

# Tunneling in bipolaron superconductors: superconductor–normal metal junctions

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The tunneling amplitude is obtained for a local pair of electrons separated by a potential barrier into two free electrons. The current-voltage characteristics of a tunnel junction between a normal metal and bipolaron (“boson”) superconductor are determined. Special features of the current-voltage characteristics are explained assuming a narrow bipolaron energy band and the Bose statistics of carriers in a superconductor.

## INTRODUCTION

Discovery of the high-temperature superconductivity<sup>1</sup> made its origin a topical subject. There are several alternative theories of the high-temperature superconductivity, which reduce mainly to the Fermi liquid representations and the BCS theory or to a model of local electron pairs (bipolarons)<sup>2,3</sup> with the Schafroth superconductivity mechanism.<sup>4</sup>

We shall obtain an expression for the tunnel term in the Hamiltonian describing a junction between a superconductor containing local electron pairs and a normal metal across an insulator. We shall report an investigation of the temperature dependence of the current-voltage characteristic of such a junction.

Studies of the current-voltage characteristics of  $S-I-N$  (superconductor–insulator–normal metal) and  $S-I-S$  (superconductor–insulator–superconductor) junctions make it possible to determine one of the most important characteristics of a superconductor, the energy gap ( $\Delta$ ) in the electron spectrum, and to find its temperature dependence. It should be pointed out that in the case of low-temperature superconductors the gap measured in the tunnel experiments agrees with that deduced from infrared radiation absorption, nuclear spin relaxation, Andreev reflection, etc.

If the  $S$  electrode in  $S-I-N$  and  $S-I-S$  junctions is a high-temperature superconductor, there are certain special features of the determination of  $\Delta$  and also of its value not observed for junctions with low-temperature superconductors.

First of all, it is difficult to determine correctly  $\Delta$  from the current-voltage characteristic<sup>5</sup> because of the presence of a fine structure.

Secondly, tunnel measurements carried out by various authors have yielded the gaps with a scatter greater than one order of magnitude for the same material. For example, in the case of the La–Sr–Cu–O compound the tunnel measurements yield the ratio of twice the gap width to the critical temperature  $2\Delta/kT_c$  ( $k$  is the Boltzmann constant) ranging from 4.5 to 7 (Refs. 5–7), whereas for  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  the values of the same ratio range from 0.7 to 13 (Refs. 8–12).

Thirdly, the current-voltage characteristics are asymmetric relative to the direction of the current.<sup>8–12</sup>

Fourthly, some investigations<sup>13</sup> have revealed that the features of the current-voltage characteristics associated with the gap do not vary with temperature, in other words, the gap is independent of temperature.

Attempts to account for these properties have been made, not without success, on the basis of a theory of reso-

nant valence bonds (RVB theory).<sup>14</sup> However, it has been shown recently that this theory is incapable of explaining the experimental data on the specific heat and electrical resistivity, so that it is doubtful whether it is applicable to high-temperature superconductors.

A polaron (bipolaron) superconductivity theory has been able to account for all the experimental data,<sup>15,16</sup> including those that cannot be explained by the RVB theory. We shall use this bipolaron theory to formulate and solve the model problem of the tunneling of charge carriers across a thin insulator layer when the carriers in the  $S$  electrode are local noninteracting charged electron pairs obeying the Bose–Einstein statistics. In the case of an  $N$  electrode the charge carriers are noninteracting electrons. When a Bose particle crosses a barrier, it is split into two free electrons. The calculated tunnel characteristics allow us to explain qualitatively all the main properties of high-temperature superconducting materials listed above by considering  $S-I-N$  junctions.

## 1. INITIAL HAMILTONIAN

We shall deduce the current-voltage characteristics of an  $S-I-N$  junction employing the familiar method of a model Hamiltonian.<sup>17</sup> We shall first describe briefly the method used in deriving in bipolaron Hamiltonian in the presence of a tunnel term.

We shall assume that the  $S$  electrode in an  $S-I-N$  junction is a material with a strong electron–phonon interaction where small bipolarons may form and the  $N$  electrode is made of a material with a weak electron–phonon interaction. We shall write down the initial Hamiltonian in the form

$$H = H_1 + H_2 + T, \quad (1)$$

where  $H_1$  is the Hamiltonian of the  $S$  electrode,  $H_2$  represents the  $N$  electrode, and  $T$  is the tunnel term. In the momentum representation we find that  $H_1$  can be described by the Fröhlich model:

$$H_1 = \sum_{\mathbf{k}, \sigma} \varepsilon_S(\mathbf{k}) c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}\sigma} + \sum_{\substack{\mathbf{k}, \mathbf{k}', \sigma, \\ \mathbf{q}, \mathbf{q}', \sigma'}} V_{\mathbf{k}\mathbf{k}'}^{q\mathbf{q}'} c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}'\sigma'} c_{\mathbf{q}'\sigma} c_{\mathbf{q}\sigma} + \sum_{\substack{\mathbf{k}, \mathbf{k}', \\ \mathbf{p}, \sigma}} c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}'\sigma} U_{\mathbf{k}\mathbf{k}'}(\mathbf{p}) \{d_{\mathbf{p}} + d_{-\mathbf{p}}^+\} + \sum_{\mathbf{p}} \omega(\mathbf{p}) d_{\mathbf{p}}^+ d_{\mathbf{p}}, \quad (2)$$

where  $\varepsilon_S(\mathbf{k})$  is the spectrum of electrons in a crystal with the lattice at rest;  $c_{\mathbf{k}}^+$  and  $c_{\mathbf{k}}$  are, respectively, the electron cre-

ation and annihilation operators for the  $S$  electrode;  $V_{\mathbf{k}\mathbf{k}'}^{\mathbf{q}\mathbf{q}'}$  and  $U_{\mathbf{k}\mathbf{k}'}(\mathbf{p})$  are the matrix element of the Coulomb and electron-phonon interactions;  $\omega(\mathbf{p})$  is the phonon spectrum;  $d_{\mathbf{p}}^+$  and  $d_{\mathbf{p}}$  are the phonon creation and annihilation operators;  $\mathbf{k}$ ,  $\mathbf{q}$ , and  $\mathbf{p}$  are the wave vectors;  $\sigma$  is the electron spin projection. We shall adopt the system of units in which the frequency, voltage, and temperature are all measured in energy units.

In the expression for  $H_2$  we shall ignore completely the Coulomb interaction of electrons with one another and the electron-phonon interaction:

$$H_2 = \sum_{\mathbf{k}, \sigma} \varepsilon_N(\mathbf{k}) a_{\mathbf{k}\sigma}^+ a_{\mathbf{k}\sigma}. \quad (3)$$

Here,  $\varepsilon_N(\mathbf{k})$  is the spectrum of electrons in the  $N$  electrode;  $a_{\mathbf{k}\sigma}^+$  and  $a_{\mathbf{k}\sigma}$  are the creation and annihilation operators.

We shall select the tunnel term in the traditional form<sup>17</sup>

$$T = \sum_{\mathbf{k}\mathbf{q}\sigma} D_{\mathbf{k}\mathbf{q}} a_{\mathbf{k}\sigma}^+ c_{\mathbf{q}\sigma} + \text{H.c.}, \quad (4)$$

where  $D_{\mathbf{k}\mathbf{q}}$  is the matrix element of a transition of an electron from the  $S$  to the  $N$  electrode.

