(4) The phonon-assisted transitions involve at most one phonon of type TA, TO, or LO of the ZnS lattice. Many fewer phonons are involved in the emission process than in the corresponding absorption process. The emission spectrum is not a mirror image of the absorption spectrum.

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General Theory of Tunneling in Oxide Diodes

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The well-known theory of tunneling in oxide diodes is the tunneling-Hamiltonian method, but this cannot describe processes happening in the oxide layer. Some new experiments necessitate the treatment of the electrons in the barrier as well. The author has elaborated a method using Green's functions to describe the whole phenomenon in an iterative procedure. The starting point is the treatment of two other problems where the metal on the left or right side of the barrier is replaced by an insulator. The current density in the barrier has been derived for normal and superconducting junctions. The phenomenon in a magnetic field has been treated using the microscopic theory, avoiding phenomenological considerations. The applicability of the tunneling Hamiltonian has been investigated; by its use the total current may be calculated. This method has proved to be very suitable for the problem of the anomalous tunneling between two normal metals with paramagnetic impurities in the barrier.

I. INTRODUCTION

IN recent years, the problem of tunneling between two normal or superconducting metals has been investigated thoroughly in numerous experimental and theoretical works. The theory of tunneling through a barrier was first investigated by Bardeen.[1] The general formalism of the problem has been given by Cohen, Falicov, and Phillips,[2] who proposed the tunneling Hamiltonian. This method has proved to be very successful in the interpretation of experimental results.

In the tunneling-Hamiltonian method the barrier is replaced by a mathematical surface, and the Hamiltonian describes processes in which an electron crosses the barrier. This method is a rather phenomenological one and fails to investigate the tunneling processes themselves. The difficulty in the elaboration of a new theory describing the electrons in the barrier, as well, comes from the choice of a set of wave functions that is complete and orthogonal. This problem has been studied very carefully by Prange,[3] and the applicability of the tunneling-Hamiltonian method has been proved in the first-order approximation. A quite different approach has been suggested by de Gennes,[4] who has derived a generalization of the Ginsburg-Landau equation for the tunneling processes. Recently, Josephson[5] proposed a very suggestive method using Green's functions, but it seems to us that the actual application of this method is not simple.

Nevertheless, a few experiments have turned up in which the region of the barrier plays a very important role, for example, the geometrical resonance and boundary effect in a superconducting tunnel junction measured by Tomasch[6] and the electron scattering on paramagnetic impurities in the barrier investigated experi-

[1] J. Bardeen, Phys. Rev. Letters **6**, 57 (1961); **9**, 147 (1962).
[2] M. H. Cohen, L. M. Falicov, and J. C. Phillips, Phys. Rev. Letters **8**, 316 (1962).
[3] P. G. Prange, Phys. Rev. **131**, 1083 (1963); in *Lectures on the Many-Body Problem*, edited by E. R. Caianiello (Academic Press Inc., New York, 1964), Vol. 2.
[4] P. G. de Gennes, Phys. Letters **5**, 22 (1963).
[5] B. D. Josephson, Advan. Phys. **14**, 419 (1965).
[6] W. J. Tomasch, Phys. Rev. Letters **15**, 672 (1965); **16**, 16 (1966); W. J. Tomasch and T. Wolfram, *ibid.* **16**, 352 (1966).

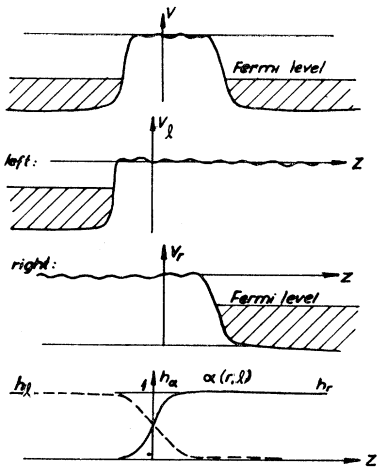

FIG. 1. The potential (a) of the original, (b) of the left problem, (c) of the right problem; and (d) the smoothed-out step functions.

mentally by Wyatt[7] and by Rowell and Shen.[8] In addition, the proximity effect has a great importance in tunneling.

A theory of tunneling between superconducting or normal metals across an insulating layer is presented here which describes the phenomenon in the barrier as well. Green's functions are used to avoid the problem of the completeness and orthogonality of the wave functions as far as possible. The starting point is the treatment of two different problems where the metal on the left (or right) side of the barrier is replaced by an insulator. In these problems, referred to as left and right problems, the main part of the boundary effects has been taken into account. This method may be applied to the calculation of the current density in the barrier, for it describes the electrons in the barrier as well. With other methods, only the total current can be calculated. Throughout the use of the current density, the effect in a magnetic field may be described in an appropriate way.

The Green's functions of the original problem are determined by the Green's functions of these two left and right problems in an interative procedure (Secs. 2 and 3). In Sec. 4 we give the calculation of the current density in the barrier. These results are applied to the Josephson current (Sec. 5), and to the long-range order in the Josephson junction in a magnetic field (Sec. 6). We discuss the applicability of the tunneling-Hamiltonian method, and we conclude that the tunneling Hamiltonian is a powerful method for the calculation of the total current (Sec. 7). Finally, the possibility of higher-order processes is discussed very briefly (Sec. 8).

2. THE MATHEMATICAL FORMULATION OF THE PROBLEM

We must describe an interacting electron gas which is divided by a potential barrier into two parts, called the left (l) and right (r) sides. The height of the potential barrier is greater than the Fermi energy for an insulating oxide layer. We shall apply the method of the thermodynamic Green's functions. The normal and anomalous one-particle Green's functions introduced by Gorkov[9] are

$$G_{\alpha\beta}(x, x') = -i\langle T\{\psi_\alpha(x)\psi_\beta^\dagger(x')\}\rangle,$$
$$F_{\alpha\beta}(x, x') = \langle T\{\psi_\alpha(x)\psi_\beta(x')\}\rangle,$$

and

$$F_{\alpha\beta}^\dagger(x, x') = \langle T\{\psi_\alpha^\dagger(x)\psi_\beta^\dagger(x')\}\rangle, \quad (1)$$

where ψ is the field operator of the electron field. The interaction of the electrons with electrons or impurities is represented by the mass operator Σ, which is calculated according to the special problem. We describe the barrier as a potential V. For brevity, we introduce the matrix notation for the Green's functions G and F,

$$\hat{G} = \begin{pmatrix} G & F \\ F^\dagger & G^T \end{pmatrix}, \quad (2)$$

where the superscript T denotes the exchange of the arguments, and the spin indices will not be written out.

The equation of motion may be written as

$$(\hat{G}_0^{-1} - \hat{\Sigma})\hat{G} = \hat{I}, \quad (3)$$

where $\hat{G}_0^{-1}$ is the inverse of the noninteracting-electron Green's function, which is

$$\hat{G}_0^{-1} = \begin{pmatrix} i(\partial/\partial x_0) + (\nabla^2/2m) + \mu - V & 0 \\ 0 & -i(\partial/\partial x_0) + (\nabla^2/2m) + \mu - V \end{pmatrix}. \quad (4)$$

In this formula x_0 denotes the time variable and μ the chemical potential. The definitions of the inverses are

$$\hat{G}^{-1}\hat{G} = \hat{I}, \quad (5a)$$

and

$$\hat{G}\hat{G}^{-1} = \hat{I}, \quad (5b)$$

where $\hat{I}$ is the unit operator. The second identity may be proven by partial integrations.

