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Theory of tunneling in superconductors

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The theory developed by Feuchtwang for tunneling in normal metals is extended to superconductors. It is shown that for metal–insulator–superconductor and metal–insulator–thin-metal–superconductor junctions, our results agree with the standard Bardeen "tunneling Hamiltonian" approach. In the latter case, however, if there exists a potential barrier at the thin-metal–superconductor interface, then the standard approach is found to be incorrect. We give the proper expansion for the tunneling current in this case.

I. INTRODUCTION

The I-V characteristic of a normal metal-oxide–superconductor tunneling junction gives detailed information on the density of states in the superconductor. This fact is inferred both from experimental observation and from the standard "tunneling Hamiltonian" theory. Analysis of experimental tunneling characteristics in terms of the standard theory and the theory of strongly coupled superconductors has produced a wealth of detailed information on the electron-phonon interaction and phonon density of states in many metals.

However, rigorous theoretical justification of the tunneling Hamiltonian theory has only been obtained recently, in a series of papers by Feuchtwang.[1] But his theory specifically describes tunneling in *normal* junctions; also, interactions such as the electron-phonon interaction are neglected.

Therefore, in this work the Feuchtwang theory is extended to deal with tunnel junctions in which one of the metallic layers is superconducting. Specifically, we consider normal-metal–insulator–superconductor and normal-metal–insulator–thin-normal-metal–superconductor junctions. The latter involves the proximity effect, which is dealt with in more detail in a separate paper.[2] The influence of interactions on tunneling is accounted for by making a local approximation for the self-energies.

As the extension of the Feuchtwang theory is not entirely straightforward, all the details of the extension of this theory have been presented here, for clarity. In Sec. II we calculate the Green's function for a three-layer system which has translational invariance in the y and z directions. The form of the results is shown to be similar to Feuchtwang's results, if the Green's functions are interpreted as matrices. In Sec. III the tunneling current is calculated, using the Kadanoff-Baym approach[3] for obtaining the Green's functions for a system which is out of equilibrium. In Sec. IV we describe the technique for calculating Green's functions for the single layers. Finally, in Sec. V, we derive the results for the dependence of the tunneling current on the densities of states for the components of a three-layer system when the central layer is a simple rectangular potential barrier. These results are shown to agree with those of the standard theory in the two cases mentioned above, providing a rigorous verification of that theory in these cases.

However, in the proximity-effect configuration with a step potential barrier at the N-S interface, such as would arise from a difference between the N and S metals in the height of the common Fermi level above the bottom of the band, we find that the standard form is altered. This leads us to conclude that the standard expression for the tunneling current may be incorrect when applied to proximity-effect tunneling, if there is a significant amount of reflection from the potential barrier at the N-S interface.

II. GREEN'S FUNCTION FOR THE TUNNELING SANDWICH

We consider three slabs of material: a left electrode, a barrier region, and a right electrode (see Fig. 1). For simplicity, we choose all interfaces to planar and parallel, so that there is translational invariance in the y and z directions. We therefore may define the quasi-one-dimensional Green's function

$$G(xx') = \int_{-\infty}^{\infty} d(y-y') \int_{-\infty}^{\infty} d(z-z') \int_{-\infty}^{\infty} d(t-t') \exp\left[-ik_y(y-y') - ik_z(z-z') + \frac{iE(t-t')}{\hbar}\right] \times G(xx', y-y', z-z'; t-t') \,. \tag{2.1}$$

Causal boundary conditions dictate that E contain a positive infinitesimal imaginary part, $i\delta$. This yields the "retarded" Green's function. The "advanced" Green's function requires an energy with negative infinitesimal imaginary part. For notational simplicity, the dependence of the Green's functions on k_1, k_2, and E will not explicitly be indicated except when confusion might arise.

The equations satisfied by the retarded or advanced Green's function are taken to be

$$\begin{aligned}[E - H_0(x) - \Sigma_l(x)]g_l(xx') &= \vec{L}_l(x)g_l(xx') \\ &= \delta(x-x'), \quad x,x' \in D_l , \\ [E - H_0(x) - \Sigma(x)]G(xx') &= \vec{L}(x)G(xx') \\ &= \delta(x-x')\end{aligned} \tag{2.2}$$

The adjoint equations are

$$\begin{aligned}g_l(xx')[E - H_0(x') - \Sigma_l(x')] \\ = g_l(xx')\overleftarrow{L}_l(x') = \delta(x-x'), \quad x,x' \in D_l , \\ G(xx')[E - H_0(x') - \Sigma(x')] \\ = G(xx')\overleftarrow{L}(x') = \delta(x-x')\end{aligned} \tag{2.3}$$

We have defined

$$\begin{aligned}H_0(x) &= \left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - \left(\mu - \frac{\hbar^2 k_\parallel^2}{2m}\right)\right]\tau_3 \\ &= \left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - \mu_1\right)\tau_3 ,\end{aligned} \tag{2.4}$$

where μ is the chemical potential, $\hbar k_\parallel$ is the magnitude of momentum parallel to the interfaces, and τ_1, τ_2, τ_3 will represent the three Pauli matrices, in the notation of Nambu.[4] The matrix self-energies $\Sigma(x)$, $\Sigma_l(x)$ apply, respectively, to the entire tunneling sandwich and to the lth slab D_l. For convenience, we define

$$s_l^+ = s_l + \delta, \quad s_l^- = s_l - \delta,$$

$$s_l^+ \in D_l, \quad s_l^- \in D_{l-1} .$$

It is assumed throughout that all self-energies are well approximated by self-energies which are local with respect to the x coordinate, i.e.,

$$\Sigma(xx'k_1k_2) \cong \Sigma(xk_1k_2)\delta(x-x')$$

for x momenta near the Fermi momentum, $p_1 \approx p_F$. These happen to be the momenta of interest in tunneling. This approximation is similar to the approximation made in bulk materials when the momentum dependence of the self-energy is neglected.

