (i\omega_n + \hat{\xi}_1) F_{l,\omega_n}(\mathbf{r}_1, \mathbf{r}_2) + \\ & + \sum_{l'} g_{l,l'} \Delta_{l'}^*(\mathbf{r}_1) G_{l,\omega_n}(\mathbf{r}_1, \mathbf{r}_2) = 0. \end{aligned}$$

It is expedient to introduce two more Green's functions according to the definition

$$\tilde{F}_l(\mathbf{r}_1, \mathbf{r}_2; \tau_1, \tau_2) = \langle T_\tau \hat{\psi}_{l,\downarrow}(\mathbf{r}_1, \tau_1) \hat{\psi}_{l,\uparrow}(\mathbf{r}_2, \tau_2) \rangle,$$

$$\tilde{G}_l(\mathbf{r}_1, \mathbf{r}_2; \tau_1, \tau_2) = - \langle T_\tau \hat{\psi}_{l,\uparrow}^+(\mathbf{r}_1, \tau_1) \hat{\psi}_{l,\uparrow}(\mathbf{r}_2, \tau_2) \rangle.$$

These functions satisfy the system of equations

$$\begin{aligned} & \left(\frac{\partial}{\partial \tau_1} + \hat{\xi}_1 \right) \tilde{F}_l(\mathbf{r}_1, \mathbf{r}_2; \tau_1, \tau_2) - \\ & - \sum_{l'} g_{l,l'} \Delta_{l'}(\mathbf{r}_1) \tilde{G}_l(\mathbf{r}_1, \mathbf{r}_2; \tau_1, \tau_2) = 0, \end{aligned} \quad (4)$$

$$\begin{aligned} & \left(\frac{\partial}{\partial \tau_1} - \hat{\xi}_1 \right) \tilde{G}_l(\mathbf{r}_1, \mathbf{r}_2; \tau_1, \tau_2) - \\ & - \sum_{l'} g_{l,l'} \Delta_{l'}^*(\mathbf{r}_1) \tilde{F}_l(\mathbf{r}_1, \mathbf{r}_2; \tau_1, \tau_2) = \\ & = -\delta(\tau_1 - \tau_2) \delta(\mathbf{r}_1 - \mathbf{r}_2). \end{aligned}$$

The application of the Fourier transformation converts system (4) into the system of equations

$$\begin{aligned} & (i\omega_n - \hat{\xi}_1) \tilde{F}_{l,\omega_n}(\mathbf{r}_1, \mathbf{r}_2) + \\ & + \sum_{l'} g_{l,l'} \Delta_{l'}(\mathbf{r}_1) \tilde{G}_{l,\omega_n}(\mathbf{r}_1, \mathbf{r}_2) = 0, \end{aligned} \quad (5)$$

$$\begin{aligned} & (i\omega_n + \hat{\xi}_1) \tilde{G}_{l,\omega_n}(\mathbf{r}_1, \mathbf{r}_2) + \\ & + \sum_{l'} g_{l,l'} \Delta_{l'}^*(\mathbf{r}_1) \tilde{F}_{l,\omega_n}(\mathbf{r}_1, \mathbf{r}_2) = \delta(\mathbf{r}_1 - \mathbf{r}_2). \end{aligned}$$

Now, by introducing the matrix Green's function

$$\hat{G}_{l,\omega_n}(\mathbf{r}, \mathbf{r}') = \begin{pmatrix} G_{l,\omega_n}(\mathbf{r}, \mathbf{r}') & -\tilde{F}_{l,\omega_n}(\mathbf{r}, \mathbf{r}') \\ -F_{l,\omega_n}(\mathbf{r}, \mathbf{r}') & \tilde{G}_{l,\omega_n}(\mathbf{r}, \mathbf{r}') \end{pmatrix},$$

we can unite systems (3) and (5) into a single matrix equation

$$\left(i\omega_n - \sigma_z \hat{\xi} - \sum_{l'} g_{l,l'} \hat{\Delta}_{l'}(\mathbf{r}) \right) \hat{G}_{l,\omega_n}(\mathbf{r}, \mathbf{r}') =$$

$$= \delta(\mathbf{r} - \mathbf{r}'), \quad (6)$$

where

$$\hat{\Delta}_l(\mathbf{r}) = \begin{pmatrix} 0 & \Delta_l(\mathbf{r}) \\ \Delta_l^*(\mathbf{r}) & 0 \end{pmatrix}.$$