The crucial point of our approach is the reduction of the solution of the above-mentioned original problem (o.p.) with the potential barrier separating the left

[7] A. F. G. Wyatt, Phys. Rev. Letters **13**, 401 (1964).
[8] J. M. Rowell and Y. Y. L. Shen, Phys. Rev. Letters **18**, 215 (1966).
[9] L. P. Gorkov, Zh. Eksperim. i Teor. Fiz. **34**, 735 (1958) [English transl.: Soviet Phys.—JETP **11**, 696 (1960)]; A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinskii, *Methods of Quantum Field Theory in Statistical Mechanics* (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1963).

and right sides to the solutions of two other problems. In the new problems, the electron gas is localized to the left or the right side of the barrier, introducing appropriate potential wells (Fig. 1). These problems are called "left and right problems" (l.p. and r.p.). The potentials introduced are chosen in such a way that the potential of the l.p. (r.p.) is equal to the potential of the o.p. on the left (right) side and inside of the barrier. The corresponding mass operators $\hat{\Sigma}_l$ and $\hat{\Sigma}_r$ may be chosen in a similar way. These definitions may be formulated mathematically if we introduce two smoothed-out step functions h_l and h_r corresponding to the left and right sides, which vary only inside the barrier [Fig. 1(d)]. Assuming the identity

$$h_l+h_r=1, \tag{6}$$

we can write[10]

$$V=h_lV_l+h_rV_r,$$

and

$$\hat{\Sigma}=h_l\hat{\Sigma}_l+h_r\hat{\Sigma}_r=\hat{\Sigma}_rh_r+\hat{\Sigma}_lh_l. \tag{7}$$

These equations are independent of the special choice of the step functions, and we shall have to show that all physical results are independent of their choice.

Let us introduce the Green's functions and their inverses for the l.p. and r.p. by the definitions

$$\hat{G}_{0\alpha}{}^{-1}=\begin{pmatrix} i(\partial/\partial x_0)+(\nabla^2/2m)+\mu-V_\alpha & 0 \\ 0 & -i(\partial/\partial x_0)+(\nabla^2/2m)+\mu-V_\alpha \end{pmatrix}, \tag{8}$$

where $\alpha=l, r$ and

$$\hat{G}_{0\alpha}{}^{-1}\hat{G}_{0\alpha}=\hat{I}. \tag{9a}$$

Furthermore,

$$\hat{G}_\alpha{}^{-1}=\hat{G}_{0\alpha}{}^{-1}-\hat{\Sigma}_\alpha, \tag{10}$$

and

$$\hat{G}_\alpha{}^{-1}\hat{G}_\alpha=\hat{I}, \qquad \hat{G}_\alpha\hat{G}_\alpha{}^{-1}=\hat{I}. \tag{9b}$$

It is easy to see from Eqs. (4), (6), (7), (9a), and (9b) that the following identities are exact:

$$\hat{G}_0{}^{-1}=\hat{G}_{0l}{}^{-1}h_l+\hat{G}_{0r}{}^{-1}h_r, \tag{11}$$

and

$$\hat{G}^{-1}=\hat{G}_l{}^{-1}h_l+\hat{G}_r{}^{-1}h_r. \tag{12}$$

Inserting (12) into (5a) and (5b) and multiplying by G_r and G_l from the left and right, respectively, and using (9b), we get the following identities:

$$(h_r+\hat{G}_r\hat{G}_l{}^{-1}h_l)\hat{G}=\hat{G}_r, \tag{13a}$$

and

$$\hat{G}(h_r+h_l\hat{G}_l{}^{-1}\hat{G}_r)=\hat{G}_r, \tag{13b}$$

or

$$r\leftrightarrow l \text{ in (13a)}, \tag{13c}$$

and

$$r\leftrightarrow l \text{ in (13a)}. \tag{13d}$$

Adding these four equations together, we get the fundamental equation of our approach, where the Green's function of o.p. is expressed by the Green's functions of the l.p. and r.p.:

$$\hat{G}=\hat{G}_r+\hat{G}_l-\tfrac{1}{2}\{(\hat{G}_r\hat{G}_l{}^{-1}h_l+r\leftrightarrow l)\hat{G}+\hat{G}(h_l\hat{G}_l{}^{-1}\hat{G}_r+r\leftrightarrow l)\}. \tag{14a}$$

Our program is to give an approximate solution of this equation, supposing that the transition rate of electrons through the barrier is very small.

3. THE ITERATIVE SOLUTION OF THE GREEN'S-FUNCTION EQUATION

We take the Fourier transform of (14a) with respect to time:

$$\hat{G}(E)=\hat{G}_r(E)+\hat{G}_l(E) -\tfrac{1}{2}\{(\hat{G}_r(E)\hat{G}_l{}^{-1}(E)h_l+r\leftrightarrow l)\hat{G}(E) +\hat{G}(E)(h_l\hat{G}_l{}^{-1}(E)\hat{G}_r(E)+r\leftrightarrow l)\}, \tag{14b}$$

to make the discussion of the physical base of our approximation easier.[11]

Equation (14b) shows quite different characteristics at small and large values of the energy variables. At small values of the energy, the Green's functions G_l and G_r are strongly localized to the left or to the right side of the barrier. Only the tails of the Green's functions penetrate into the barrier. In this case the expression in the bracket is very small, for it contains products

[10] The sufficient condition of the given form of Σ is that it may be written in the following form:

$$\Sigma=\tilde{\Sigma}_l+\tilde{\Sigma}_r+\Sigma_B,$$

where $\tilde{\Sigma}_l$ and $\tilde{\Sigma}_r$ are the parts of the mass operator which are well localized to the left or right sides of the barrier and Σ_B is localized to the barrier and its neighborhood. Furthermore, we have to suppose that Σ_B is a local function in the space

$$\Sigma_B(x_1x')=\Sigma_B(x_1x_0-x_0')\delta(x-x').$$

This condition is fulfilled if Σ describes interaction of electrons with impurities corresponding to the Hamiltonian:

$$H=g\psi_\alpha{}^\dagger(\mathbf{R})\psi_\alpha(\mathbf{R})-J\psi_\alpha{}^\dagger(\mathbf{R})\sigma_{\alpha\beta}\psi_\beta(\mathbf{R})\mathbf{S},$$

where $\psi_\alpha{}^\dagger\sigma_{\alpha\beta}\psi_\beta$ is the spin density and $\psi_\alpha{}^\dagger\psi_\alpha$ is the electron density at the position of the impurity with spin S. In this notation we may write

$$\Sigma_l=\tilde{\Sigma}_l+\Sigma_B \quad \text{and} \quad \Sigma_r=\tilde{\Sigma}_r+\Sigma_B.$$

[11] The definition of an arbitrary Fourier transform according to time is

$$f(E)=\int_{-\infty}^{\infty}dt\,f(t)\,\exp(iEt).$$

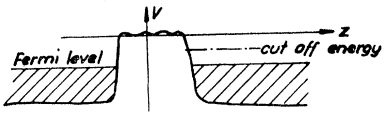

FIG. 2. The cutoff energy between the top of the potential barrier and the Fermi energy.

like $\hat{G}_r\hat{G}_l^{-1}h_l$, which are proportional to the rate of penetration into the barrier. Therefore, $\hat{G}_l+\hat{G}_r$ is the zero-order approximation to the Green's function near the Fermi energy.