Following Feuchtwang's prescription, we construct

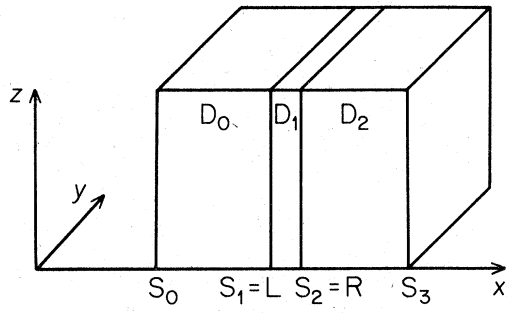

FIG. 1. Geometry of the tunneling junction considered here. The layers are labeled by D_0, D_1, D_2.

$$\int_{s_l^+}^{s_{l+1}^-} dx''\,[G(xx'')\vec{L}_l(x'')g_l(x''x') - G(xx'')\overleftarrow{L}(x'')g_l(x''x')] = G(xx')\Theta(x' \in D_l) - g_l(xx')\Theta(x \in D_l) . \tag{2.5}$$

The Θ function $\Theta(x \in D_l)$ vanishes if x is *not* in D_l, and is unity otherwise. Partial integration yields

$$\begin{aligned}G(xx')\Theta(x' \in D_l) = g_l(xx')\Theta(x \in D_l) + \Bigg(\frac{-\hbar^2}{2m}[G(xx'')'\tau_3 g_l(x''x') - G(xx'')\tau_3 g_l'(x''x')]\Big|_{s_l^+}^{s_{l+1}^-} \\ + \int_{s_l^+}^{s_{l+1}^-} dx''\,G(xx'')[\Sigma(x'') - \Sigma_l(x'')]g_l(x''x')\Bigg) ,\end{aligned} \tag{2.6}$$

where we define

$$G'(xx') = \frac{\partial}{\partial x}G(xx'), \quad G(xx')' = \frac{\partial}{\partial x'}G(xx'), \quad G'(xx')' = \frac{\partial}{\partial x}\frac{\partial}{\partial x'}G(xx') \tag{2.7}$$

Similarly,

$$\int_{s_i^+}^{s_{i+1}^-} dx''\,[g_i(xx'')\vec{L}_i(x'')G(x''x') - g_i(xx'')\overleftarrow{L}(x'')G(x''x')]$$

$$= G(xx')\Theta(x \in D_i) - g_i(xx')\Theta(x' \in D_i)$$

$$= \left(\frac{-\hbar^2}{2m}[g_i(xx'')\tau_3 G'(x''x') - g_i(xx'')'\tau_3 G(x''x')]\right)\Bigg|_{s_i^+}^{s_{i+1}^-} + \int_{s_i^+}^{s_{i+1}^-} g_i(xx'')[\Sigma(x'') - \Sigma_i(x'')]\,G(x''x')\,dx'' \quad . \tag{2.8}$$

These equations are similar to Eqs. (2.6) and (2.7) of Ref. 1(b) except for the matrices and the self-energy difference within the ith region. We will assume that the self-energy $\Sigma_i(x'')$ can be chosen such that this term vanishes. Because $\Sigma(x'')$ must be determined self-consistently from the Green's function $G(xx')$, which one is trying to calculate, this is not a trivial requirement. We shall assume that it can be met to accuracy sufficient to leave the self-energy difference within the ith region as a small perturbative correction.

It is sometimes convenient to interpret these results in terms of a pseudo "tunneling Hamiltonian" [see Eqs. (2.15) and (2.16) of Ref. 1(b)]:

$$G(xx') = g(xx') + \int_{s_0}^{s_3} dx''\,g(xx'')H_T(x'')G(x''x')$$

$$= g(xx') + \int_{s_0}^{s_3} dx''\,G(xx'')H_T^\dagger(x'')g(x''x') \quad , \tag{2.9}$$

where

$$g(xx') = g_i(xx'), \quad x,x' \in D_i \quad ,$$

and (neglecting the self-energy difference at the boundaries)

$$H_T(x'') = \frac{\hbar^2}{2m}\tau_3\left\{\sum_{i=0}^{2}[\delta(x''-s_i^+) - \delta(x''-s_{i+1}^-)], \frac{\partial}{\partial x''}\right\}$$

$$= -H_T^\dagger(x'') \quad . \tag{2.10}$$

The large parentheses indicate an anticommutator. The δ functions $\delta(x''-s_0^+)$ and $\delta(x''-s_3^-)$ may be set equal to zero because all the Green's functions will be required to vanish at s_0 and s_3.

It must be understood that the limits $s_0 \to -\infty$ and $s_3 \to +\infty$ are to be taken, otherwise the Dirichlet boundary condition would lead to no net current. In these limits, the temporal boundary condition on the Green's functions (retarded) *automatically* leads to the required outgoing-wave behavior, as we show for a specific case in Sec. V, Eq. (5.3). This procedure assumes that what occurs at s_0 and s_3, the free surfaces, has no effect on the observed current, so that the finite-sized sample may be regarded as effectively infinite in extent.

The boundary conditions on the $g_i(xx')$ at s_1 and s_2 may be chosen for convenience.[1(c)] We shall require that the first derivative of $g_i(xx')$ (with respect to x or x') vanish at s_1 and s_2. At $(x,x') = s_0$ or s_3 we require that $g_0(xx')$ and $g_2(xx')$ vanish, again with the implied limits $s_0 \to -\infty$, $s_3 \to +\infty$, and the temporal boundary condition, which combine to produce the correct outgoing-wave behavior.