For convenience in polaron and bipolaron transformations, we shall adopt the Wannier function representation in Eqs. (2)-(4). After the necessary transformation of the electron operators

$$a_{\mathbf{k}\sigma} = \frac{1}{\sqrt{N_N}} \sum_{\mathbf{m}} a_{\mathbf{m}\sigma} \exp(-i\mathbf{k}\mathbf{R}_{\mathbf{m}}), \quad (5)$$

$$c_{\mathbf{q}\sigma} = \frac{1}{\sqrt{N_S}} \sum_{\mathbf{n}} c_{\mathbf{n}\sigma} \exp(-i\mathbf{q}\mathbf{R}_{\mathbf{n}}),$$

where  $\mathbf{R}_{\mathbf{m}}$  and  $\mathbf{R}_{\mathbf{n}}$  are the radius vectors of the  $m$ th and  $n$ th lattice sites in the  $N$  and  $S$  electrodes, and  $N_N$  and  $N_S$  are the numbers of sites in the  $N$  and  $S$  electrodes, we find that  $H_1$ ,  $H_2$ , and  $T$  are described by

$$H_1 = \sum_{\mathbf{m}, \mathbf{m}', \sigma} T_{\mathbf{m}\mathbf{m}'}^{(S)} c_{\mathbf{m}\sigma}^+ c_{\mathbf{m}'\sigma} + \sum_{\substack{\mathbf{m}, \mathbf{m}', \sigma, \\ \mathbf{n}, \mathbf{n}', \sigma'}} V_{\mathbf{m}\mathbf{m}'}^{\mathbf{n}\mathbf{n}'} c_{\mathbf{m}\sigma}^+ c_{\mathbf{m}'\sigma} c_{\mathbf{n}\sigma} c_{\mathbf{n}'\sigma} \quad (6)$$

$$+ \sum_{\substack{\mathbf{m}, \mathbf{m}', \\ \mathbf{p}, \sigma}} c_{\mathbf{m}\sigma}^+ c_{\mathbf{m}'\sigma} U_{\mathbf{m}\mathbf{m}'}(\mathbf{p}) \{d_{\mathbf{p}} + d_{-\mathbf{p}}^+\} + \sum_{\mathbf{p}} \omega(\mathbf{p}) d_{\mathbf{p}}^+ d_{\mathbf{p}},$$

$$H_2 = \sum_{\mathbf{ll}'\sigma} T_{\mathbf{ll}'}^{(N)} a_{\mathbf{l}\sigma}^+ a_{\mathbf{l}'\sigma}, \quad (7)$$

$$T = \sum_{\mathbf{ml}\sigma} D_{\mathbf{ml}} a_{\mathbf{l}\sigma}^+ c_{\mathbf{m}\sigma} + \text{H.c.} \quad (8)$$

The hopping integrals for the  $S$  and  $N$  electrodes are, respectively,

$$T_{\mathbf{mm}'}^{(S)} = \frac{1}{N_S} \sum_{\mathbf{k}} \varepsilon_S(\mathbf{k}) \exp[i\mathbf{k}(\mathbf{R}_{\mathbf{m}} - \mathbf{R}_{\mathbf{m}'})], \quad (9)$$

$$T_{\mathbf{mm}'}^{(N)} = \frac{1}{N_N} \sum_{\mathbf{k}} \varepsilon_N(\mathbf{k}) \exp[i\mathbf{k}(\mathbf{R}_{\mathbf{m}} - \mathbf{R}_{\mathbf{m}'})].$$

The matrix elements of the Coulomb, electron-phonon, and tunnel interactions can be written in the form

$$V_{\mathbf{m}\mathbf{m}'}^{\mathbf{n}\mathbf{n}'} = \frac{1}{N_S^2} \sum_{\substack{\mathbf{k}, \mathbf{k}', \\ \mathbf{q}, \mathbf{q}'}} V_{\mathbf{k}\mathbf{k}'}^{\mathbf{q}\mathbf{q}'} \exp(i\mathbf{k}\mathbf{R}_{\mathbf{m}} + i\mathbf{k}'\mathbf{R}_{\mathbf{m}'} - i\mathbf{q}\mathbf{R}_{\mathbf{n}} - i\mathbf{q}'\mathbf{R}_{\mathbf{n}'}), \quad (10)$$

$$U_{\mathbf{m}\mathbf{m}'}(\mathbf{p}) = \frac{1}{N_S^2} \sum_{\mathbf{k}, \mathbf{k}'} U_{\mathbf{k}\mathbf{k}'}(\mathbf{p}) \exp(i\mathbf{k}\mathbf{R}_{\mathbf{m}} - i\mathbf{k}'\mathbf{R}_{\mathbf{m}'}), \quad (11)$$

$$D_{\mathbf{ml}} = \frac{1}{(N_S N_N)^{1/2}} \sum_{\mathbf{k}, \mathbf{k}'} D_{\mathbf{k}\mathbf{k}'} \exp(i\mathbf{k}\mathbf{R}_{\mathbf{m}} - i\mathbf{k}'\mathbf{R}_{\mathbf{l}}). \quad (12)$$

In the subsequent calculations we shall allow only for the direct electron-phonon and Coulomb interactions, i.e., in Eqs. (10) and (11) we shall assume that  $\mathbf{n} = \mathbf{n}'$  and  $\mathbf{m} = \mathbf{m}'$ .

If the electron-phonon interaction is sufficiently strong to form polarons in the  $S$  electrode, we can apply the familiar Lang-Firsov transformation<sup>18</sup> to the Hamiltonian (1):

$$H_p = e^S H e^{-S} = H_{1p} + H_{2p} + T_p, \quad (13)$$

$$S_1 = \sum_{\mathbf{mp}\sigma} c_{\mathbf{m}\sigma}^+ c_{\mathbf{m}\sigma} \omega^{-1}(\mathbf{p}) U_{\mathbf{m}\mathbf{m}}(\mathbf{p}) (d_{\mathbf{p}}^+ - d_{-\mathbf{p}}). \quad (14)$$

This transformation does not alter  $H_2$  ( $H_2 = H_{2p}$ ), whereas  $H_{1p}$  and  $T_p$  become

$$H_{1p} = \sum_{\mathbf{m}, \sigma} E_{\mathbf{m}} c_{\mathbf{m}\sigma}^+ c_{\mathbf{m}\sigma} + \sum_{\substack{\mathbf{m}, \mathbf{m}', \sigma \\ (\mathbf{m} \neq \mathbf{m}')}} \sigma_{\mathbf{m}\mathbf{m}'} c_{\mathbf{m}\sigma}^+ c_{\mathbf{m}'\sigma} \\ + \sum_{\substack{\mathbf{m}, \mathbf{m}', \sigma, \sigma' \\ (\mathbf{m} \neq \mathbf{m}', \sigma \neq \sigma')}} V_{\mathbf{m}\mathbf{m}'}^{\mathbf{m}\mathbf{m}'} c_{\mathbf{m}\sigma}^+ c_{\mathbf{m}'\sigma'}^+ c_{\mathbf{m}'\sigma} c_{\mathbf{m}\sigma} + \sum_{\mathbf{p}} \omega(\mathbf{p}) d_{\mathbf{p}}^+ d_{\mathbf{p}}, \quad (15)$$

simultaneously)

$$T_p = \sum_{\mathbf{ml}, \sigma} \hat{D}_{\mathbf{ml}} a_{\mathbf{l}\sigma}^+ c_{\mathbf{m}\sigma} + \text{H.c.},$$

where

$$E_{\mathbf{m}} = T_{\mathbf{m}\mathbf{m}}^{(S)} - \sum_{\mathbf{p}} U_{\mathbf{m}\mathbf{m}}(\mathbf{p}) \omega^{-1}(\mathbf{p}), \quad (16)$$

$$\sigma_{\mathbf{m}\mathbf{m}'} = T_{\mathbf{m}\mathbf{m}'}^{(S)} \exp \left\{ \sum_{\mathbf{p}} \omega^{-1}(\mathbf{p}) [U_{\mathbf{m}\mathbf{m}}(\mathbf{p}) - U_{\mathbf{m}'\mathbf{m}'}(\mathbf{p})] (d_{\mathbf{p}}^+ - d_{-\mathbf{p}}) \right\}, \quad (17)$$

$$V_{\mathbf{m}\mathbf{m}'}^{\mathbf{m}\mathbf{m}'} = V_{\mathbf{m}\mathbf{m}'}^{\mathbf{m}\mathbf{m}'} - \sum_{\mathbf{p}} U_{\mathbf{m}\mathbf{m}}(\mathbf{p}) U_{\mathbf{m}'\mathbf{m}'}(\mathbf{p}) \omega^{-1}(\mathbf{p}), \quad (18)$$

$$\hat{D}_{\mathbf{ml}} = D_{\mathbf{ml}} \exp \left[ - \sum_{\mathbf{p}} \omega^{-1}(\mathbf{p}) U_{\mathbf{m}\mathbf{m}}(\mathbf{p}) (d_{\mathbf{p}}^+ - d_{-\mathbf{p}}) \right]. \quad (19)$$