At high values of the energy variable, the effect of the potentials V_l and V_r may be neglected. In this case both of the two terms in the bracket of Eq. (14b) are approximately the solution of Eq. (14b) itself. We are interested in the solution of this equation only in the first case, and it seems reasonable to solve the equation by iteration starting with the zero-order approximation $\hat{G}_l+\hat{G}_r$.

To get rid of the physically uninteresting part of the Green's functions with large values of the energy variable, we apply a cutoff in the spectral functions of the Green's functions at some energy between the top of the potential barrier and the Fermi energy (Fig. 2). The prime on the Green's function will denote that the cutoff procedure is applied. It is worth mentioning that Eqs. (9b) are to be corrected for the truncated Green's functions. The corresponding new equations are

$$\int d^4x''\hat{G}_\alpha^{-1}(x, x'')\hat{G}_\alpha'(x'', x') = \hat{D}_\alpha(x, x') = \delta(x_0-x_0')\hat{D}_\alpha(\mathbf{x}, \mathbf{x}') \neq \hat{I}, \tag{15}$$

where the application of the cutoff results in a smeared-out Dirac delta function $\hat{D}$. Since the Green's functions $\hat{G}_l'$ and $\hat{G}_r'$ are strongly localized to the left or right sides, $\hat{D}_l'$ is very small on the right side and $\hat{D}_r'$ on the left side.

Our fundamental equation (14a) after the application of the cutoff is

$$\hat{G}'(E) = \hat{G}_l'(E)+\hat{G}_r'(E) - \tfrac{1}{2}\{(\hat{G}_r'(E)\hat{G}_l^{-1}(E)h_l+r\leftrightarrow l)\hat{G}'(E) + \hat{G}'(E)(h_l\hat{G}_l^{-1}(E)\hat{G}_r(E)+r\leftrightarrow l)\}, \tag{16}$$

where the terms in the bracket are small, because we have supposed that the penetration of the wave function into the barrier is weak. By iterating this equation, we get some typical terms which we will now investigate.

It will be useful to transform some terms, e.g., in the following ways,

$$\hat{G}_r'\hat{G}_l^{-1}h_l\hat{G}_l' = \hat{G}_r'([\hat{G}_l^{-1}h_l]_-+h_l\hat{G}_l^{-1})\hat{G}_l' = \hat{G}_r'[\hat{G}_l^{-1}h_l]_-\hat{G}_l'+\hat{G}_r'h_l\hat{D}_l, \tag{17}$$

where we have made use of the identity (15), and $[\ ]_-$ denotes the commutator. The commutator in (17) may be calculated using (8) and (10):

$$[G_\alpha^{-1}h_\alpha]_- = m^{-1}(\vec{\nabla}_i h_\alpha)\vec{\nabla}_i+(2m)^{-1}\vec{\Delta}h_\alpha-[\hat{\Sigma}_\alpha h_\alpha]_-, \tag{18}$$

where the direction of an arrow above a differential operator indicates the operand. The cyclic rule is to be followed in the absence of an adjacent operand.

We suppose that the commutator on the right side of (18) vanishes:

$$[\hat{\Sigma}_\alpha h_\alpha]_- = 0; \tag{19}$$

the identities in Eq. (19) are fulfilled if the mass operators are local functions in that region of space where the corresponding smoothed-out step functions vary, i.e., inside the barrier (see Ref. 10).

Inserting (18) and (19) into (17), we get finally

$$\hat{G}_r'\hat{G}_l^{-1}h_l\hat{G}_l' = \hat{G}_r'(m^{-1}(\vec{\nabla}_i h_l)\vec{\nabla}_i+2m^{-1}(\vec{\Delta}h_l))\hat{G}_l'+\hat{G}_r'h_l\hat{D}. \tag{20}$$

It is easy to prove the following identity for another typical term appearing in the iteration of (16):

$$\begin{aligned}\hat{G}_r'\hat{G}_l^{-1}h_l\hat{G}_r' &= \hat{G}_r'(\hat{G}_r^{-1}-(\Delta V_l-\Delta V_r)-(\Delta\Sigma_l-\Delta\Sigma_r))h_l\hat{G}_r' \\ &= \hat{D}_r h_l\hat{G}_r'-\hat{G}_r'(\Delta V_l-\Delta V_r)h_l\hat{G}_r' \\ &\quad -\hat{G}_r'(\Delta\hat{\Sigma}_l-\Delta\hat{\Sigma}_r)h_l\hat{G}_r',\end{aligned} \tag{21}$$

where we have introduced the new notation

$$\Delta V_\alpha = V_\alpha - V, \quad \text{and} \quad \Delta\hat{\Sigma}_\alpha = \Sigma_\alpha-\Sigma, \tag{22}$$

and the following identity has been applied:

$$\hat{G}_r^{-1}-\hat{G}_l^{-1} = (V_l-V_r)+(\Sigma_l-\Sigma_r), \tag{23}$$

which follows from (8) and (10). It is worth mentioning that ΔV_l is different from zero only on the right side of the barrier. Similar results may be obtained by the exchange of the indices r and l.

The result in the first-order iteration of (16) may be written as the sum of four terms with different physical interpretations:

$$\hat{G}' = \hat{G}_l'+\hat{G}_r'+\delta\hat{G}_T+\delta\hat{G}_R+\delta\hat{G}_D. \tag{24}$$

We will give the order of the particular terms in powers of the tunneling rate t. The tunneling rate is the relative decrease of the wave functions at the Fermi energy in the barrier:

$$t = \exp\{-[2m(V-\mu)]^{1/2}d\}, \tag{25}$$

where d denotes the thickness of the barrier and V is the energy of the top of the barrier.

FIG. 3. The first-order diagrams corresponding to the tunneling contribution of the Green's function. B denotes the barrier and x denotes the current coupling.

The particular terms of the Green's function are:

(1) The tunneling term $\delta\hat{G}_T$;

$$\delta\hat{G}_T(x,x')=\int\left\{\hat{G}_l'(x,y)\left(\frac{\vec{\nabla}_y-\bar{\vec{\nabla}}_y}{2m}\right)_i\hat{G}_r'(y,x')-\hat{G}_r'(x,y)\left(\frac{\vec{\nabla}_y-\bar{\vec{\nabla}}_y}{2m}\right)_i\hat{G}_l'(y,x')\right\}\times(\vec{\nabla}_y h_l(\mathbf{y}))_i d^4y, \tag{26}$$

where h_r is eliminated by h_l using (6). In Appendix A another form of this term is derived to eliminate h_l as well;

$$\delta G_T(x,x')=\int_S\left\{\hat{G}_l'(x,y)\left(\frac{\vec{\nabla}_y-\bar{\vec{\nabla}}_y}{2m}\right)_i\hat{G}_r'(y,x')-r\leftrightarrow l\right\}d^2f_{y,i}dy, \tag{27}$$

where the integral is taken on an arbitrary surface S lying in the barrier. The surface element vector $df_{y,i}$ is directed from left to right, and it may be shown that the value of this integral is independent of the special choice of the surface S to a good approximation. Namely, we can prove that that part of δG_T which is dependent on the choice of the step function h is similar to the third type of correction $\delta\hat{G}_D$ [see Eq. (33) and Appendix A], which is always neglected.

It is easy to see that this term corresponds to the one-particle tunneling and therefore is proportional to the tunneling rate t, and that its part depending on the choice of h is of order t^2. These corrections give the coupling between the Green's functions corresponding to the two different sides of the barrier by the current coupling derived by Bardeen.[1] They may be illustrated by the diagrams in Fig. 3.