Thus Eqs. (2.6) and (2.8) reduce to

$$G(xx')\Theta(x' \in D_i) = g_i(xx')\Theta(x \in D_i) + \frac{\hbar^2}{2m}[G(x,s_i^+)'\tau_3 g_i(s_i^+,x') - G(x,s_{i+1}^-)'\tau_3 g_i(s_{i+1}^-,x')] \quad , \tag{2.11}$$

$$G(xx')\Theta(x \in D_i) = g_i(xx')\Theta(x' \in D_i) + \frac{\hbar^2}{2m}[g_i(x,s_i^+)\tau_3 G'(s_i^+,x') - g_i(x,s_{i+1}^-)\tau_3 G'(s_{i+1}^-,x')] \quad . \tag{2.12}$$

The first derivatives in Eq. (2.12) are found by evaluating the first derivative of (2.11) at s_i^+ and s_{i+1}^-. One thereby obtains

$$G(xx')\Theta(x \in D_i) = g_i(xx')\Theta(x' \in D_i) - \frac{\hbar^2}{2m}g_i(x,s_i^+)[\Gamma(s_i^+,s_i^+)g_i(s_i^+,x') - \Gamma(s_i^+,s_{i+1}^-)g_i(s_{i+1}^-,x')]$$

$$+ \frac{\hbar^2}{2m}g_i(x,s_{i+1}^-)[\Gamma(s_{i+1}^-,s_i^+)g_i(s_i^+,x') - \Gamma(s_{i+1}^-,s_{i+1}^-)g_i(s_{i+1}^-,x')] \quad , \tag{2.13}$$

where

$$\Gamma(xx') \equiv -(\hbar^2/2m)\tau_3 G'(xx')'\tau_3 \quad . \tag{2.14}$$

All functions in Eq. (2.13) are now *continuous*, so that the limits

$$s_i^+ \to s_i, \quad s_{i+1}^- \to s_{i+1}$$

may be taken.

The only remaining unknowns are the Γ matrices. To determine these, we derive equations from the equation for the discontinuity of the first derivative of the Green's function at the source point $x' = x = s_{i+1}$:

$$\tau_3[G'(s_{i+1},s_{i+1}^-) - G'(s_{i+1},s_{i+1}^+)] = 2m/\hbar^2 \ . \tag{2.15}$$

In combination with the first derivative of (2.11) at s_{i+1}, this yields

$$-\Gamma(s_{i+1},s_i)g_i(s_i,s_{i+1}) + \Gamma(s_{i+1},s_{i+1})g_i(s_{i+1},s_{i+1}) + \Gamma(s_{i+1},s_{i+1})g_{i+1}(s_{i+1},s_{i+1}) - \Gamma(s_{i+1},s_{i+2})g_{i+1}(s_{i+2},s_{i+1}) = 2m/\hbar^2 \ . \tag{2.16}$$

Since the first derivative of $G(xx')$ is continuous in x' away from the source point ($x = x'$), we have

$$\tau_3[G'(s_{i+1},s_i^-) - G'(s_{i+1},s_i^+)] = 0 \quad \tau_3[G'(s_i,s_{i+1}^-) - G'(_i,s_{i+1}^+)] = 0 \ .$$

In combination with the first derivative of (2.11) at s_{i+1}, the first of these yields

$$-\Gamma(s_{i+1},s_{i-1})g_{i-1}(s_{i-1},s_i) + \Gamma(s_{i+1},s_i)g_{i-1}(s_i,s_i) + \Gamma(s_{i+1},s_i)g_i(s_i,s_i) - \Gamma(s_{i+1},s_{i+1})g_i(s_{i+1},s_i) = 0 \ , \tag{2.17}$$

and the second yields

$$-\Gamma(s_i,s_i)g_i(s_i,s_{i+1}) + \Gamma(s_i,s_{i+1})g_i(s_{i+1},s_{i+1}) + \Gamma(s_i,s_{i+1})g_{i+1}(s_{i+1},s_{i+1}) - \Gamma(s_i,s_{i+2})g_{i+1}(s_{i+2},s_{i+1}) = 0 \ . \tag{2.18}$$

To facilitate comparison of these results with Eq. (2.10) of Ref. 1(b), we relabel the regions $D_0 \to D_L$, $D_1 \to D_B$, $D_2 \to D_R$ and set $s_1 = R$, $s_2 = L$. Using the boundary conditions on the $g_i(xx')$, one finds [from (2.16), (2.17), and (2.18)]

$$\begin{pmatrix} \Gamma(LL) & \Gamma(LR) \\ \Gamma(RL) & \Gamma(RR) \end{pmatrix} \begin{pmatrix} g_L(LL) + g_B(LL) & -g_B(LR) \\ -g_B(RL) & g_R(RR) + g_B(RR) \end{pmatrix} = \frac{2m}{\hbar^2} \ . \tag{2.19}$$

In the normal state, where all the matrices Γ and g are *diagonal,* this is identical to Eq. (2.10) of Ref. 1(b).

In the limit $L = R$, all of the Γ's above must be equal. To show what the result for Γ is in this limit, we consider the case in which the barrier region is a rectangular potential barrier of height V. Then, using the appropriate boundary conditions at L and R (Ref. 5):

$$g_B(RR) = g_B(LL) = m/\hbar^2 \begin{pmatrix} \coth[K_+(L-R)]/K_+ & 0 \\ 0 & -\coth[K_-(L-R)]/K_- \end{pmatrix} \tag{2.20}$$

$$g_B(RL) = g_B(LR) = m/\hbar^2 \begin{pmatrix} \{K_+ \sinh[K_+(L-R)]\}^{-1} & 0 \\ 0 & -\{K_- \sinh[K_-(L-R)]\}^{-1} \end{pmatrix} \tag{2.21}$$

where $K_\pm \equiv [(2m/\hbar^2)(V - \mu_\nu \mp E)]^{1/2}$.

Note that all of these functions diverge at $L = R$. We now consider the solution for $\Gamma(LL)$,

$$\Gamma(LL) = (2m/\hbar^2)\{g_L(LL) + g_B(LL) - g_B(LR)[1 + g_B(RR)^{-1}g_R(RR)]^{-1}g_B(RR)^{-1}g_B(RL)\}^{-1} \tag{2.22}$$

Thus we find, in the appropriate limit,

$$\lim_{R \to L} \Gamma(LL) = (2m/\hbar^2)[g_L(LL) + g_R(LL)]^{-1} \tag{2.23}$$

Equation (2.23) follows from (2.22) if one expands

$$[1 + g_B(RR)^{-1}g_R(RR)]^{-1}$$

to first order in the small quantity $g_B(RR)^{-1}g_R(RR)$ as $L \to R$. One thus obtains

$$\lim_{R \to L} \Gamma(LL) = (2m/\hbar^2)[g_L(LL) + g_B(LL) - g_B(LR)g_B(RR)^{-1}g_B(RL) + g_B(LR)g_B(RR)^{-1}g_R(RR)g_B(RR)^{-1}g_B(RL)]^{-1}$$

Using Eqs. (2.20) and (2.21), it is easy to show that the second term minus the third term is diagonal with diagonal elements equal to

$$\pm\frac{m}{\hbar^2 K_\pm}\left\{\coth[K_\pm(L-R)] - \frac{1}{\cosh[K_\pm(L-R)]}\right\} = \pm\frac{m}{\hbar^2 K_\pm}\sinh[K_\pm(L-R)]$$

Thus, this term vanishes as $L \to R$. Again using (2.20) and (2.21), one finds that

$$\lim_{L\to R} g_B(RR)^{-1} g_B(RL) = 1 ,$$

so that the fourth term becomes $g_R(RR) = g_R(LL)$, by continuity.