If the polaron-polaron interaction  $V_{\mathbf{m}\mathbf{m}'}^{\mathbf{m}\mathbf{m}'}$  is strong ( $V_{\mathbf{m}\mathbf{m}'}^{\mathbf{m}\mathbf{m}'} \gg \sigma_{\mathbf{m}\mathbf{m}'}, \hat{D}_{\mathbf{ml}}$ ) and the Coulomb interaction is masked

by the electron-phonon interaction [i.e., if the second term in Eq. (18) is larger than the first], it follows from Refs. 1 and 2 that polarons form bound pairs in the form of small bipolarons. We shall consider only bipolarons localized at one lattice site. We shall assume that  $E_m = 0$ , which corresponds simply to a new reference point for the polaron and energy and in Eq. (18) we shall assume that only the diagonal terms with  $\mathbf{m} = \mathbf{m}'$  differ from zero:

$$V_{\mathbf{m}\mathbf{m}'}^{\mathbf{m}\mathbf{m}'} = -1/2 \Delta \delta_{\mathbf{m}\mathbf{m}'}. \quad (20)$$

We shall show below that  $\Delta$  determines the reduction in the ground-state energy of bipolarons compared with the energy of the ground state of polarons.

Following the treatment in Refs. 1 and 2, we shall apply the second canonical transformation

$$H_b = e^{S_2} H_p e^{-S_2}. \quad (20)$$

We shall write down the Hamiltonian  $H_p$  in the form

$$H_p = H_0 + H_1, \quad (21)$$

where

$$H_0 = \sum_{\substack{\mathbf{m}, \mathbf{m}', \sigma, \sigma' \\ (\mathbf{m} \neq \mathbf{m}', \sigma \neq \sigma') \\ \text{simultaneously}}} V_{\mathbf{m}\mathbf{m}'}^{\mathbf{m}\mathbf{m}'} c_{\mathbf{m}\sigma}^+ c_{\mathbf{m}'\sigma'}^+ c_{\mathbf{m}'\sigma'} c_{\mathbf{m}\sigma} \\ + \sum_{\mathbf{p}} \omega(\mathbf{p}) d_{\mathbf{p}}^+ d_{\mathbf{p}} + \sum_{\mathbf{l}\mathbf{l}'} T_{\mathbf{l}\mathbf{l}'}^{(N)} a_{\mathbf{l}\sigma}^+ a_{\mathbf{l}'\sigma'}, \quad (22)$$

and

$$H_1 = \sum_{\substack{\mathbf{m}, \mathbf{m}', \sigma \\ (\mathbf{m} \neq \mathbf{m}')}} \sigma_{\mathbf{m}\mathbf{m}'} c_{\mathbf{m}\sigma}^+ c_{\mathbf{m}'\sigma} + \sum_{\mathbf{m}, \mathbf{l}\sigma} (\bar{D}_{\mathbf{m}\mathbf{l}} a_{\mathbf{l}\sigma}^+ c_{\mathbf{m}\sigma} + \text{H.c.}). \quad (23)$$

In order to remove terms that destroy bipolarons, we must select  $S_2$  subject to the condition<sup>17</sup>

$$H_1 + [S_2 H_0] = 0, \quad (24)$$

which gives

$$\langle f | S_2 | f' \rangle = \frac{\langle f | H_1 | f' \rangle}{E_f - E_{f'}}, \quad (25)$$

where  $|f\rangle$  and  $|f'\rangle$  are the eigenvectors of the Hamiltonian  $H_0$  with the energies  $E_f$  and  $E_{f'}$ .

Using Eqs. (20)–(25) for the matrix element of the operator  $H_b$ , we obtain

$$(H_b)_{ff'} = E_f \delta_{ff'} + \frac{1}{2} \sum_{\lambda} \langle f | \\ \times \sum_{\mathbf{m}, \mathbf{m}', \sigma} \sigma_{\mathbf{m}\mathbf{m}'} c_{\mathbf{m}\sigma}^+ c_{\mathbf{m}'\sigma} | \lambda \rangle \langle \lambda | \sum_{\mathbf{n}, \mathbf{n}', \sigma} \sigma_{\mathbf{n}\mathbf{n}'} c_{\mathbf{n}\sigma}^+ c_{\mathbf{n}'\sigma} | f' \rangle \\ \times \frac{2E_{\lambda} - E_f - E_{f'}}{(E_f - E_{\lambda})(E_{\lambda} - E_{f'})} + \frac{1}{2} \sum_{\lambda'} \frac{2E_{\lambda'} - E_f - E_{f'}}{(E_f - E_{\lambda'})(E_{\lambda'} - E_{f'})} \\ \times \left( \langle f | \sum_{\mathbf{m}, \mathbf{l}\sigma} \bar{D}_{\mathbf{m}\mathbf{l}} a_{\mathbf{l}\sigma}^+ c_{\mathbf{m}\sigma} | \lambda' \rangle \langle \lambda' | \sum_{\mathbf{m}', \mathbf{l}'\sigma'} \bar{D}_{\mathbf{m}'\mathbf{l}'}^+ c_{\mathbf{m}'\sigma'}^+ a_{\mathbf{l}'\sigma'} | f' \rangle + \text{H.c.} \right) \\ + \frac{1}{2} \sum_{\lambda''} \langle f | \sum_{\mathbf{m}, \mathbf{l}\sigma} D_{\mathbf{m}\mathbf{l}} c_{\mathbf{m}\sigma}^+ a_{\mathbf{l}\sigma} | \lambda'' \rangle \langle \lambda'' | \sum_{\mathbf{m}', \mathbf{l}'\sigma'} D_{\mathbf{m}'\mathbf{l}'}^+ a_{\mathbf{l}'\sigma'}^+ c_{\mathbf{m}'\sigma'} | f' \rangle \\ \times \frac{(2E_{\lambda''} - E_f - E_{f'})}{(E_f - E_{\lambda''})(E_{\lambda''} - E_{f'})}. \quad (26a)$$

The states  $|f\rangle$  and  $|f'\rangle$  are diagonal in the number of particles in the  $S$  and  $N$  electrodes; the state  $|\lambda'\rangle$  corresponds to the number of polarons in the  $S$  electrode which is one more and in the  $N$  electrodes to the number of electrons is one less than in the  $|f\rangle$ ,  $|f'\rangle$ , and  $|\lambda\rangle$  states. In the  $|\lambda''\rangle$  case the reverse is true: in the  $S$  electrode the number of polarons is one less and in the  $N$  electrode the number of electrons is one more.

The off-diagonal (in respect of the number of particles) matrix elements of the operator  $H_b$  are as follows:

$$(H_b)_{ff''} = \frac{1}{2} \sum_{\lambda''} \frac{2E_{\lambda''} - E_f - E_{f''}}{(E_f - E_{\lambda''})(E_{\lambda''} - E_{f''})} \langle f | \sum_{\mathbf{m}, \mathbf{l}\sigma} D_{\mathbf{m}\mathbf{l}} c_{\mathbf{m}\sigma}^+ a_{\mathbf{l}\sigma} | \lambda'' \rangle \\ \times \langle \lambda'' | \sum_{\mathbf{m}', \mathbf{l}'\sigma'} D_{\mathbf{m}'\mathbf{l}'}^+ a_{\mathbf{l}'\sigma'}^+ c_{\mathbf{m}'\sigma'} | f'' \rangle, \quad (26b)$$

$$(H_b)_{ff'''} = \frac{1}{2} \sum_{\lambda'''} \frac{2E_{\lambda'''} - E_f - E_{f'''}}{(E_f - E_{\lambda'''})(E_{\lambda'''} - E_{f'''})} \langle f | \sum_{\mathbf{m}, \mathbf{l}\sigma} D_{\mathbf{m}\mathbf{l}} a_{\mathbf{l}\sigma}^+ c_{\mathbf{m}\sigma} | \lambda''' \rangle \\ \times \langle \lambda''' | \sum_{\mathbf{m}', \mathbf{l}'\sigma'} D_{\mathbf{m}'\mathbf{l}'}^+ a_{\mathbf{l}'\sigma'}^+ c_{\mathbf{m}'\sigma'} | f''' \rangle. \quad (26c)$$

In the  $|f''\rangle$  ( $|f'''\rangle$ ) state we find that the  $S$  electrode contains two polarons more (less), whereas the  $N$  electrode contains two electrons less (more) than in the state  $|f\rangle$ .