(2) The renormalization terms $\delta\hat{G}_R$ due to the potential and mass operator corresponding to the opposite sides;

$$\delta\hat{G}_R=\tfrac{1}{2}\{\hat{G}_r'(\Delta V_l-\Delta V_r)h_l\hat{G}_r'+\hat{G}_r'h_l(\Delta V_l-\Delta V_r)\hat{G}_r'+\hat{G}_r'(\Delta\hat{\Sigma}_l-\Delta\hat{\Sigma}_r)h_l\hat{G}_r'+\hat{G}_r'h_l(\Delta\hat{\Sigma}_l-\Delta\hat{\Sigma}_r)\hat{G}_r'\}+\tfrac{1}{2}\{r\leftrightarrow l\}. \tag{28}$$

Using the definitions of ΔV_l, ΔV_r, $\Delta\hat{\Sigma}_l$, and $\Delta\hat{\Sigma}_r$, the following identities may be proven:

$$\Delta V_\alpha h_\alpha=h_\alpha\Delta V_\alpha=0, \tag{29}$$

$$\Delta\hat{\Sigma}_\alpha h_\alpha=h_\alpha\Delta\hat{\Sigma}_\alpha=0. \tag{30}$$

Inserting (29) and (30) into (28) and making use of (6) we have gotten rid of the smoothed-out step functions h_l and h_r:

$$\delta\hat{G}_R(x,x')=-\int\{\hat{G}_r'(x,y)\Delta\hat{M}_r(y,y')\hat{G}_r'(y',x')+(r\leftrightarrow l)\}d^4yd^4y'. \tag{31}$$

Here we have introduced the new notation

$$\Delta\hat{M}_\alpha(y,y')=\Delta V_\alpha(y)\delta(y-y')+\Delta\Sigma_\alpha(y,y'). \tag{32}$$

A certain part of $\delta\hat{G}_R$ provides a contribution to the proximity effect. δG_R is proportional to the square of the tunneling rate t^2, and is represented by the diagrams in Fig. 4.

(3) Terms corresponding to the nonorthogonality:

$$\delta\hat{G}_D(x,x')=-\frac{1}{2}\left\{\int\hat{G}_r'(x,y)h_l(\mathbf{y})\hat{D}_l(y,x')d^4y+\int\hat{D}_l(x,y)h_l(\mathbf{y})\hat{G}_r'(y,x')d^4y+\int\hat{G}_r'(x,y)h_l(\mathbf{y})\hat{D}_r(y,x')d^4y+\int\hat{D}_r(x,y)h_l(\mathbf{y})\hat{G}_r'(y,x')d^4y\right\}-\tfrac{1}{2}\{r\leftrightarrow l\}. \tag{33}$$

These terms are slightly dependent on the choice of the smeared-out step functions. A careful analysis of these terms shows that this correction renormalizes the one-particle wave functions inside the barrier and in the neighborhood of it. These correction terms are very strongly oscillating outside the barrier and quickly damp with increasing distance from the barrier. They are the effect of breaks in the orthogonality and completeness of the used one-particle wave functions, discussed by Prange.[3] Because this correction is like a renormalization of the wave functions, the direct contribution to current via (34) is zero, but in higher-order approximations it might give a correction to the current proportional to t^3. We conjecture that the correction terms are concerned with some mathematical problems of our approach and never with some real physical problems. We will neglect them in the following.

FIG. 4. The diagrams corresponding to the renormalization of the Green's function by the opposite side.

We may get higher-order approximations to the Green's functions in this way using the corrections of the first and second type.

The surface and the proximity effect may be taken into account in two steps:

(1) The Green's functions G_α' have been calculated

in the case where the metal on the opposite side and the barrier are replaced by a single insulator. In this way, the decrease of the gap function near the barrier and the surface effects have been taken into account.

(2) Actually, there is another metal behind the barrier and this may cause a slight modification of the gap function near the barrier. This can be calculated in perturbation theory using the diagrams in Figs. 3 and 4.

4. THE CURRENT DENSITY IN THE BARRIER

The current density in an arbitrary point x can be calculated using the Green's function.

$$j_i(x)=\lim_{x'\to x_0+0,x'_i\to x_i}\{e((\nabla_x-\nabla_{x'})/2m)_iG'(x,\mathbf{x}')\}. \quad (34)$$

The zeroth-order approximation to G will not give any contribution to the current density. Using the first-order approximation to the Green's functions, we get the leading term of current density, which is given by diagrams in Fig. 5, where the lower-case $j(x)$ represents the current operator. The corresponding mathematical expression is

$$j_i(x)=e\int_S d^2f_{y,i'}\int_{-\infty}^{\infty}dy_0 \times\left\{\left(\frac{\vec{\nabla}_x-\overleftarrow{\nabla}_x}{2m}\right)_i\hat{G}_r'(x,y)\left(\frac{\vec{\nabla}_y-\overleftarrow{\nabla}_y}{2m}\right)_{i'}\hat{G}_l'(y,x)-r\leftrightarrow l\right\}. \quad (35)$$

In the statistical mechanics of nonequilibrium processes, the current density is calculated as a response to an external force; in the present case, it is calculated as a response to the tunneling coupling:

$$j_i(x)=\int_S d^2f_{x',i'}\int_{-\infty}^{\infty}dy_0K_i(x,x')\,T_{i'}(\mathbf{x}'), \quad (36)$$

where T is the general symbol of the tunneling coupling. The causal kernel $K_c(x,x')$ is calculated using the causal Green's functions, but here we need the retarded one. Investigation of the analytical properties of the kernels shows[12] that the retarded kernel may be obtained by shifting the poles of the Fourier transform of K_c below the real axis in the complex energy plane. If the operator $(C\to R)$ stands for this operation, then the expression of the current density is finally

$$j_i(x)=(C\to R)\,e\int_S d^2f_{x',i'}\int dx_0'\left\{\left(\frac{\vec{\nabla}_x-\overleftarrow{\nabla}_x}{2m}\right)_i\hat{G}_r'(x,x')\left(\frac{\vec{\nabla}_{x'}-\overleftarrow{\nabla}_{x'}}{2m}\right)_{i'}\hat{G}'(x',x)-r\leftrightarrow l\right\}. \quad (37a)$$

The current density derived here satisfies the equation of continuity in the barrier. This can be shown by a calculation similar to the one in Appendix A. We will return later to discuss the connection of (37) and the current formula derived by using the tunneling Hamiltonian.[13]

A similar formula can be obtained in the case of an external magnetic field:

$$j_i(x)=(C\to R)\,e\int d^2f_{x',i'}\int dx_0' \times\left\{\left(\frac{[\vec{\nabla}_x+i(e/c)\mathbf{A}(\mathbf{x})]-[\overleftarrow{\nabla}_x-i(e/c)\mathbf{A}(\mathbf{x})]}{2m}\right)_i\hat{G}'(x,x')\left(\frac{[\vec{\nabla}_{x'}+i(e/c)\mathbf{A}(\mathbf{x}')]-[\overleftarrow{\nabla}_{x'}-i(e/c)\mathbf{A}(\mathbf{x}')]}{2m}\right)_{i'}\hat{G}_l'(x',x) -r\leftrightarrow l\right\}, \quad (37b)$$

where $\mathbf{A}(x)$ stands for the vector potential.