In the case of an external potential $U(\mathbf{r})$, the matrix equation (6) reads

$$\begin{aligned} & (i\omega_n - \sigma_z (\hat{\xi} + U(\mathbf{r}))) \hat{G}_{l,\omega_n}(\mathbf{r}, \mathbf{r}') - \\ & - \sum_{l'} g_{l,l'} \hat{\Delta}_{l'}(\mathbf{r}) \hat{G}_{l,\omega_n}(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}'). \end{aligned}$$

3. Quasiclassical Equations

In order to develop the method of quasiclassical equations in the framework of the two-gap superconductivity theory, let us introduce the matrix Green's functions in the momentum space,

$$\hat{G}_{l,\omega_n}^{i,k}(\mathbf{p}, \mathbf{p}') = \int d\mathbf{r} \int d\mathbf{r}' \psi_{\mathbf{p}}^{*(i)}(\mathbf{r}) \psi_{\mathbf{p}'}^{(k)}(\mathbf{r}') \hat{G}_{l,\omega_n}(\mathbf{r}, \mathbf{r}').$$

The superscripts i and k can acquire values of 1 and 2. The functions $\psi_{\mathbf{p}}^{(k)}(\mathbf{r})$ are solutions of the Schrödinger equation with the potential

$$U(\mathbf{r}) = U(z) = U_0 \delta(z),$$

which simulates a thin dielectric film. In this case, the order parameters and the current density depend only on the z -coordinate. Using a calculation scheme similar to that described in monograph [25], we arrive at the following matrix equations in terms of the variables t and t' :

$$\begin{aligned} & (i\omega_n + i\sigma_z \frac{\partial}{\partial t}) \hat{G}_{l,\omega_n}^{i,k}(t, t') - \\ & - \sum_{l'} \hat{E}_l^{i,i'}(t, x) \hat{G}_{l,\omega_n}^{i',k}(t, t') = \delta_{i,k} \delta(t - t'). \end{aligned} \quad (7)$$

Here, we use the notation

$$\begin{aligned} \hat{E}_l^{i,i'}(t, x) &= \\ &= \begin{pmatrix} 0 & \sum_{l'} g_{l,l'} \Delta_{l'}^{i,i'}(t, x) \\ (-1)^{i+i'} \sum_{l'} g_{l,l'} \Delta_{l'}^{*i,i'}(t, x) & 0 \end{pmatrix}, \end{aligned}$$

where

$$\Delta_l^{1,1}(t, x) = D\Delta_l(v_0 x t) +$$

$$+ R[\theta(-t)\Delta_l(v_0 x t) + \theta(t)\Delta_l(-v_0 x t)],$$

$$\Delta_l^{1,2}(t, x) = i\sqrt{DR}\theta(t)[\Delta_l(-v_0 x t) - \Delta_l(v_0 x t)],$$

$$\Delta_l^{2,1}(t, x) = i\sqrt{DR}\theta(t)[\Delta_l(v_0 x t) - \Delta_l(-v_0 x t)],$$

$$\Delta_l^{2,2}(t, x) = D\Delta_l(-v_0 x t) +$$

$$+ R[\theta(t)\Delta_l(v_0 x t) + \theta(-t)\Delta_l(-v_0 x t)].$$

The physical quantity v_0 is called the Fermi velocity. It is worth noting that

$$x = \frac{p_z}{\sqrt{p_x^2 + p_y^2 + p_z^2}}.$$

The coefficients of electron reflection from, R , and transmission through, D , the potential barrier are calculated by the following formulas:

$$R(x) = \frac{m^2 U_0^2}{p_0^2 x^2 + m^2 U_0^2}, \quad D(x) = \frac{p_0^2 x^2}{p_0^2 x^2 + m^2 U_0^2}.$$

The quantity p_0 is called the Fermi momentum. When determining the matrix equations for Green's functions in the t -representation, all required calculations were performed in a vicinity of this momentum value.