We shall now introduce bipolaron operators:

$$b_{\mathbf{m}} = c_{\mathbf{m}\downarrow} c_{\mathbf{m}\uparrow}, \quad b_{\mathbf{m}}^+ = c_{\mathbf{m}\uparrow}^+ c_{\mathbf{m}\downarrow}^+. \quad (27)$$

Following Ref. 19, we shall write down the denominators and the corresponding factors in the numerators of Eq. (26) allowing for the following relationships:

$$E_f - E_{\lambda} = E_{f'} - E_{\lambda} = -\Delta + \sum_{\mathbf{q}} (n_{\mathbf{q}}^f - n_{\mathbf{q}}^{\lambda}) \omega(\mathbf{q}), \quad (28)$$

$$E_f - E_{\lambda'} = E_{f'} - E_{\lambda'} = -\frac{\Delta}{2} + \sum_{\mathbf{q}} (n_{\mathbf{q}}^f - n_{\mathbf{q}}^{\lambda'}) \omega(\mathbf{q}),$$

where  $n_{\mathbf{q}}^f$  and  $n_{\mathbf{q}}^{\lambda'}$  are the numbers of phonons with the momentum  $\mathbf{q}$  in the states  $|f\rangle$  and  $|\lambda'\rangle$ , respectively. The differences  $E_f - E_{\lambda''}$ ,  $E_{f'} - E_{\lambda''}$ ,  $E_{f''} - E_{\lambda''}$ ,  $E_{f'''} - E_{\lambda''}$  are exactly equal to the difference  $E_f - E_{\lambda'}$ , defined by Eq. (28).

After averaging Eq. (26) with the phonon density matrix

$$\rho = \frac{\exp(-H_{\text{ph}}/T)}{\text{Sp} \exp(-H_{\text{ph}}/T)} \quad (29)$$

[ $H_{\text{ph}} = \sum_{\mathbf{q}} \omega(\mathbf{q}) d_{\mathbf{q}} + d_{\mathbf{q}}$  is the phonon part of the Hamiltonian], and allowing for Eqs. (27) and (28), we find that the bipolaron Hamiltonian becomes

$$H_b = \sum_{\mathbf{q}} \omega_{\mathbf{q}} d_{\mathbf{q}}^+ d_{\mathbf{q}} + \sum_{\mathbf{l}, \mathbf{l}'\sigma} T_{\mathbf{l}\mathbf{l}'}^{(N)} a_{\mathbf{l}\sigma}^+ a_{\mathbf{l}'\sigma} - \sum_{\mathbf{m} \neq \mathbf{m}'} t_{\mathbf{m}\mathbf{m}'} b_{\mathbf{m}}^+ b_{\mathbf{m}'} \\ + \sum_{\mathbf{m} \neq \mathbf{m}'} \tilde{v}_{\mathbf{m}\mathbf{m}'} b_{\mathbf{m}}^+ b_{\mathbf{m}'} b_{\mathbf{m}'}^+ b_{\mathbf{m}} + \sum_{\mathbf{m}, \mathbf{l}\mathbf{l}'} (\bar{D}_{\mathbf{m}\mathbf{l}}^+ b_{\mathbf{m}}^+ a_{\mathbf{l}\sigma}^+ a_{\mathbf{l}'\sigma} - \bar{D}_{\mathbf{m}\mathbf{l}'} b_{\mathbf{m}} a_{\mathbf{l}\sigma}^+ a_{\mathbf{l}'\sigma}^+). \quad (30)$$

We shall assume that the renormalized energy of the sites vanishes and ignore the terms proportional to  $D_{\mathbf{m}\mathbf{l}}^* D_{\mathbf{m}\mathbf{l}'}^*$ ,

which are small compared with the other terms when the bipolaron concentration is low.

The bipolaron hopping integral is

$$t_{mm'} = 2i \int_0^{\infty} d\tau \exp[-(i\Delta + \delta)\tau] \langle \sigma_{mm'}(\tau) \sigma_{m'm}(0) \rangle, \quad (31)$$

the dynamic bipolaron-bipolaron interaction is described by

$$\tilde{v}_{mm'} = 4V_{mm'}^{mm'} + 2i \int_0^{\infty} d\tau \exp[-(i\Delta + \delta)\tau] \langle D_{m1}(\tau) D_{m1}(0) \rangle, \quad (32)$$

and the matrix element of the tunneling interaction is

$$\tilde{D}_{m11'} = i \int d\tau \exp\left[-\left(i\frac{\Delta}{2} + \delta\right)\tau\right] \langle D_{m1}(\tau) D_{m1'}(0) \rangle. \quad (33)$$

The following notation is introduced in Eqs. (31)–(33):

$$\begin{aligned} \sigma_{mm'}(\tau) &= \exp(iH_{ph}\tau) \sigma_{mm'} \exp(-iH_{ph}\tau), \\ D_{m1}(\tau) &= \exp(iH_{ph}\tau) D_{m1} \exp(-iH_{ph}\tau). \end{aligned}$$

The following analytic expressions for  $t_{mm'}$  and  $\tilde{v}_{mm'}$  are obtained in Ref. 19:

$$\begin{aligned} t_{mm'} &= 2T_{mm'} T_{m'm} / \Delta, \\ \tilde{v}_{mm'} &= 4V_{mm'}^{mm'} + (2T_{mm'}^2 / \Delta) \exp(-4g^2). \end{aligned} \quad (34a)$$

If  $\Delta \gg \omega = \varepsilon_p / g^2$ , where  $\omega$  is the characteristic phonon frequency of the system, we have  $\varepsilon_p = \sum_{\mathbf{q}} \omega^{-1}(\mathbf{q}) U^2(\mathbf{q})$  for the polaron shift,  $U(\mathbf{p}) = U_{kk}(\mathbf{p})$  [see Eq. (2)], and the dimensionless electron-phonon interaction constant  $g$  is described by

$$g^2 = \sum_{\mathbf{q}} \omega^{-2}(\mathbf{q}) \text{cth}\left(\frac{\omega(\mathbf{q})}{2T}\right) |U(\mathbf{q})|^2 [1 - \cos \mathbf{q}(\mathbf{R}_m - \mathbf{R}_{m'})]. \quad (34b)$$

In the same approximation, we have

$$\tilde{D}_{m11'} = (4/\Delta) \exp(-2\eta^2) D_{m1} D_{m1'}, \quad (34c)$$

where

$$\eta^2 = \sum_{\mathbf{q}} \omega^{-2}(\mathbf{q}) \text{cth}\left(\frac{\omega(\mathbf{q})}{2T}\right) |U(\mathbf{q})|^2. \quad (34d)$$

If  $T \ll \Delta \ll \omega$ , it follows that

$$\begin{aligned} t_{mm'} &= (2/\Delta) T_{mm'} T_{m'm} \exp(-2g^2), \\ \tilde{v}_{mm'} &= 4V_{mm'}^{mm'} + (2/\Delta) T_{mm'}^2 \exp(-2g^2), \\ \tilde{D}_{m11'} &= (4/\Delta) D_{m1} D_{m1'} \exp(-\eta^2). \end{aligned} \quad (35)$$

In the subsequent calculations we shall make a number of simplifications in the bipolaron Hamiltonian of Eq. (30). We shall consider the case of a low bipolaron concentration (i.e., we shall assume that the number of sites at which there are bipolarons is less than that of unoccupied sites) and we shall ignore the interaction between bipolarons:  $\tilde{v}_{mm'} = 0$ . It is shown in Ref. 16 that in the same approximation the operators  $b_n$  and  $b_n^+$  can be regarded as of the Bose type.