5. JOSEPHSON CURRENT

To calculate the actual value of the current, we have to insert the matrix form of the Green's functions (2) into the expression of the current (37). Then using the symbolic notation T for the coupling constant we obtain the following formula:

$$\mathbf{j}_i(x)=e\{TG_r'TG_l'+TF_r'TF_l^{\dagger\prime}\}-e\{r\leftrightarrow l\}. \quad (38)$$

It is well known that the anomalous Green's functions are dependent on the special choice of phases and the absolute value of the time arguments. Therefore we may write

$$F_\alpha'(x,x')=\exp(-2i\mu_\alpha x_0)\phi_\alpha'(\mathbf{x},\mathbf{x}';x_0-x_0') \times\exp(-(2e/c)i\varphi_\alpha),$$

and

$$F_\alpha^{\dagger\prime}(x',x)=\exp(+2i\mu_\alpha x_0)\phi_\alpha^{\dagger\prime}(\mathbf{x}',\mathbf{x};x_0'-x_0) \times\exp[+(2e/c)i\varphi_\alpha], \quad (39)$$

where μ_α is the chemical potential and φ_α is the phase

[12] V. Ambegaokar and L. P. Kadanoff, Nouvo Cimento **22**, 914 (1961); A. A. Abrikosov *et al.* (see Ref. 9).
[13] See Sec. 7.

of the pair wave functions on the α side of the barrier. Here ϕ_α ($\alpha=l$, r) are independent of the choice of phases.

The current density may be written as the sum of two terms:

$$\mathbf{j}(x)=\mathbf{j}_N(x)+\mathbf{j}_J(x), \tag{40}$$

where

$$\mathbf{j}_N(x)=TG_r'TG_l'-(r\leftrightarrow l) \tag{41a}$$

is the one-particle current density and

$$\mathbf{j}_J(x)=\exp\{2[(e/c)\Delta\varphi+\Delta\mu x_0]\}T\phi_r'T\phi_l^{\dagger\prime}-(r\leftrightarrow l) \tag{41b}$$

is the current density due to the pair tunneling, first suggested by Josephson.[14] Here we have used the notations

$$\Delta\mu=\mu_l-\mu_r=eV, \tag{42}$$

where V is the applied voltage, and

$$\Delta\varphi=\varphi_l-\varphi_r. \tag{43}$$

The actual value of the current density is given in Appendix B. At zero applied voltage, the expression for the current density reduces to the following:

$$\mathbf{j}_J=\mathbf{J}_{J,0}\sin[2(e/c)\Delta\varphi]. \tag{44}$$

6. JOSEPHSON EFFECT IN MAGNETIC FIELD

We will also very briefly treat the Josephson effect in the presence of an external magnetic field. This treatment is based on the compensation of the long-range phase modulation of the pair wave function F' by an appropriate transformation discussed by the author in the case of fluxoid quantization.[15] Inside large superconductors the magnetic field vanishes; the vector potential A_i may be written as a gradient of a function φ_α, i.e.,

$$A_{\alpha,i}(\mathbf{x})=\nabla_i\varphi_\alpha(\mathbf{x})+\delta\tilde{A}_{\alpha,i}, \qquad (\alpha=l,\ r) \tag{45}$$

where $\delta\tilde{A}_{\alpha,i}$ vanishes except at the surface layers and at the neighborhood of the barrier where the magnetic field appears. It is useful to apply the following transformation:

$$G_\alpha'(x,x')=\tilde{G}_\alpha(x,x')\exp\{-i(e/c)[\varphi_\alpha(\mathbf{x})-\varphi_\alpha(\mathbf{x}')]\},$$

$$F_\alpha^{\dagger\prime}(x,x')=\exp(+2i\mu_\alpha x_0)\tilde{\phi}_\alpha^{\dagger\prime}(\mathbf{x}',\mathbf{x};x_0'-x_0)\times\exp\{+i(e/c)[\varphi_\alpha(\mathbf{x})+\varphi_\alpha(\mathbf{x}')]\},$$

and

$$F_\alpha'(x,x')=\exp(-2i\mu_\alpha x_0)\tilde{\phi}_\alpha'(\mathbf{x},\mathbf{x}';x_0-x_0')\times\exp\{-i(e/c)[\varphi_\alpha(\mathbf{x})+\varphi_\alpha(\mathbf{x}')]\}. \tag{46}$$

This transformation has a form similar to that of a gauge transformation; therefore, using the gauge-invariant structure of our approach, it is easy to see

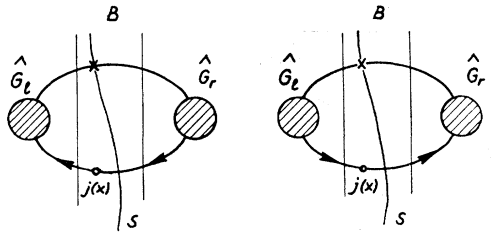

FIG. 5. The diagrams of the current density. S is the surface occurring in (34) and $j(x)$ stands for the current operator.

that in the system of equations for the Green's functions of the particular problems only $\delta\tilde{A}_\alpha$ occurs, and in the system of equations of the original problem $\delta\tilde{A}_\alpha$ and $\Delta\varphi(x)=\varphi_l(x)-\varphi_r(x)$ occur.[16] Inside the superconductors, $\tilde{G}_\alpha$ and $\tilde{\phi}_\alpha$ satisfy field-free equations, and so they are equal to the Green's function in the absence of an external field and will be denoted by $G_{0,\alpha}'$ and $\phi_{0,\alpha}'$ later in this section. We introduce a notation similar to (45),

$$\tilde{G}_\alpha=G_{0,\alpha}'+\delta\tilde{G}_\alpha \quad\text{and}\quad \tilde{\phi}_\alpha=\phi_{0,\alpha}'+\delta\tilde{\phi}_\alpha, \tag{47}$$

where $\delta\tilde{G}_\alpha$ and $\delta\tilde{\phi}_\alpha$ are the deviations from the field-free Green's functions. These deviations are induced by the vector potential $\delta\tilde{A}_\alpha$ according to the Meissner effect, and produce the current which cancels the magnetic field in the superconductor and supplies the current in the barrier. $\delta\tilde{A}_\alpha$ has to be determined in a self-consistent way as discussed by Ferrel and Prange.[17] This vector potential is small and therefore can be treated in perturbation theory.

We can calculate the Josephson current very simply if we suppose that the phase difference $\Delta\varphi$ is slowly varying in the barrier.[18] Inserting (46) into (41b) and replacing $\Delta\varphi(x')$ by $\Delta\varphi(x)$, we have the formula for the Josephson current density:

$$\mathbf{j}_J(x)=\exp\{2ei(c^{-1}\Delta\varphi(\mathbf{x})+Vx_0)\}\times T\phi_{0,r}'T\phi_{0,l}'-(r\leftrightarrow l). \tag{48}$$

At zero applied voltage, this formula becomes more simple as (B11) has been simplified to (B12):

$$\mathbf{j}_J(\mathbf{x})=J_J(\mathbf{x})\sin[2(e/c)\Delta\varphi(\mathbf{x})], \tag{49}$$

where some part of the phase shift $\Delta\varphi$ is due to the magnetic field at the junction. If $\Delta\varphi$ changes by $(\pi c/e)n$, where $n=\pm1,\pm2,\cdots$, the Josephson current density does not alter.

We will treat the connection between the direction of the Josephson current and the magnetic field enclosed by the junction which has been discussed by Anderson.[19] In Fig. 6 we have illustrated a junction

[14] B. D. Josephson, Phys. Letters **1**, 251 (1962).
[15] A. Zawadowski, Phys. Rev. Letters **14**, 557 (1965).
[16] The variable x is taken on the surface S.
[17] R. A. Ferrel and R. E. Prange, Phys. Rev. Letters **10**, 479 (1963).
[18] The opposite case is discussed later in this section.
[19] P. W. Anderson, in *Lectures on the Many Body Problem*, edited by E. R. Caianiello (Academic Press Inc., New York, 1963), Vol. 2.