4. Current Density

The current density in the case of superconductivity with two energy gaps was calculated using the formula

$$\mathbf{j}(\mathbf{r}) = \frac{ie}{m} T \sum_{l,\omega_n} \lim_{\mathbf{r}' \rightarrow \mathbf{r}} (\nabla_{\mathbf{r}'} - \nabla_{\mathbf{r}}) G_{l,\omega_n}(\mathbf{r}, \mathbf{r}'). \quad (8)$$

With the help of Green's functions in the t -representation, this expression can be transformed as follows:

$$\begin{aligned} j(z) &= 2\pi e v_0 N(0) T \times \\ &\times \sum_{l,\omega_n} \int_0^1 x dx \left[D \left\{ G_{l,\omega_n}^{1,1}(t, t) - G_{l,\omega_n}^{2,2}(-t, -t) \right\} + \right. \\ &+ R \left\{ \theta(-z) \left[G_{l,\omega_n}^{1,1}(t, t) - G_{l,\omega_n}^{1,1}(-t, -t) \right] + \right. \\ &+ \theta(z) \left[G_{l,\omega_n}^{2,2}(t, t) - G_{l,\omega_n}^{2,2}(-t, -t) \right] \left. \right\} + \\ &+ i\sqrt{DR} \left\{ \theta(z) \left[G_{l,\omega_n}^{1,2}(t, t) - G_{l,\omega_n}^{2,1}(t, t) \right] + \right. \\ &+ \theta(-z) \left[G_{l,\omega_n}^{1,2}(-t, -t) - G_{l,\omega_n}^{2,1}(-t, -t) \right] \left. \right\} \left. \right]. \end{aligned}$$

This formula includes the notation $t = \frac{z}{v_0 x}$ and the quantity $N(0) = \frac{m^2 v_0}{2\pi^2}$. Below, we use a model with piecewise constant order parameters. In this approximation, the absolute values of order parameters are assumed to be constant within each superconductor, whereas the phases are different. Then, one may write that

$$\Delta_l(z) = \Delta_l [\theta(-z) \exp(i\varphi_l) + \theta(z) \exp(i\chi_l)].$$

After having solved Eq. (7) for Green's functions in the t -representation for the case of small transparency and in the selected order parameter approximation, we can calculate the current density in the plane $z = 0$:

$$j = \sum_{i,k} j_{i,k} \sin(\chi_i - \varphi_k), \quad (9)$$

where

$$j_{i,k} = \pi e v_0 N(0) T \Delta_i \Delta_k \times \\ \times \sum_l g_{l,i} g_{l,k} \sum_{\omega_n} \frac{1}{\Omega_{l,\omega_n}^{1,1} \Omega_{l,\omega_n}^{2,2}} \int_0^1 x D(x) dx,$$

$$\Omega_{l,\omega_n}^{k,k} = \sqrt{|\omega_n|^2 + |E_l^{k,k}|^2},$$

$$E_l^{1,1} = \sum_{l'} g_{l,l'} \Delta_{l'} \exp(i\varphi_{l'}),$$

$$E_l^{2,2} = \sum_{l'} g_{l,l'} \Delta_{l'} \exp(i\chi_{l'}).$$

5. Conclusions

In this work, the method of quasiclassical equations, which is known in the theory of one-gap superconductors, is extended onto the case of superconductors with two energy gaps. The equation for Green's functions in the t -representation is obtained, and the formula for the current density is found, by using Green's functions in this representation. All calculations are made at the Fermi surface. By considering the case of low transparency, we have obtained a quite compact dependence of the current density on the phase difference. By its mathematical structure, the final result is similar to that obtained in the framework of the phenomenological approach [22].

Our work clearly demonstrates the advantage of the microscopic approach, because it allows one to obtain

the dependence for the current density with parameters that can be calculated. Those parameters have a physical sense, which is hidden in the phenomenological theory of superconductivity.

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*А.М. Шутовський, А.В. Свідзинський,
В.Є. Сахнюк, О.Ю. Пастух*

МІКРОСКОПІЧНИЙ РОЗРАХУНОК
ДЖОЗЕФСОНІВСЬКОГО СТРУМУ В ТУНЕЛЬНИХ
НАДПРОВІДНИХ КОНТАКТАХ НА ОСНОВІ
ДВОЩІЛІННИХ НАДПРОВІДНИКІВ

Резюме

Метод квазікласичних рівнянь, побудований у теорії однощільної надпровідності, застосовано для випадку надпровідників з двома енергетичними щілинами. Побудовані рівняння для функцій Гріна у t -представленні дають можливість обчислювати густину струму, який протікає крізь тонку діелектричну плівку у тунельних джозефсонівських контактах на основі двощільних надпровідників. Отримана залежність густини струму від різниць фаз містить коефіцієнти зрозумілого походження.