Allowing for the approximations and going back to the momentum representation, we obtain

$$\begin{aligned} H_b &= \sum_{\mathbf{k}} \varepsilon_b(\mathbf{k}) b_{\mathbf{k}}^+ b_{\mathbf{k}} + \sum_{\mathbf{q}, \sigma} \varepsilon_N(\mathbf{q}) a_{\mathbf{q}\sigma}^+ a_{\mathbf{q}\sigma} \\ &+ \sum_{\mathbf{k}, \mathbf{q}_1, \mathbf{q}_2} (D_{\mathbf{k}\mathbf{q}_1\mathbf{q}_2}^* b_{\mathbf{k}}^+ a_{\mathbf{q}_1\uparrow} a_{\mathbf{q}_2\downarrow} - D_{\mathbf{k}\mathbf{q}_1\mathbf{q}_2} b_{\mathbf{k}} a_{\mathbf{q}_1\uparrow}^+ a_{\mathbf{q}_2\downarrow}^+), \end{aligned} \quad (36)$$

where  $\varepsilon_b(\mathbf{k})$  is the energy of the bipolaron with a momentum  $\mathbf{k}$ :

$$\begin{aligned} \varepsilon_b(\mathbf{k}) &= 2 \frac{\exp(-\theta g^2)}{\Delta N_s} \sum_{\mathbf{k}'} \varepsilon_s(\mathbf{k}') \varepsilon_s(\mathbf{k} - \mathbf{k}'), \\ \theta &= 0 \text{ for } \Delta \gg \omega, \theta = 2 \text{ for } T \ll \Delta \ll \omega; \end{aligned} \quad (37)$$

where

$$D_{\mathbf{k}\mathbf{q}_1\mathbf{q}_2} = \frac{4}{\Delta N_s^{1/2}} \exp(-\theta \eta^2) \sum_{\mathbf{k}'} D_{\mathbf{k}'\mathbf{q}_1} D_{\mathbf{k}-\mathbf{k}',\mathbf{q}_2}, \quad (38)$$

where  $\theta = 1$  for  $\Delta \gg \omega$  and  $\theta = 2$  for  $T \ll \Delta \ll \omega$ .

We shall regard  $\varepsilon_s(\mathbf{k})$  as the energy of electrons in a crystal, obtained in the tight-binding approximation for a cubic lattice:

$$\varepsilon_s(\mathbf{k}) = \varepsilon_0 [3 - \cos k_x a - \cos k_y a - \cos k_z a]. \quad (39)$$

If the mass of an electron near the bottom of the band is denoted by  $m$ , then the dimensional expression is  $\varepsilon_0 = \hbar^2 / (a^2 m)$ .

We shall describe the matrix element  $D_{\mathbf{k}\mathbf{q}}$  using the WKB approximation,<sup>17</sup> according to which

$$D_{\mathbf{k}\mathbf{q}} = \left[ \frac{\partial \varepsilon_s(\mathbf{k})}{\partial k_x} \right]^{1/2} \left[ \frac{\partial \varepsilon_N(\mathbf{q})}{\partial q_x} \right]^{1/2} D_0, \quad (40)$$

where  $k_x$  and  $q_x$  are the projections of the wave vectors perpendicular to the tunnel contact plane and  $D_0$  is a constant which depends weakly on the wave vector.

Substitution of Eq. (39) into Eq. (37) gives the dispersion law of bipolarons which is exactly the same as Eq. (39) where we have to replace  $\varepsilon_0 = \hbar^2 / (a^2 m)$  with  $\varepsilon_{0b} = \hbar^2 / (a^2 m_b)$ . The effective mass of a bipolaron is

$$m_b = \frac{2m_0^2 \Delta a \exp(\theta g^2)}{24\hbar^2}. \quad (41)$$

If  $|k| \ll 1/a$ , the bipolaron energy is a quadratic function of the momentum. In the same limit the matrix element  $D_{\mathbf{k}, \mathbf{q}_1\mathbf{q}_2}$  is

$$D_{\mathbf{k}\mathbf{q}_1\mathbf{q}_2} = \Phi_0 k_x^2 (q_{1x} q_{2x})^{1/2}, \quad (42)$$

if the conditions  $k_x, q_{1x}, q_{2x} > 0$  are satisfied simultaneously, but it vanishes if at least one of the projections is negative. In Eq. (42), we have

$$\Phi_0 = \frac{N_s^{1/2}}{4\Delta} D_0^2 \exp(-\theta \eta^2) \frac{\hbar}{(m_b m_0)^{1/2}}. \quad (42a)$$

The expression for the tunnel term in the Hamiltonian is obtained from the electron tunnel Hamiltonian by applying consecutively two canonical transformations. The matrix element occurring in the tunnel term and responsible for the transition of bipolarons across the tunnel junction can be expressed in terms of the matrix elements of the ordinary

electron tunnel Hamiltonian. However, the term  $T$  representing the tunneling of electrons [see Eq. (1)] is generally introduced phenomenologically, so that in solving the problem of the tunneling of a bipolaron we can use an approach different from that developed above. In the new approach the tunnel term may be introduced into the Hamiltonian exactly in the same way as is done phenomenologically after the canonical transformations. At present we are unable to decide in favor of one of these methods and we therefore thought it suitable to give in the present paper the results obtained by the second approach to the problem of tunneling of a bipolaron across a barrier accompanied by decay into two electrons. In the second approach the nature of the tunnel term is exactly the same as in the first approach, but the dependence of the matrix element on the momenta of a bipolaron and electrons has to be determined, which is done in the next section.

## 2. TUNNEL HAMILTONIAN (SECOND APPROACH)

We shall now describe the second (alternative) method for deriving the tunnel bipolaron Hamiltonian. In full analogy as in the tunneling of electrons, we shall modify the initial Hamiltonian describing bipolarons in the  $S$  electrode and electrons in the  $N$  electrode by introducing the tunnel term  $T$  describing a sub-barrier transition of a bipolaron followed by decay into two electrons in the  $N$  electrode.

More exactly, the initial Hamiltonian is similar to that given by Eq. (36), but  $D_{kq_1q_2}$  is a quantity which has to be determined. We recall that a similar quantity for one-electron tunneling is found by comparison with the corresponding results of a quantum-mechanical problem of a sub-barrier transition of an electron from one material to another. We shall therefore consider the following problem: in the initial state we have a bound system of two particles moving toward a barrier. In the final state, we have two free particles. Clearly, this process involves not only the tunneling but also the dissociation (decay) of the bound system. It is this decay that introduces a considerable indeterminacy into the amplitude of the process, because it depends on the nature of the interaction in the bound system and on the properties of the junction layer where the decay occurs. Nevertheless, we can follow this approach to obtain useful information on the transition amplitude (it should be noted that even in the one-electron case the height of the barrier occurring in the expression for the amplitude remains unknown and it can be estimated only from the experimental data).

Let us assume that a bound system goes over from a region I (Fig. 1) to a region II via a region III, where the dissociation takes place. A sub-barrier transition occurs in a region defined by  $0 < y < l$ .

By definition, the transition amplitude is<sup>20</sup>

$$A = \int dx_1 dx_2 dx'_1 dx'_2 \psi_{II}(x'_1, x'_2) \times K(x'_1, x'_2, t'; x_1, x_2, t) \psi_I(x_1, x_2). \quad (43)$$

Here,  $\psi_I$  and  $\psi_{II}$  are the initial and final steady states of the system,  $K$  is the amplitude of conversion of particles with the coordinates  $x_1$  and  $x_2$  at a moment  $t \rightarrow -\infty$  into particles with the coordinates  $x'_1$  and  $x'_2$  at a moment  $t' \rightarrow +\infty$ . The wave functions are selected in the form

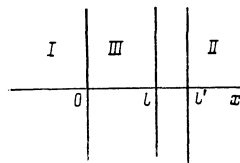


FIG. 1. Schematic representation of a tunnel junction.

$$\psi_I(x_1, x_2) = \varphi(x) \exp(iPX), \quad \psi_{II}(x_1, x_2) = \exp(ip_1x'_1 + ip_2x'_2) \quad (44)$$

with normalization to one particle per unit volume. The following notation is used above:  $x = x_1 - x_2$ ,  $X = (x_1 + x_2)/2$ ,  $P$  is the momentum of the bound system,  $p_1$  and  $p_2$  are the momenta of the final particles.