III. TUNNELING CURRENT

In the Nambu formalism,[4] the Green's function is defined by

$$G(11') = \frac{1}{i}\langle T(\Psi(1)\Psi^\dagger(1'))\rangle , \tag{3.1}$$

where (illustrating the notation)

$$\Psi(1) = \begin{pmatrix} \Psi_\uparrow(\vec{r}_1 t_1) \\ \Psi_\downarrow^\dagger(\vec{r}_1 t_1) \end{pmatrix} , \quad \Psi^\dagger(1') = (\Psi_\uparrow^\dagger(\vec{r}_1' t_1') , \Psi_\downarrow(\vec{r}_1' t_1')) ,$$

and $\Psi_\uparrow(\vec{r}_1 t_1)$ $[\Psi_\downarrow^\dagger(\vec{r}_1 t_1)]$ is a destruction (creation) operator for a fermion of spin up (down) at $\vec{r}_1$ at time t_1. The brackets indicate a grand canonical ensemble average with respect to the exact Hamiltonian. The operator T orders the operators in parentheses in order of increasing time from right to left.

It is useful to define two auxiliary functions,[6]

$$G(11') = G(11')^< \Theta(t_1' - t_1) + G(11')^> \Theta(t_1 - t_1') . \tag{3.2}$$

We also need the retarded and advanced functions $G(11')^r, G(11')^a$, which obey the same equation as the "full" Green's function, with a temporal boundary condition that requires $G(11')^r$ to vanish for $t_1' > t_1$, and $G(11')^a$ to vanish for $t_1' < t_1$. The latter two functions are related to those in Eq. (3.2) by

$$\begin{aligned} G(11')^r &= [G(11')^> - G(11')^<]\Theta(t_1 - t_1') , \\ G(11')^a &= -[G(11')^> - G(11')^<]\Theta(t_1' - t_1) . \end{aligned} \tag{3.3}$$

Thus,

$$G(11')^a - G(11')^r = G(11')^< - G(11')^> \equiv -\delta G(11') . \tag{3.4}$$

The last definition above is made for later convenience.

In Ref. 3 [see Eqs. (8.27) and (8.28) of this reference] equations are derived for $G(11')^{<(>)}$ in the normal state. Since the generalization of these equations to the superconducting case is straightforward, we merely quote the necessary results,

$$\left(i\frac{\partial}{\partial t_1} - H_0(r_1)\right) G(11')^{>(<)} - \int d\bar{1}\,[\delta\Sigma(1\bar{1})G(\bar{1}1')^{>(<)}\Theta(t_1 - \bar{t}_1) - \Sigma(1\bar{1})^{>(<)}\delta G(\bar{1}1')\Theta(t_1' - \bar{t}_1)] = H_T(1)G(11')^{>(<)} \tag{3.5}$$

and

$$-i\frac{\partial}{\partial t_1'} G(11')^{>(<)} - G(11')^{>(<)} H_0(r_1') - \int d\bar{1}\,[G(1\bar{1})^{>(<)}\delta\Sigma(\bar{1}1')\Theta(t_1 - \bar{t}_1) - \delta G(1\bar{1})\Sigma(\bar{1}1')^{>(<)}\Theta(t_1' - \bar{t}_1)] = G(11')^{>(<)} H_T(1') , \tag{3.6}$$

where

$$\delta\Sigma(1\bar{1}) \equiv \Sigma(1\bar{1})^> - \Sigma(1\bar{1})^< , \quad \delta\Sigma(1\bar{1})\Theta(t_1 - \bar{t}_1) \equiv \Sigma(1\bar{1})^r$$

Making use of these results, one can readily verify [using (3.3)] that the retarded or advanced Green's function satisfies

$$\left(i\frac{\partial}{\partial t_1} - H_0(r_1)\right) G(11') - \int d\bar{1}\,\Sigma(1\bar{1})G(\bar{1}1') = H_T(1)G(11') + \delta(1-1') \tag{3.7}$$

and

$$-i\frac{\partial}{\partial t_1'} G(11') - G(11')H_0(r_1') - \int d\bar{1}\,G(1\bar{1})\Sigma(\bar{1}1') = G(11')H_T(1') + \delta(1-1') . \tag{3.8}$$

A Fourier transform of this equation, defined as in Eq. (2.1), yields Eq. (2.9), since $g(xx')$ is to be constructed to satisfy Eq. (3.7) for $H_T = 0$. A similar Fourier transform of Eqs. (3.5) and (3.6) likewise leads to

$$G^<(xx') = g^<(xx') + \int_{x_0}^{x_3} dx_1 \, [g(xx_1)^r H_T(x_1) G(x_1x')^< + g(xx_1)^< H_T(x_1) G(x_1x')^a] \tag{3.9}$$

or

$$G^<(xx') = g^<(xx') + \int_{x_0}^{x_3} dx_1 \, [G(xx_1)^< H_T^\dagger(x_1) g(x_1x')^a + G(xx_1)^r H_T^\dagger(x_1) g(x_1x')^<] \tag{3.10}$$