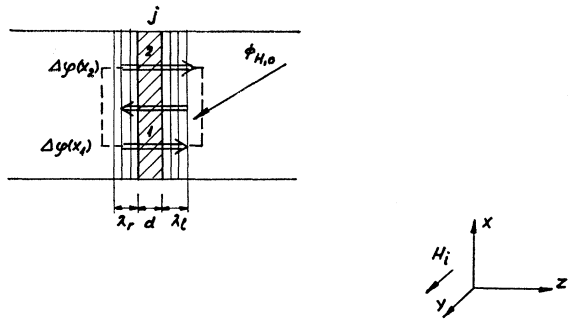

FIG. 6. Junction with penetration region of the magnetic field. The arrows represent the direction of the Josephson current density.

and the penetration of the magnetic field into it. The penetration depths are denoted by λ_l and λ_r, respectively. The magnetic field may be found from the magnetic field H (which is directed along the axis y):

$$A_x(x, z) = \int_0^z H_y(x, z)\, dz. \tag{50}$$

The appropriate transformations discussed before are determined by the functions

$$\varphi_l(x) = \int_{x_0}^{x} dx \int_0^{-\infty} dz H_y(x, z),$$

and

$$\varphi_r(x) = \int_{x_0}^{x} dx \int_0^{\infty} dz H_y(x, z), \tag{51}$$

where x_0 determines the boundary condition for the relative phases. The corresponding change of the phase difference between the points x_2 and x_1 is

$$\Delta\varphi(x_2) - \Delta\varphi(x_1) = \int_{x_1}^{x_2} dx \int_{-\infty}^{\infty} dz H_y(x, z) = \Delta\phi_H(x_2, x_1), \tag{52}$$

which is the magnetic flux enclosed by the dashed line in Fig. 6. The Josephson current is unaltered if the flux changes by $n\phi_{H,0}$, where $\phi_{H,0} = \pi c/e$ is the flux quantum, as has been found by Anderson.[19] The current density (49) and the phase difference (52) determine the total current as a function of the enclosed magnetic field, which is similar to a Fraunhoffer interference-pattern formula.[20]

It might be expected that a similar interference effect would occur in the local current density at a fixed point x. One of the electrons of a tunneling pair crosses the barrier at point x, but the other one crosses somewhere else in the region of the coherence length around the fixed point x. The phase difference for the second electron might strongly vary as a function of the tunneling place if the magnetic field were strong enough. Then the integrand of the current density expression (37a) would oscillate as a function of x'. In fact, this effect cannot be observed because the required magnetic field would be comparable with the critical magnetic field.

[20] B. D. Josephson, Rev. Mod. Phys. **36**, 216 (1964).

7. THE TUNNELING HAMILTONIAN METHOD

The tunneling Hamiltonian has been proposed by Cohen, Falicov, and Phillips[2] to describe the electron transitions through the barrier in a phenomenological way. The Hamiltonian containing the field operators of both sides of the barrier is

$$H_T = \sum_{\lambda,\lambda'} \tilde{T}_{\lambda',\lambda;l,r} a_{\lambda',l}^{\dagger} a_{\lambda,r} + \text{conj.}$$

The transition amplitude T in the tunneling-Hamiltonian method has been fitted to the electron scattering amplitude corresponding to the transition from one side of the barrier to the other. According to Bardeen's investigations which are in agreement with our results,[21] they are

$$\tilde{T}_{\lambda',\lambda;l,r} = \int_S d^2 f_{\mathbf{x},i} \chi_{\lambda',l}^{*}(\mathbf{x}) \left(\frac{\vec{\nabla}_{\mathbf{x}} - \overleftarrow{\nabla}_{\mathbf{x}}}{2m}\right)_i \chi_{\lambda,r}(\mathbf{x}) = -iT_{\lambda',\lambda;l,r}, \tag{53}$$

where the χ's are the one-electron wave functions.

The value of the total current is the same if we calculate from the tunneling-Hamiltonian method[22] or from the present Green's-function method. However, we need not automatically expect corresponding agreement in the case of the energy density.[23]

8. HIGHER-ORDER PROCESSES

A diagram technique is proposed in Sec. 3 which is similar to the one suggested by Josephson.[5] The typical structure of the nth-order diagrams is illustrated in Fig. 7.

The contribution of the fourth-order diagrams to the tunneling current has been calculated by Schrieffer and Wilkins.[24] In the processes calculated by them one pair has been broken up and two electrons have tunneled through the barrier. Such processes were first observed by Taylor and Burstein[25] as peaks in tunneling characteristics. Recently, $2\Delta/n$ structure has been observed.[26] These processes may be interpreted as the breaking of one pair and the tunneling of n electrons in the same quantum-mechanical process.

[21] See Appendix B.

[22] Our results may be compared with, e.g., those of V. Ambegaokar and A. Baratoff, Phys. Rev. Letters **10**, 486 (1963); **11**, 104 (1963).

[23] Recently, K. L. Ngai, J. A. Appelbaum, M. H. Cohen, and J. C. Phillips [Phys. Rev. (to be published)] investigated this problem and have concluded that the tunneling Hamiltonian is accurate for the calculation of the energy density as well.

[24] J. R. Schrieffer and J. W. Wilkins, Phys. Rev. Letters **10**, 17 (1963).

[25] B. N. Taylor and E. Burstein, Phys. Rev. Letters **10**, 14 (1963).

[26] I. K. Yanson, V. M. Svistunov, and I. M. Dmitrenko, Zh. Eksperim. i Teor. Fiz. **47**, 2091 (1964) [English transl.: Soviet Phys.—JETP **20**, 1404 (1965)]; S. M. Marcus, Phys. Letters **19**, 623 (1966); **20**, 236 (1966).

We may argue that there is no reason to suppose that there would be a great difference between the amplitudes for the break of one or several electron pairs in processes of the same order. The proposed process is the breaking of p pairs and the tunneling of n electrons. The voltage threshold of these processes is $eV=2\Delta(p/n)$, due to the conservation of energy. The experimental results of Rochlin and Douglass[27] may be interpreted as a $2\Delta(p/n)$ structure in the tunneling characteristics, as is discussed elsewhere.[28]

It must be stressed that the proposed method is not correct to any order, as the first term of the Green's function in the iteration procedure given in Sec. 3 contains unphysical corrections of higher order to the lowest nonvanishing one. It seems reasonable to suppose that if we consider only the leading corrections of the higher-order processes and neglect the unphysical corrections, we will obtain the interesting contributions of these processes. On the other hand, the amplitudes of the higher-order corrections strongly decrease as the order increases. Therefore the processes of this type may be much more intensive if the transitions of the electrons through the barrier occur at some imperfections of the barrier. In the last case our approach cannot be applied.

9. CONCLUSION

A many-body treatment of the tunneling processes has been elaborated. The present approach has dealt with the behavior of the electrons in the barrier, as well. The Green's functions have been calculated by an iteration procedure. The contributions to the Green's functions in the lowest approximation might be classified into three different groups:

(1) The tunneling term $\delta\hat{G}_T$ which describes the electron transition through the barrier[29];

(2) the renormalization term $\delta\hat{G}_R$ for the metal on one of the sides due to presence of the metal on the opposite side; and

(3) the term $\delta\hat{G}_D$ due to nonorthogonality and noncompleteness of the wave functions.[30] These terms are dependent on the choice of the step functions introduced in Sec. 2. These terms have been neglected.