The amplitude  $K$  can be expressed in terms of the path integral in the following way:<sup>20</sup>

$$K(x'_1, x'_2, t'; x_1, x_2, t) = \int_{x_1, x_2}^{x'_1, x'_2} Dy_1 Dy_2 e^{iS}, \quad (45)$$

where  $S$  is the action of the system. We shall select it in the form

$$S = \int_t^{t'} d\tau \left[ \frac{\mu \dot{y}_1^2}{2} + \frac{\mu \dot{y}_2^2}{2} - U(y_1) - U(y_2) - u(y_1, y_2) \right], \quad (46)$$

where  $U(y)$  is the potential which is constant everywhere apart from the region of the tunnel junction (it is this junction which is the barrier to the motion of the particles) and  $u(y_1, y_2)$  is the interparticle potential. In the region II, we have  $u = 0$ . We shall now make simplifying assumptions which are quite permissible for our purpose. We shall assume that the characteristic size of the bound system  $d$  satisfies the condition  $d \ll l$ .

It is then convenient to introduce the coordinate of the center of mass of the bound system  $Y = \frac{1}{2}(y_1 + y_2)$  and to assume that the potential  $u(y_1, y_2)$  is such that

$$u(Y, y_1 - y_2) = v(y_1 - y_2) \quad \text{for } Y < l, \quad (47)$$

$$u(Y, y_1 - y_2) = 0 \quad \text{for } Y > l'.$$

Our task is to obtain a closed expression for the amplitude of Eq. (43) using the definitions of Eqs. (44)–(47).

Calculation of Eq. (45) by the steepest-descent method, gives<sup>20,21</sup>

$$K = \left( \det \frac{\partial^2 S_{cl}}{\partial x_i \partial x'_j} \right)^{1/2} e^{iS_{cl}}, \quad i, j = 1, 2. \quad (48)$$

In this case the preexponential factor represents generalization to the two-particle process of the familiar Van Vleck determinant,<sup>21</sup>  $S_{cl} = S[y_{1cl}, y_{2cl}]$ , and the classical paths  $y_{1cl}(\tau)$  and  $y_{2cl}(\tau)$  are found from the equations

$$\left. \frac{\delta S}{\partial y_k} \right|_{y_{kcl}} = 0 \quad (k=1, 2) \quad (49)$$

subject to the additional conditions

$$y_k(t) = x_k, \quad y_k(t') = x'_k.$$

Substituting Eqs. (44) and (48) into Eq. (43) and applying the steepest-descent method in the course of integration with respect to the variables  $x'_1$  and  $x'_2$ , we obtain the following expression for the amplitude:

$$A = \int dx_1 dx_2 \varphi(x) \left[ \det \frac{\partial^2 S_{cl}}{\partial x_i \partial x_j} / \det \frac{\partial^2 S_{cl}}{\partial x'_i \partial x'_j} \right]_{x'_i = x_{icl}}^{1/2} \times \exp [i(PX - p_1 x'_{1cl} - p_2 x'_{2cl} + S_{cl})]. \quad (50)$$

The quantities  $x'_{icl}$  are found from the conditions for an extremum

$$\partial S_{cl} / \partial x'_{icl} - p_k = 0. \quad (51)$$

The main task thus reduces to finding the value of  $S_{cl}$  and of the determinants which occur in the preexponential factor. The results of the solution of Eq. (49) which give  $S_{cl}$  can be obtained everywhere except for the region III, where the decay of the bound system takes place, and it depends strongly on the potentials  $U(y)$  and  $u(Y, y)$ . Nevertheless, the general properties of the classical equations allow us to move further. Moreover, we need the fact that the derivative of the action with respect to the final coordinate of a path is the momentum, i.e.,

$$\frac{\partial S_{cl}}{\partial x_k} = \tilde{p}_k \equiv \frac{\mu(x'_k - z'_k)}{(t' - t^*)}. \quad (52)$$

Moreover, the law of conservation of energy should be satisfied along a classical path:

$$\varepsilon_P + \varepsilon_B = \varepsilon_1 + \varepsilon_2. \quad (53)$$

Here,  $t^{**}$  is the moment in time when the center of mass of a closed system reaches the region III, i.e.,  $Y(t^{**}) = l'$ ;  $z'_1$  and  $z'_2$  are the coordinates of the particles at the moment  $t^{**}$ ;  $z' = z'_1 - z'_2$ ;  $\tilde{\varepsilon}_k = \tilde{p}_k^2 / 2\mu$ ;  $\varepsilon_B$  is the binding energy;  $\varepsilon_P$  is the kinetic energy of the closed system:  $\varepsilon_P = \tilde{P}^2 / 4\mu$ , where  $\tilde{P} = 2\mu X / (t - t^*)$ ;  $t^*$  is the moment in time when the center of mass of the bound system reaches the region II, i.e.,  $Y(t^*) = l$ . Using the equalities given above, we can find the preexponential factor in Eq. (50) and the expression for the amplitude becomes

$$A = \int dX dx \varphi(x) \left[ \frac{\partial z'}{\partial x} \frac{(p_1 + p_2)}{P} \right]^{1/2} \exp \left\{ iS_3 - \mathcal{F}_B - it^* \left[ -P \left( \frac{e_P}{\mu} \right)^{1/2} + \varepsilon_P - \varepsilon_B + \varepsilon_1 + \varepsilon_2 \right] - \int_x^z d\xi \left[ \frac{\mu}{2} (\varepsilon_B - v(\xi)) \right]^{1/2} \right\}. \quad (54)$$

Allowance is made above for the fact that Eqs. (51) and (52) yield  $\tilde{p}_k = p_k \equiv (2\mu\varepsilon_k)^{1/2}$  and whenever possible the quantities  $z = z_1 - z_2$  and  $t^* - t^{**}$  are ignored, which is justified for  $|t|, |t'| \rightarrow \infty$ ;  $S_3$  is the classical action for two particles which at the moment  $t^*$  are at the points  $z_1$  and  $z_2$  and at the moment  $t^{**}$  are at the points  $z'_1$  and  $z'_2$ . Using the semi-classical form of the function  $\varphi(x)$  and substituting the variables, we obtain

$$A = \int dX \left( \frac{p_1 + p_2}{P} \right)^{1/2} \Phi(p_1, p_2) \times \exp [it^* (\varepsilon_P + \varepsilon_1 + \varepsilon_2 - \varepsilon_B) + iPX - \mathcal{F}_B],$$

$$\Phi(p_1, p_2) = \int dz \varphi(z) \frac{\partial z'}{\partial z} \exp [iS_3 + i(p_1 - p_2)z].$$

Integration with respect to  $X$  is a trivial matter if we allow for the fact that  $\mu X = \varepsilon_P^{1/2} (t - t^*)$ . Finally, the amplitude of the process is

$$A(P, p_1, p_2) = 2\pi D_{Pp_1p_2} \delta(\varepsilon_1 + \varepsilon_2 - \varepsilon) \quad D_{Pp_1p_2} = \Phi_0 [P(p_1 + p_2)]^{1/2}, \quad (55)$$

$$\Phi_0 = (2\mu)^{-1} e^{-\mathcal{F}} \Phi(p_1, p_2), \quad (55a)$$

where  $\varepsilon_1, \varepsilon_2, p_1$ , and  $p_2$  are the energies and momenta of the final particles;  $\varepsilon$  and  $P$  are the energy and momentum of the bound system. It should be pointed out that it is the matrix element  $D_{Pp_1p_2}$  that occurs in this case in the Hamiltonian (36).