By conservation of current, we obtain the total current through the planar junction of Fig. 1 ($\hat{x}$ is a unit vector in the x direction),

$$j(x) = \int\int \hat{x} \cdot \vec{j}(\vec{r}) \, dy \, dz = \int\int \hat{x} \cdot \left(\frac{2|e|\hbar}{2im} \right) \left[\left(\frac{\partial}{\partial \vec{r}} - \frac{\partial}{\partial \vec{r}'} \right) \frac{1}{2} \mathrm{Tr}[G(\vec{r}t\,\vec{r}'t')^<]_{t=t'} (1+\tau_3) \right] dy \, dz \tag{3.11}$$

The symbol "Tr" signifies a trace in the two-dimensional space. The 11 component of the Green's function is projected out by means of the matrix $(1+\tau_3)$. A Fourier transformation according to Eq. (2.1) yields

$$j(x) = \frac{|e|}{2im} \int \frac{dk_y \, dk_z \, dE}{(2\pi)^3} \left[\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial x'} \right) \mathrm{Tr}[G(xx')^<]_{x=x'} (1+\tau_3) \right] \tag{3.12}$$

To evaluate the x derivative we use Eq. (3.10), while for the x' derivative we use (3.9), in order to obtain results in terms of the Γ matrices. Thus

$$\begin{aligned} j(x) = \frac{-|e|\hbar}{2im} \int \frac{dk_y}{2\pi} \int \frac{dk_z}{2\pi} \int \frac{dE}{2\pi\hbar} \mathrm{Tr} \Bigg\{ \sum_{i=0}^{2} \{ \tau_3 [& \Gamma(xs_i^+)^< g_i(s_i^+x)^a - \Gamma(xs_{i+1}^-)^< g_i(s_{i+1}^-x)^a \\ & + \Gamma(xs_i^+)^r g_i(s_i^+x)^< - \Gamma(xs_{i+1}^-)^r g_i(s_{i+1}^-,x)^<] \\ & - [g_i(xs_i^+)^r \Gamma(s_i^+x)^< - g_i(xs_{i+1}^-)^r \Gamma(s_{i+1}^-,x)^< \\ & + g_i(xs_i^+)^< \Gamma(s_i^+x)^a - g_i(xs_{i+1}^-)^< \Gamma(s_{i+1}^-x)^a] \tau_3 \} (1+\tau_3) \Bigg\} , \end{aligned} \tag{3.13}$$

where

$$\Gamma(ab)^{>(<)} = \frac{-\hbar^2}{2m} \tau_3 \frac{\partial}{\partial x} \frac{\partial}{\partial x'} G(xx')^{>(<)} \tau_3 \big|_{x=a, x'=b}$$

It is most convenient to calculate the current either at $x = s_1 \equiv L$ or $x = s_2 \equiv R$. Using the fact that the Green's functions for the ith region vanish outside this region, we find

$$\begin{aligned} j(L) = \frac{+|e|}{2m} \int \frac{dk_y}{2\pi} \int \frac{dk_z}{2\pi} \int \frac{dE}{2\pi} \mathrm{Tr} (\{ & \tau_3 [\Gamma(LL)^< g_L(LL)^a + \Gamma(LL)^r g_L(LL)^<] \\ & - [g_L(LL)^r \Gamma(LL)^< + g_L(LL)^< \Gamma(LL)^a] \tau_3 \} (1+\tau_3)) \end{aligned} \tag{3.14}$$

after evaluating (3.13) at $x = s_1^- = L^-$, and taking the limit $L^- \to L$. The equation for $j(R)$ is the negative of the above with L replaced everywhere by R. Using Eq. (3.4), we see that

$$\Gamma^a - \Gamma^r = \Gamma^< - \Gamma^> \quad \text{and} \quad g_L^a - g_L^r = g^< - g^>$$

Equation (3.14) can therefore be written

$$\begin{aligned} \frac{2m}{|e|} j(L) = \int \frac{dE}{2\pi} \int\int \frac{dk_y \, dk_z}{(2\pi)^2} \mathrm{Tr} (\{ & \tau_3 [\Gamma(LL)^> g_L(LL)^< - \Gamma(LL)^< g_L(LL)^>] + \tau_3 \Gamma^<(LL) g_L^a(LL) \\ & - g_L^a(LL) \Gamma^<(LL) \tau_3 + \tau_3 \Gamma^a(LL) g_L^<(LL) - g_L^<(LL) \Gamma^a(LL) \tau_3 \} (1+\tau_3)) \end{aligned} .$$

This form is obtained by making the indicated substitutions into the first two terms of Eq. (3.14). A similar substitution in the last two terms of this equation yields

$$j(L)=\frac{|e|}{2m}\int\frac{dE}{2\pi}\int\frac{dk_x\,dk_z}{(2\pi)^2}\,\mathrm{Tr}\{(1+\tau_3)[g_L(LL)^<\Gamma(LL)^>-g_L(LL)^>\Gamma(LL)^<]$$
$$+(1+\tau_3)[\Gamma(LL)^<g_L(LL)^a-g_L(LL)^a\Gamma(LL)^<+\Gamma(LL)^r g_L(LL)^<$$
$$-g_L(LL)^<\Gamma(LL)^r]\}\ .$$

One-half the sum of these expressions yields (after using the cyclic property of the trace)

$$j(L)=\frac{|e|}{2m}\int\frac{dE}{2\pi}\int\frac{dk_x\,dk_z}{(2\pi)^2}\frac{1}{2}\,\mathrm{Tr}\{(1+\tau_3)\{[\Gamma(LL)^>,g_L(LL)^<]_+-[\Gamma(LL)^<,g_L(LL)^>]_+\}$$
$$+\tau_3[\Gamma(LL)^<,g_L(LL)^a+g_L(LL)^r]_-$$
$$+\tau_3[\Gamma(LL)^a+\Gamma(LL)^r,g_L(LL)^<]_-)\ . \tag{3.15}$$

To complete the calculation of the current, it is necessary to determine the matrix $\Gamma^{>(<)}$. For convenience, we reproduce here the approach in Appendix A of Ref. 1(b). Using the results in Eqs. (3.5)–(3.10) we have, symbolically,

$$G^{>(<)}=g^{>(<)}+g^rH_TG^{>(<)}+g^{>(<)}H_TG^a\ ,$$
$$G^r=g^r+g^rH_TG^r=g^r+G^rH_T^\dagger g^r\ .$$