We have found that only the term of the first type gives contributions to the current density in the barrier. We may conclude that our approach, computing the current density, is correct to order t^2. The advantage of working with the current density occurs in the consequent treatment of the electromagnetic properties of Josephson junctions.

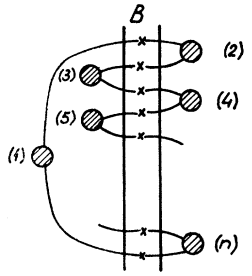

FIG. 7. Typical nth-order diagram. B denotes the barrier and the circles stand for the different Green's functions G, F, and F^+.

In a few cases, the description of the electrons in the region of the barrier is very important. One of them is the geometrical resonance effect discovered by Tomasch[31] where the surface and the boundary effects play important roles. This method may be very powerful in the discussion of this effect, because the boundary and surface effects could be taken into account in the solution of the so-called left and right problems and a direct calculation of the tunneling current becomes possible using the solutions of the particular thin-film problems.

Recently, some new tunneling anomalies have been discovered,[32] and Anderson[33] and Suhl[34] have called attention to the Kondo scattering in the barrier as the possible explanation of this effect. Appelbaum[35] has calculated the tunneling current using the tunneling Hamiltonian. Recently, Sólyom and the author have applied this Green's-function method to this problem,[36] summing up a wide class of diagrams. The resonant scattering on the paramagnetic impurities has been taken into account by finding the solution of the particular left and right problems considering also the paramagnetic impurities.

Finally, it has been concluded that the phenomenological tunneling Hamiltonian can be applied to the calculation of the current in those cases in which the barrier effects are not important.

ACKNOWLEDGMENTS

I should like to thank Professor L. Pál for his continuous interest in this work and Professor Morrel H. Cohen for a stimulating discussion and correspondence. I am very grateful to K. L. Ngai, J. A. Appelbaum, M. H. Cohen, and J. C. Phillips for communication of their work on the free energy of the Josephson junction prior to its publication and for pointing out an error in the first version of this manuscript, to Professor L. P. Gor'kov for calling the proximity effect to my attention, and to Dr. T. Wolfram for a suggestive dis-

[27] G. I. Rochlin and D. H. Douglass, Jr., Phys. Rev. Letters **16**, 359 (1966).

[28] A. Zawadowski, Phys. Letters **23**, 225 (1966).

[29] The term $\hat{G}_T-\hat{G}_{T,D}$ would be better described as the tunneling term. See Appendix B.

[30] According to Ref. 35, it is correctly $\hat{G}_D+\hat{G}_{T,D}$.

[31] See Ref. 3; W. L. McMillan and P. W. Anderson, Phys. Rev. Letters **16**, 85 (1966).

[32] See Refs. 7 and 8.

[33] P. W. Anderson, Phys. Rev. Letters **17**, 95 (1966).

[34] H. Suhl, lecture at the International School of Physics, Varenna, Italy, 1966 (unpublished).

[35] J. A. Appelbaum, Phys. Rev. Letters **17**, 91 (1966).

[36] A. Zawadowski, in Proceedings of the Tenth International Conference on Low Temperature Physics (to be published); J. Sólyom and A. Zawadowski (to be published).

cussion on the Tomasch effect. I wish to acknowledge numerous helpful discussions with Dr. Cs. Hargitai, Dr. N. Menyhárd, and Dr. J. Sólyom.

APPENDIX A

We have derived the tunneling term of the Green's function, but (26) contains the smoothed-out step function h_l. We must show that $\delta\hat{G}_T$ is independent of the choice of h_l to a good approximation. The following expression is to be calculated:

$$[\delta/\delta h_l(\mathbf{y})]\delta\hat{G}_T(x, x'), \quad \text{if} \quad \mathbf{y}\in B \tag{A1}$$

or taking the Fourier transform with respect to the time variable,

$$[\delta/\delta h_l(\mathbf{y})]\delta\hat{G}_T'(\mathbf{x}, \mathbf{x}'; E), \quad \text{if} \quad \mathbf{y}\in B. \tag{A2}$$

A straightforward calculation gives the derivative

$$\nabla_{y,i}\{\hat{G}_l'(\mathbf{x}, \mathbf{y}; E) \times((\vec{\nabla}_y-\overleftarrow{\nabla}_y)/2m)_i\hat{G}_r'(\mathbf{y}, \mathbf{x}'; E)-(r\leftrightarrow l)\}, \tag{A3}$$

or

$$\{\hat{G}_l'(\mathbf{x}, \mathbf{y}; E)((\vec{\Delta}_y-\overleftarrow{\Delta}_y)/2m)\hat{G}_r'(\mathbf{y}, \mathbf{x}'; E)-(r\leftrightarrow l)\}. \tag{A4}$$

We express the Laplacian operators by the inverses of the Green's functions, using (8) and (9):

$$\vec{\Delta}_y/2m=-(E+\mu-V(\mathbf{y})-\hat{\Sigma}_B(\mathbf{y}; E))+\vec{\hat{G}}_\alpha^{-1}(\mathbf{y}; E), \tag{A5}$$

and

$$\overleftarrow{\Delta}_y/2m=-(E+\mu-V(\mathbf{y})-\hat{\Sigma}_B(\mathbf{y}; E))+\overleftarrow{\hat{G}}_\alpha^{-1}(\mathbf{y}; E),$$

where we made use of the structure of the mass operator[10] and the arrow above a differential operator indicates the operand.

Inserting (A5) into (A4) and using (15), we get the following formula:

$$\begin{aligned}&[\delta/\delta h_l(\mathbf{y})]\delta\hat{G}_T'(\mathbf{x}, \mathbf{x}'; E)\\&=\{G_l'(\mathbf{x}, \mathbf{y}; E)\hat{D}_r(\mathbf{y}, \mathbf{x}')-\hat{D}_l(\mathbf{x}, \mathbf{y})\hat{G}_r'(\mathbf{y}, \mathbf{x}')\}-\{r\leftrightarrow l\}\\&=[\delta/\delta h_l(\mathbf{y})]\delta\hat{G}_{T,D}(\mathbf{x}, \mathbf{x}'; E),\end{aligned} \tag{A6}$$

where we have introduced the new notation

$$\begin{aligned}&\delta\hat{G}_{T,D}(\mathbf{x}, \mathbf{x}'; E)\\&=\int\{\hat{G}_l'(\mathbf{x}, \mathbf{y}; E)\hat{D}_r(\mathbf{y}, \mathbf{x}')-\hat{D}_l(\mathbf{x}, \mathbf{y})\hat{G}_r'(\mathbf{y}, \mathbf{x}'; E)\}\\&\qquad\times h_l(\mathbf{y})d^3\mathbf{y}-(r\leftrightarrow l).\end{aligned}$$

We may conclude that $\delta\hat{G}_T$ could be cut into two parts $\delta\hat{G}_T-\delta\hat{G}_{T,D}$ and $\delta\hat{G}_{T,D}$. The first term contributes directly to the physical quantities (e.g., current density), but the second one is similar to δG_D, which is due to the break of completeness and orthogonality. In Sec. 3 we neglected the contribution $\delta\hat{G}_D$ so we do the same with $\delta\hat{G}_{T,D}$. Finally we conclude that $\delta\hat{G}_T$ is independent of the choice of h_l in this approximation.