The factor  $\exp(-\mathcal{F})$  usually appears in calculations dealing with sub-barrier transitions. When the bound system dissociates before such a transition, we have

$$\mathcal{F} = \mathcal{F}_e = \int_0^{l'} d\xi \{ [2\mu(U(\xi) - \varepsilon_1)]^{1/2} + [2\mu(U(\xi) - \varepsilon_2)]^{1/2} \},$$

whereas in the case of dissociation of the system after the sub-barrier transition, we obtain

$$\mathcal{F} = \mathcal{F}_B = \int_0^{l'} d\xi 2 \{ \mu [U(\xi) - \varepsilon_P] \}^{1/2}.$$

If the bound state dissociates after crossing a region  $0 < y < l'$ , then the function  $\Phi(p_1, p_2)$  depends on the properties of the decay region and on the potential of the interparticle interaction in the bound system. In the extremely simplified formation of the problem, when the size of the decay region III vanishes, we have

$$\Phi(p_1, p_2) = \int dz \varphi(z) \exp [i(p_1 - p_2)z],$$

where  $\varphi(z)$  is the wave function of the bound system. Attempts to derive rigorously the function  $\Phi$  on the basis of the two-particle problem are doomed to failure because inelastic processes occur in the decay region. Therefore, the selection of the type of function must be made on the basis of physical considerations.

In addition to the usual factor  $\sqrt{P}$ , we also have a factor  $[(p_1 + p_2)/2]^{1/2}$ , indicating that the probability of a tunnel transition vanishes if the center of mass of a system of two particles is at rest. However, if the momentum of one particle vanishes, the tunneling is nevertheless possible since a particle at rest may form a bound system with an incident particle, but in this case the momentum of the system does not vanish.

Generalization to the three-dimensional case is carried out in the same way as for the one-electron tunneling.<sup>22</sup>

$$D_{\mathbf{p}_1, \mathbf{p}_2} = [P_x(p_{1x} + p_{2x})]^{1/2} \Phi_0 \delta^{(2)}(\mathbf{P}_\perp - \mathbf{p}_{1\perp} - \mathbf{p}_{2\perp}). \quad (56)$$

The two-dimensional  $\delta$  function in Eq. (56) reflects the law of conservation of the component of the momentum parallel to the tunnel junction plane. This is true only in the case of an ideal junction when we can ignore the influence of inhomogeneities, because otherwise Eq. (56) must be averaged over  $\mathbf{P}_\perp$ ,  $\mathbf{p}_{1\perp}$  and  $\mathbf{p}_{2\perp}$ , so that the  $\delta$ -functional dependence is lost. The expressions (42) and (56) obtained for the matrix element  $D_{\mathbf{k}q_1q_2}$  are different. The difference between the momentum dependences of Eqs. (42) and (56) can be explained qualitatively by the fact that they are obtained for different limiting cases: Eq. (42) on the assumption of low-mobility bipolarons (narrow energy bands) tunneling from a site adjoining the tunnel junction into the metal. Equation (56) is obtained using the concept of bipolarons considered as free particles (wide energy band). The final answer of the correctness of one or the other expression can be obtained only by comparison with experimental results.

Nevertheless, as shown below, the difference between the matrix elements (42) and (56) has only a quantitative effect on the final results. The main qualitative conclusions are independent of the initial model of the Hamiltonian because both models rely on the hypothesis of bipolarons as charge carriers and on the finite width of the bipolaron energy band.

### 3. EXPRESSION FOR THE TUNNEL CURRENT

We shall define the tunnel current using the standard expression<sup>17</sup>

$$I = -2e \left\langle \frac{d}{dt} \sum_{\mathbf{k}} b_{\mathbf{k}}^+ b_{\mathbf{k}} \right\rangle, \quad (57)$$

where  $e$  is an elementary positive charge and the factor 2 appears because a bipolaron consists of two polarons; the angular brackets denote the Gibbs averaging procedure.

If a junction is subjected to a voltage, chemical potentials of the  $S$  and  $N$  electrodes become different. The difference between them can be allowed for by introducing an additional term  $-2V \sum_{\mathbf{k}} b_{\mathbf{k}}^+ b_{\mathbf{k}}$  in the Hamiltonian of Eq. (36), i.e., it can be allowed for by renormalization of the origin of the bipolaron energy scale.

Averaging in Eq. (57) and allowing for the specific form of the Hamiltonian (36), we find that the tunnel current can be described by

$$I = -4e \operatorname{Im} \sum_{\mathbf{k}, q_1, q_2} |D_{\mathbf{k}q_1q_2}|^2 \frac{\langle b_{\mathbf{k}}^+ b_{\mathbf{k}} \rangle (1 - f_{q_1} - f_{q_2}) - f_{q_1} f_{q_2}}{\varepsilon_N(\mathbf{q}_1) + \varepsilon_N(\mathbf{q}_2) - \varepsilon_b(\mathbf{k}) + 2V - i0} \quad (58)$$

( $f_q$  is the Fermi distribution function).

The first term in the Hamiltonian of Eq. (36) is the kinetic energy of bipolarons similar to the total Hamiltonian of a noninteracting Bose gas, apart from the momentum dependence of the energy. An ideal Bose gas condenses at low temperatures and the degeneracy temperature is also the critical superconducting transition temperature.

If the temperature of a junction is below the critical value, then the  $S$  electrode contains not only condensate charge carriers, but also those in excess of the condensate. However, the condensate particles make no contribution to

the tunnel current because they are characterized by  $k = 0$  and  $D_{0q_1q_2} = 0$ .

For this reason we can simplify the sum in Eq. (58) by excluding the term with  $k = 0$  and it is also why the average of the operators

$$\langle b_{\mathbf{k}}^+ b_{\mathbf{k}} \rangle = \varphi_{\mathbf{k}} \quad (59)$$

is the Bose distribution function.

Going over from summation to integration with respect to the momenta in Eq. (58), we obtain

$$I(V, T) = \frac{4\Phi_0^2}{(2\pi)} \int d^3\mathbf{k} \int d^3\mathbf{q}_1 \int d^3\mathbf{q}_2 L(k_x, q_{1x}, q_{2x}) \times [\varphi_{\mathbf{k}} (1 - f_{q_1} - f_{q_2}) - f_{q_1} f_{q_2}] \delta(\varepsilon_N(\mathbf{q}_1) + \varepsilon_N(\mathbf{q}_2) - \varepsilon_b(\mathbf{k}) + 2V),$$

$$L(k_x, q_{1x}, q_{2x}) = \begin{cases} k_x^4 q_{1x} q_{2x} & \text{for first model} \\ k_x (q_{1x} + q_{2x})^{1/2} & \text{for second model,} \end{cases} \quad (60)$$

where  $T$  is the temperature in energy units.

In Eq. (60) we used  $k_x k \cos \theta$ ,  $q_{1,2x} = q_{1,2} \cos \theta$  (the angle  $\theta$  is measured from the  $x$  axis perpendicular to the junction plane);  $\Phi_0$  is governed by Eqs. (42a) and (55a) for the first and second models, respectively.

If the dispersion law of polarons and electrons is quadratic (we shall assume that near the Fermi surface of the  $N$  electrode we can still use the quadratic dispersion law, which is quite obvious in the case of bipolarons because at low temperatures the main contribution to the tunnel current is made by the bottom of the bipolaron band), after changing from integration with respect to the momenta to integration with respect to the energies, we find that  $I(V, T)$  is given by

$$I = I_0 \int_0^W \varepsilon^n (\varepsilon - 2V) [(e^{\varepsilon/T} - 1)^{-1} - (e^{(\varepsilon - 2V)/T} - 1)^{-1}] d\varepsilon, \quad (61)$$

where

$$I_0 = \frac{\Phi_0^2 m_b^{1/2} m_0^4 \varepsilon_F^2}{2^{1/2} 5\pi^6}$$

and  $n = 5/2$  for the first model, whereas

$$I_0 = \frac{\Phi_0^2 m_b^2 m_0^{1/2} \varepsilon_F^5}{2^{5/2} \pi^6}$$

and  $n = 1$  for the second model;  $W$  is the width of the bipolaron energy band;  $\varepsilon_F$  is the Fermi energy of electrons in the  $N$  electrode.

In the derivation of Eq. (61) it is assumed that the width of the electron energy band in the  $N$  electrode is considerably greater than  $W$ . In this case the density of the electron states  $N(\varepsilon)$  formed on transition from integration with respect to the momenta to integration with respect to the energy can be described by its value at the Fermi level  $N(0)$ , as is usually done in calculations of the tunneling characteristics. This cannot be done in the case of the density of the bipolaron states  $N_b(\varepsilon)$ , because near the bottom of the band there is a strong dependence of the energy on the momentum  $N_b(\varepsilon) \propto \sqrt{\varepsilon}$ , so that  $\varepsilon_b(\mathbf{k}) \propto \mathbf{k}^2$  [Eq. (61) is derived on the assumption that  $N_b(\varepsilon) \propto \sqrt{\varepsilon}$  for  $\varepsilon < W$  and  $N_b(\varepsilon) = 0$  for  $\varepsilon > W$ ].