Thus

$$G^{>(<)}=(1-g^rH_T)^{-1}\times(g^{>(<)}+g^{>(<)}H_TG^a)$$

and

$$G^r(g^r)^{-1}=(1-g^rH_T)^{-1}=1+G^rH_T^\dagger\ .$$

The combination of these last two equations gives the required result,

$$G^{>(<)}=g^{>(<)}+g^{>(<)}H_TG^a+G^rH_T^\dagger g^{>(<)}+G^rH_T^\dagger g^{>(<)}H_TG^a\ . \tag{3.16}$$

Using Eq. (3.16) and the boundary conditions on the Green's functions, one may obtain

$$-\frac{2m}{\hbar^2}\Gamma^{>(<)}(xx)=\sum_{i=0}^{2}\{\Gamma^r(xs_i^+)[g_i^{>(<)}(s_i^+s_i^+)\Gamma^a(s_i^+x)-g_i^{>(<)}(s_i^+s_{i+1}^-)\Gamma^a(s_{i+1}^-x)]$$
$$-\Gamma^r(xs_{i+1}^-)[g_i^{>(<)}(s_{i+1}^-s_i^+)\Gamma^a(s_i^+x)-g_i^{>(<)}(s_{i+1}^-s_{i+1}^-)\Gamma^a(s_{i+1}^-x)]\}\ . \tag{3.17}$$

The quantities of interest are now easily found to be

$$-\frac{2m}{\hbar^2}\Gamma^{>(<)}(LL)=\Gamma^r(LL)[g_L^{>(<)}(LL)+g_B^{>(<)}(LL)]\Gamma^a(LL)-\Gamma^r(LL)g_B^{>(<)}(LR)\Gamma^a(RL)$$
$$-\Gamma^r(LR)g_b^{>(<)}(RL)\Gamma^a(LL)+\Gamma^r(LR)[g_R^{>(<)}(RR)+g_B^{>(<)}(RR)]\Gamma^a(RL) \tag{3.18}$$

Equations (2.19), (3.15), and (3.18) determine the tunneling current once the single-layer Green's functions are obtained.

One has the relationship

$$g_i(xx')^{>(<)}=\mp i\rho_i(xx')f_i^{(\pm)}(E) \tag{3.19}$$

where $f_i^{(-)}(E)=1-f_i^{(+)}(E)\equiv f_i(E)$ is the Fermi distribution function for the ith layer and $\rho_i(xx')$ is the complex spectral density function defined by Eqs. (3.14) and (3.15) of Ref. 1(b). As noted in this reference (just below the aforementioned equations) this function vanishes over energy intervals in which $\rho_i(xx)$ vanishes. But

$$i\rho_i(xx)=[g_i(xx)^a-g_i(xx)^r]=-2i\,\mathrm{Im}[g_i(xx)^r]\ ,$$

because $\rho_i(xx)$ is real. Thus, at energies for which

$g_B(xx)'$ is real, we find

$$g_B(xx')^{>(<)}=0 . \tag{3.20}$$

That is, (3.20) holds if there are no states in B at the energies of interest for tunneling. One can verify this statement for the special case of a simple rectangular barrier by examining Eqs. (2.20) and (2.21). Barriers for which (3.20) holds at the energies of interest for tunneling will be termed "structureless barriers" in the following.

For a structureless barrier, the first two terms of Eqs. (3.15) can be written

$$\frac{|e|}{2m}\int\frac{dE}{2\pi}\int\frac{dk_y\,dk_z}{(2\pi)^2}\frac{1}{2}\mathrm{Tr}\left\{(1+\tau_3)\frac{\hbar^2}{2m}[\Gamma'(LR)\rho_R(RR)\Gamma^a(RL),\rho_L(LL)]_+\right\}[f_L(E)-f_R(E)] . \tag{3.21}$$

When the tunneling junction is biased with a voltage V, this term is nonzero. Otherwise, it vanishes, since $f_L(E)-f_R(E)=f(E-eV)-f(E)\to 0$.

The last two terms of (3.15) are finite even when $V=0$. Hence they represent the "zero-bias anomaly" or Josephson effect (in the absence of a magnetic field). Using the identity

$$\mathrm{Tr}(A[B,C])=\mathrm{Tr}([C,A]B),$$

we may rewrite the "anomalous" terms

$$j_{\mathrm{an}}(L)=\frac{|e|}{2m}\int\frac{dE}{2\pi}\int\frac{dk_y\,dk_z}{(2\pi)^2}\frac{1}{2}\mathrm{Tr}\{[g_L(LL)^a+g_L(LL)',\tau_3]\Gamma(LL)^<+[g_L(LL)^<,\tau_3][\Gamma(LL)^a+\Gamma(LL)']\} . \tag{3.22}$$

If L is the normal state then the Green's functions g_L contain elements on the diagonal only, and the commutators vanish. Since only one of the three layers of the tunneling sandwich we consider is a superconductor, there will be no Josephson current. Thus, the current is given by (3.21).

IV. SINGLE-LAYER GREEN'S FUNCTIONS

An important approximation is made in the neglect of the self-energy difference at the metal boundaries [see Eqs. (2.6) and (2.8)]. If one can make an accurate initial guess for the local self-consistent self-energy of the sandwich, then this neglect will be justified. A crude, but tractable, ansatz for the self-energy in each layer will be adopted here: the self-energy will be assumed spatially constant in each layer, with step-function discontinuities at the boundaries. Such an ansatz is generally taken in studies of normal metal-oxide–superconductor tunneling. The accuracy of this is to be evaluated by calculating the self-consistent self-energy using the Green's functions obtained by means of this ansatz.