APPENDIX B

The tunneling current can be obtained by computing expressions (41a) and (41b).

The Green's functions may be expressed by a complete set of appropriate one-particle wave functions:

$$\hat{G}_\alpha'(x, x')=\sum_\lambda \chi_{\lambda,\alpha}(\mathbf{x})\hat{G}_{\lambda,\alpha}(x_0-x_0')\chi_{\lambda,\alpha}^*(\mathbf{x}). \tag{B1}$$

The spectral representation of the normal and anomalous Green's functions are[22]

$$G_{\lambda,\alpha}'(E)=\int dt\exp(iEt)G_{\lambda,\alpha}'(t)=\int d\omega\left(\frac{1-n_{\omega,\alpha}}{E-\omega+i\epsilon}+\frac{n_{\omega,\alpha}}{E-\omega-i\epsilon}\right)A_{\lambda,\alpha}(\omega), \tag{B2}$$

$$\phi_{\lambda,\alpha}'(E)=\int dt\exp(iEt)\phi_{\lambda,\alpha}'(t)=\int d\omega\left(\frac{1-n_{\omega,\alpha}}{E-\omega+i\epsilon}+\frac{n_{\omega,\alpha}}{E-\omega-i\epsilon}\right)B_{\lambda,\alpha}(\omega),$$

and

$$\phi_{\lambda,\alpha}(E)=\phi_{\lambda,\alpha}^\dagger(E), \tag{B3}$$

where $t=x_0-x_0'$, and

$$n_{\omega,\alpha}=\{\exp[\beta(\omega-\mu_\alpha)]+1\}^{-1}. \tag{B4}$$

Here the spectral functions $A_\lambda(\omega)$ and $B_\lambda(\omega)$ are real. The current density may be expressed by the Fourier transform of the causal response function

$$j_i(x)=\lim_{E\to 0}(C\to R)\int_S d^2f_{x',i'}\int_{-\infty}^{\infty}dt\exp(iEt)K_{c,i}(x, x')T_{i'}(x'). \tag{B5}$$

We calculate first the one-particle current using (37) and (B1)–(B5) and introducing the transition matrix

elements

$$T_{\lambda',\lambda;i,l,r}(\mathbf{x}) = \chi_{\lambda',l}{}^{x}(\mathbf{x})\left(\frac{\vec{\nabla}_x - \overleftarrow{\nabla}_x}{2m}\right)_i \chi_{\lambda,r}(\mathbf{x})$$
$$= -T^*{}_{\lambda,\lambda';i,r,\lambda}(\mathbf{x}), \tag{B6}$$

and

$$T_{\lambda,\lambda';r,l} = \int_S d^2 f_{x',i} T_{\lambda,\lambda';i,r,l}(\mathbf{x}')$$
$$= -T_{\lambda',\lambda;r,l}{}^*. \tag{B7}$$

The current density calculated in a straightforward manner is

$$j_{N,i}(x) = 2\lim_{E\to 0}(C\to R)e\int dt \exp(iEt)\{\sum_{\lambda,\lambda'} T_{\lambda',\lambda;i,l,r}(\mathbf{x}) G_{\lambda,r}'(t) G_{\lambda',l}'(-t) T_{\lambda,\lambda';r,l} - (r\leftrightarrow l)\}$$
$$= 2\lim_{E\to 0}(C\to R)e\left\{\sum_{\lambda,\lambda'} T_{\lambda',\lambda;i,l,r}(\mathbf{x}) T_{\lambda,\lambda';r,l}\int \frac{dE'}{2\pi} G_{\lambda,r}(E'+E) G_{\lambda',l}(E') - (r\leftrightarrow l)\right\}$$
$$= 2i\lim_{E\to 0}(C\to R)e\left\{\sum_{\lambda,\lambda'} T_{\lambda',\lambda;i,l,r}(\mathbf{x}) T_{\lambda,\lambda';r,l}\int d\omega'' A_{\lambda,r}(\omega'')\int d\omega' A_{\lambda',l}(\omega')\right.$$
$$\left.\times\left(\frac{(1-n_{\omega'',r})n_{\omega',l}}{E+\omega'-\omega''+i\epsilon} - \frac{n_{\omega'',r}(1-n_{\omega',l})}{E+\omega'-\omega''-i\epsilon}\right) - (r\leftrightarrow l)\right\}$$
$$= 2i\lim_{E\to 0} e\left\{\sum_{\lambda,\lambda'} T_{\lambda',\lambda;i,l,r}(\mathbf{x}) T_{\lambda,\lambda';r,l}\int d\omega'' A_{\lambda,r}(\omega'')\int d\omega' A_{\lambda',l}(\omega')\frac{n_{\omega',l}-n_{\omega'',r}}{E+\omega'-\omega''+i\epsilon} - (r\leftrightarrow l)\right\}, \tag{B8}$$

where the factor two is due to the spin orientations. Finally we have

$$j_{N,i}(x) = -4e\,\mathrm{Im}\left\{\sum_{\lambda,\lambda'} T_{\lambda',\lambda;i,l,r}(x) T_{\lambda,\lambda';r,l}\int d\omega'' A_{\lambda,r}(\omega'')\int d\omega' A_{\lambda',l}(\omega')\frac{n_{\omega',l}-n_{\omega'',r}}{E+\omega'-\omega''+i\epsilon}\right\}, \tag{B9}$$

or

$$j_{N,i}(x) = 4\pi e\sum_{\lambda,\lambda'} T_{\lambda',\lambda;i,l,r}(\mathbf{x}) T_{\lambda,\lambda';r,l}\int d\omega A_{\lambda,r}(\omega) A_{\lambda',l}(\omega)(n_{\omega,l}-n_{\omega,r}). \tag{B10}$$

The Josephson current density can be calculated in a similar way and the result is

$$j_{J,i}(x) = -4e\,\mathrm{Im}\left\{\exp\{2ie(c^{-1}\Delta\varphi + Vx_0)\}\sum_{\lambda,\lambda'} T_{\lambda',\lambda;i,l,r}(x) T_{\lambda,\lambda';r,l}\int d\omega'' B_{\lambda,r}(\omega'')\int d\omega' B_{\lambda',l}(\omega')\frac{n_{\omega',l}-n_{\omega'',r}}{\omega'-\omega''+i\epsilon}\right\}$$
$$= J_{S,i}{}^{V}(\mathbf{x})\,\sin[2e(c^{-1}\Delta\varphi + Vx_0)] + J_{C,i}{}^{V}(\mathbf{x})\,\cos[2e(c^{-1}\Delta\varphi + Vx_0)], \tag{B11}$$

where we have introduced the notations (42) and (43) and the amplitudes $J_S{}^V$ and $J_C{}^V$.

At zero applied voltage we have a much more simple expression of the Josephson current:

$$j_{J,i}(\mathbf{x}) = -4e\sin[(2e/c)\Delta\varphi]\left\{\sum_{\lambda,\lambda'} T_{\lambda',\lambda;i,l,r}(\mathbf{x}) T_{\lambda,\lambda';r,l}\int d\omega'' B_{\lambda,r}(\omega'')\int d\omega' B_{\lambda',l}(\omega')\frac{n_{\omega'}-n_{\omega''}}{\omega'-\omega''}\right\}$$
$$= J_{J,0,i}(\mathbf{x})\,\sin[2(e/c)\Delta\varphi], \tag{B12}$$

where $n_\omega = n_{\omega,r} = n_{\omega,l}$ and $J_{J,0} > 0$.