In the  $T = 0$  case it follows from Eq. (61) that an analytic expression can be obtained for the tunnel current. In the first model, we have

$$I = \begin{cases} 0, & 2V \leq 0 \\ (1/6)I_0(2V)^{3/2}, & 0 < 2V \leq W \\ 2I_0W^{1/2}(-W/9 + 2V/7), & 2V > W \end{cases} \quad (62a)$$

In the second model, we have

$$I = \begin{cases} 0, & V < 0 \\ 1/6 I_0 (2V)^3, & 0 \leq 2V \leq W \\ I_0 \frac{W^2}{2} (-2/3 W + 2V), & 2V > W \end{cases} \quad (62b)$$

For negative directions the current vanishes because the chemical potential of bipolarons exceeds by  $2V$  the chemical potential of electrons. Electrons cannot cross the tunnel barrier because there are no allowed states below the chemical potential of bipolarons. Moreover, since  $D_{0q_1, q_2} = 0$ , the transition of bipolarons across the tunnel barrier is also impossible.

If  $0 < 2V < W$ , the current-voltage characteristics are nonlinear because of the strong energy dependence of the density of bipolaron states and because of the energy dependence of the matrix element  $L(k_x, q_{1x}, q_{2x})$ .

If  $2V > W$ , then the upper boundary of the bipolaron band lies at an energy below the Fermi level in the normal electrode, the current-voltage characteristic becomes linear because the tunnel current includes contributions of electron transitions to the whole of the bipolaron band.

Numerical calculations of the current-voltage characteristic of a junction are carried out for a nonzero temperature using Eq. (61) for  $T < T_c$  ( $T_c$  is the Bose condensation temperature, which is identical in the bipolaron model with the superconducting transition temperature) and also using the relationship

$$I = I_0 \int_0^W d\varepsilon \varepsilon^n (\varepsilon - 2V) \left\{ \left[ \exp\left(\frac{\varepsilon - \mu(T)}{T}\right) - 1 \right]^{-1} \times \left[ \exp\left(\frac{\varepsilon - \mu(T) - 2V}{T}\right) - 1 \right]^{-1} \right\}. \quad (63)$$

In Eq. (63) at temperatures  $T > T_c$  the chemical potential of bipolarons  $\mu(T)$  is found from the normalization condition

$$n_b = \int_0^W N_b(\xi) d\xi \left[ \exp\left(\frac{\xi - \mu(T)}{T}\right) - 1 \right]^{-1}. \quad (64)$$

The results of the calculations carried out using the first and second models are presented in Fig. 2 for different temperatures and a fixed value  $W = 1.5T_c$ .

Since at  $T \neq 0$  some bipolarons ( $T < T_c$ ) or all of them ( $T > T_c$ ) leave the condensate at  $2V < 0$ , the current becomes greater than zero and its absolute value increases with temperature. The nonlinear part of the current-voltage characteristic is retained both at  $T < T_c$  and  $T > T_c$ , and in both cases we have  $0 < 2V < W$ . This is demonstrated most clearly in Fig. 3, which gives the dependence of the derivative  $dI/dV$  on the voltage across the junction. The curves representing this dependence consist of three regions. If  $2V < 0$  and  $2V > W$ , the regions are flat, whereas for  $0 < 2V < W$ , there is

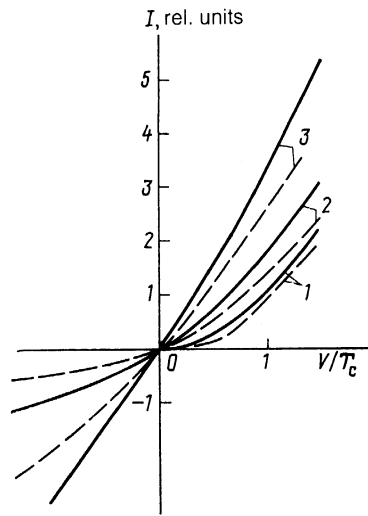


FIG. 2. Current-voltage characteristic of an  $S-I-N$  junction. The width of the bipolaron band is  $W = 1.5T_c$ ; the dashed lines represent the first model and the continuous lines represent the second model; 1)  $T = 0.05T_c$ ; 2)  $T = 0.5T_c$ ; 3)  $T = 1.1T_c$ .

a monotonic rise. The results of calculations of the current-voltage characteristics are qualitatively the same for both models.

#### 4. CONCLUSIONS

We calculated the current-voltage characteristics of superconductor-insulator-normal metal junctions in the case when the superconductivity can be described by the bipolaron theory developed by Alexandrov and Ranninger.<sup>2,3</sup> We used the approximation of noninteracting bipolarons. The approximation of a strong electron-phonon interaction and the model of a tunnel Hamiltonian were used to obtain expressions for the tunnel current. The calculations showed the following.

1) The current-voltage characteristics of the junctions are strongly asymmetric when the polarity of the voltage across the junction is reversed, which is typical<sup>4-7</sup> of the experimentally observed current-voltage characteristics of the  $S-I-N$  junctions, where the  $S$  electrode is a high-tem-

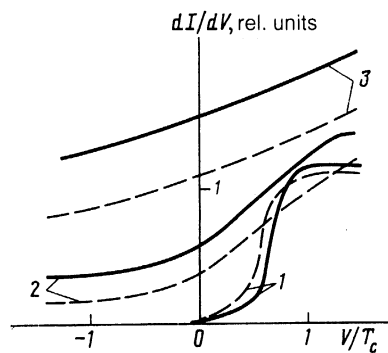


FIG. 3. Differential conductance of an  $S-I-N$  junction. The width of the bipolaron band is  $W = 1.5T_c$ ; the dashed curves represent the first model and the continuous curves the second model; 1)  $T = 0.05T_c$ ; 2)  $T = 0.5T_c$ ; 3)  $T = 1.1T_c$ .



perature metal oxide superconductor.

2) The current-voltage characteristics and the dependence of  $dI/dV$  on  $V/T_c$  at the junction voltage  $V = W/2$  reveals a singularity associated with a strong energy dependence of the bipolaron states density and also with the fact that the bipolaron energy band is narrow.

3) This singularity does not disappear either in the case when  $T > T_c$ , i.e., when the  $S$  electrode goes over to the normal state.

As pointed out in the Introduction, it is experimentally difficult to extract the information on the gap from the spectrum of electrons using the  $S-I-N$  tunnel characteristic if the  $S$  electrode is a metal oxide superconductor. The difficulty is that the current-voltage characteristic does not then show a steep rise of the current at some value of the voltage, which is identified within the framework of the BCS theory with the superconducting gap, even at very low temperatures<sup>5-12</sup> when an abrupt junction should form if  $T \ll \Delta$ . It follows from our calculations that the singularity of the current-voltage characteristic may be related not to the presence of the gap in the electron spectrum, but to the existence of the bipolaron band.

The same conclusion is supported by the observation<sup>13</sup> of a singularity in the current-voltage characteristics of an  $S-I-N$  junction at a position along the voltage axis independent of temperature. According to the BCS theory the gap should depend strongly on temperature and, therefore, this experimental result cannot be understood. However, in the bipolaron theory,<sup>2-4</sup> the coordinate of a singularity on the voltage axis should be independent of temperature, because the bipolaron band width is independent of  $T$ .

It should be pointed out that some of the experimental features of the current-voltage characteristics of the  $S-I-N$  junctions can be explained only qualitatively for a structure in which the  $S$  electrode is a metal-oxide superconductor. This is due to the fact that we have considered so far only the simplest model of noninteracting bipolarons. In this model there is no tunnel current because of the condensate particles whose momentum vanishes. In a quantitative description of

the experimental results we have to allow for the interaction between bipolarons.

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