The quasi-one-dimensional Nambu Green's function can be written

$$G(xx')=\sum_g d_g\Psi_g(x_>)\Phi_g(x_<)^\dagger , \tag{4.1}$$

where $\Psi_g(x_>)$ is a two-component vector wave function satisfying the Bogolyubov equations with boundary conditions appropriate to the right of the source point at $x=x'$, $\Phi_g(x_<)$ a solution for boundary conditions applying to the left-hand side of the source point. The index g accounts for the inherent (twofold) degeneracy in the solutions of the Bogolyubov equations. The constants d_g are to be determined from the discontinuity in the first derivative of the Green's function,

$$\tau_3\left(\frac{d}{dx_>}-\frac{d}{dx_<}\right)G(xx')\Big|_{x=x'}=\frac{2m}{\hbar^2} , \tag{4.2}$$

where $x_>$ ($x_<$) is the greater (lesser) of the two coordinates x,x'.

The self-energy ansatz is

$$\Sigma(x)=(1-Z_i)E+\phi_i\tau_1+V_i\tau_3,\quad x\in D_i . \tag{4.3}$$

Thus, for x in the ith layer, the Bogolyubov equations are

$$\left[Z_iE+\left(\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\mu_\nu-V_i\right)\tau_3-\phi_i\tau_1\right]\Psi_g^{(i)}(x)=0 . \tag{4.4}$$

The general solutions are

$$\Psi_\pm^{(i)}(x)=\begin{bmatrix}[(E\pm\Omega_i)/\Omega_i]^{1/2}\\ [(E\mp\Omega_i)/\Omega_i]^{1/2}\end{bmatrix}[A\cos(K_\pm^{(i)}x)+B\sin(K_\pm^{(i)}x)] , \tag{4.5}$$

where

$$\begin{aligned}&\Delta_i\equiv\phi_i/Z_i ,\\ &\Omega_i\equiv(E^2-\Delta_i^2)^{1/2} ,\\ &K_\pm^{(i)}\equiv[k_{F\nu}^2-(2m/\hbar^2)(V_i\mp Z_i\Omega_i)]^{1/2}\\ &k_{F\nu}\equiv(2m\mu_\nu/\hbar^2)^{1/2}\end{aligned} \tag{4.6}$$

and A,B are constants.

Using Eqs. (4.2) and (4.5), we write

$$\Psi_{\pm}^{(\prime)}(x_>) = \begin{pmatrix} (E \pm \Omega_\prime/\Omega_\prime)^{1/2} \\ (E \mp \Omega_\prime/\Omega_\prime)^{1/2} \end{pmatrix} \psi_{\pm}^{(\prime)}(x_>) \ ,$$

$$[\Phi_{\pm}^{(\prime)}(x_<)]^\dagger = \left(\frac{E \pm \Omega_\prime}{\Omega_\prime}\right)^{1/2}, \left(\frac{E \mp \Omega_\prime}{\Omega_\prime}\right)^{1/2} \phi_{\pm}^{(\prime)}(x_<) \ ,$$

and find the solutions for $d_\pm$,

$$d_\pm = \pm m/\hbar^2 W_{\pm}^{(\prime)} \ , \tag{4.7}$$

where $W_{\pm}^{(\prime)}$ is the Wronskian

$$W_{\pm}^{(\prime)} = \frac{d\psi_{\pm}^{(\prime)}(x)}{dx}\phi_{\pm}^{(\prime)}(x) - \psi_{\pm}^{(\prime)}(x)\frac{d\phi_{\pm}^{(\prime)}(x)}{dx} \ , \tag{4.8}$$

which is independent of x. One can now write the Green's function for any of the layers.

$$g_L(xx') = \begin{pmatrix} \dfrac{m\cos[K_+^L(x_> - L)]\sin[K_+^L(x_< - s_0)]}{\hbar^2 K_+^L \cos[K_+^L(L - s_0)]} & 0 \\ 0 & \dfrac{-m\cos[K_-^L(x_> - L)]\sin[K_-^L(x_< - s_0)]}{\hbar^2 K_-^L \cos[K_-^L(L - s_0)]} \end{pmatrix} , \tag{5.2}$$

since we choose to have the left-hand slab in the normal state. In all cases, we assume that the left-hand slab will be so thick that, since the current [according to Eq. (3.21)] is being probed at L, the boundary conditions at s_0 will have negligible influence. Thus, we take the limit $s_0 \to -\infty$. Since the function in (5.2) is a retarded Green's function, the energy E has a positive imaginary infinitesimal part. Thus

$$\lim_{s_0 \to -\infty} \frac{\sin[K_\pm^L(x_< - s_0)]}{\cos[K_\pm^L(L - s_0)]} = +-ie^{\pm iK_\pm^L(L - x_<)} , \tag{5.3}$$

and therefore, at the energies of interest,

$$g_L(LL) \approx im/\hbar^2 k_{FN} \ . \tag{5.4}$$

Here we have assumed that $K_+^L \approx K^{(L)} \approx k_{FN}$. From Eq. (4.6) we observe that this requires

$$\frac{\hbar^2}{2m}k_{FN}^2 = \mu_\nu = \mu - \frac{\hbar^2 k_\parallel^2}{2m} >> V_L \pm Z_L E$$

($\Omega_L = E$ since L is in the normal state). Except for values of $k_\parallel$ *very* near $k_F = (2m\mu/\hbar^2)^{1/2}$ this is an excellent approximation. As noted in Ref. 7, the dominant values of $k_\parallel$ for tunneling electrons are very near zero, because the effective thickness of the structureless barrier which must be traversed by a tunneling electron increases rapidly as $k_\parallel$ increases, exponentially decreasing the tunneling probability for such electrons. A general form for the Green's function $g_R(RR)$ is

$$g_R(RR) = (m/\hbar^2)(A + B\tau_1 + C\tau_3) \ . \tag{5.5}$$

Now, neglecting terms of second or higher order in $e^{-K(R-L)}$, we obtain

$$\Gamma(LR) \approx (2m/\hbar^2)[g_L(LL) + g_B(LL)]^{-1} \times g_B(LR)[g_R(RR) + g_B(RR)]^{-1} \ , \tag{5.6}$$

$$\Gamma(RL) = \Gamma(LR)^\dagger \ .$$

Using (5.1), (5.4), and (5.5), we obtain the "tunneling matrix"

$$\Gamma(LR) = -(4e^{-K(R-L)}/K)(i/k_{FN} - 1/K\tau_3)^{-1} \times \tau_3[A + (C - 1/K)\tau_3 + B\tau_1]^{-1} \ . \tag{5.7}$$

Now, from Eqs. (3.19) and (5.5),

$$\rho_R(RR) = -2\,\mathrm{Im}g_R(RR)' = -(2m/\hbar^2)\,\mathrm{Im}(A + B\tau_1 + C\tau_3) \ , \tag{5.8}$$

and, from (5.4),

$$\rho_L(LL) = \begin{cases} -2m/\hbar^2 k_{FN}, & k_\parallel < k_F \\ 0, & k_\parallel > k_F \end{cases} , \tag{5.9}$$

V. TUNNELING CURRENT: EXAMPLES

Using the technique described in Sec. IV, one may construct the Green's function for the barrier of width $R - L$. The results are given in (2.20) and (2.21). Assuming that $K_\pm(R - L) \approx K(R - L) >> 1$ for the energies of interest, we find

$$g_B(RR) = g_B(LL) \approx -(m/\hbar^2 K)\tau_3 \ ,$$
$$g_B(RL) = g_B(LR) \approx -(2m/\hbar^2 K)e^{-K(R-L)}\tau_3 \ . \tag{5.1}$$

Referring to the expression just after (2.21), one observes that the approximate equality of K_+ and K_- requires $V - \mu_\nu$ to be much greater than E, the energy of interest (measured relative to the equilibrium chemical potential μ). The barrier height (i.e., $V - \mu$) is typically of the order of an electron volt or more, while the energies of interest (E) in superconducting tunneling are of the order of phonon energies, so that this approximation is well justified.

The solution for the Green's function of the left-hand slab (D_0) in Fig. 1 is

Using (5.6)–(5.9) in (3.21), we find that the current is given by

$$j(L)=\frac{|e|}{\hbar^2}\int_{-\infty}^{\infty}\frac{dE}{2\pi}\int_0^{k_F}\frac{k_{\parallel}dk_{\parallel}}{(2\pi)^2}T^2\frac{(1/k_{FX}^R)^2+(1/K)^2}{(1/k_{FX})^2+(1/K)^2}\frac{f_L(E)-f_R(E)}{|A^2-B^2-(1/K-C)^2|^2}$$

$$\times\mathrm{Tr}[(1+\tau_3)M_{LR}k_{FX}^R\,\mathrm{Im}(A+B\tau_1+C\tau_3)M_{LR}^{\dagger}]\ , \tag{5.10}$$

where

$$T^2=16e^{-2K(R-L)}k_{FX}k_{FX}^RK^2\times\{(k_{FX}^2+K^2)[k_{FX}^R)^2+K^2]\}^{-1} \tag{5.11}$$

is the transmission coefficient of the barrier, with $k_{FX}^R=[(k_F^R)^2-k_{\parallel}^2]^{1/2}$, k_F^R being the Fermi wave vector of the right-hand layer of Fig. 1, k_F the Fermi wave vector of the left-hand layer. We have also defined

$$M_{LR}\equiv(i/k_{FX}+1/K\tau_3)\tau_3[A-B\tau_1+(1/K-C)\tau_3]\ . \tag{5.12}$$

Using the fact that region D_B is a structureless barrier in the evaluation of (5.10), we obtain for the integrand in (5.10)

$$-T^2[(1/k_{FX}^R)^2+(1/K)^2](mk_{FX}^R/\hbar^2)\times\mathrm{Im}(\mathrm{Tr}\{(1+\tau_3)[g_R(RR)+g_B(RR)]^{-1}\})\times[f_L(E)-f_R(E)]\ . \tag{5.13}$$

The imaginary part of the trace is readily evaluated as

$$(\hbar^2/m)\,\mathrm{Im}\{(A-C+1/K)/[A^2-B^2-(C-1/K)^2]\}\ . \tag{5.14}$$

Using (5.1) and (5.5) we identify

$$A^2-B^2-(C-1/K)^2=(\hbar^2/m)^2\times\det[g_R(RR)+g_B(RR)]$$

Using this result in combination with (5.14) and (5.13) we obtain for (5.10),

$$j(L)=\frac{|e|}{\hbar^2}\int_{-\infty}^{\infty}\frac{dE}{2\pi}\int_0^{k_F}\frac{k_{\parallel}dk_{\parallel}}{(2\pi)^2}T^2(m/\hbar^2)^2k_{FX}^R\,\mathrm{Im}\left[\left(\frac{(1/k_{FX}^R)^2+(1/K)^2}{\det[g_R(RR)+g_B(RR)]}\right)(A-C+1/K)\right][f_L(E)-f_R(E)]\ . \tag{5.15}$$

Now, according to the standard tunneling Hamiltonian[7] theory, the expression in (5.14) should reduce to $2k_{FX}^R\,\mathrm{Im}A$,[8] i.e., the result should be given solely by the *diagonal* part of the Green's function in the superconductor. This means that $\mathrm{Im}C$ must vanish and

$$\det[g_R(RR)+g_B(RR)]=-(m/\hbar^2)^2[(1/k_{FX}^R)^2+(1/K)^2]\ . \tag{5.16}$$

if the standard result is correct.

We have verified (5.16) in two cases. For the normal metal–insulator–superconductor junction, we calculate the Green's function for a semi-infinite superconductor and find that

$$A=i|E|/(k_{FX}^R\Omega_R),\quad B=iE\Delta/(k_{FX}^R\Omega_R|E|),\quad C=0\ , \tag{5.17}$$

which satisfies (5.16).

For a normal metal–insulator–thin-normal-metal-(N) superconductor (S) junction we can also show that (5.16) holds. In this case we solve for the Green's function in the right-hand layer of Fig. 1 by calculating the Green's functions in the thin N layer (of width d) and the semi-infinite S layer.

We assume that the metals N and S are identical except for the strengths of their electron-phonon and Coulomb interactions. Thus, k_F^N, the Fermi wave vector in N, is equal to k_F^S. Using the technique described in Sec. II for $R=L$ [see below Eq. (2.19)], we obtain the Green's function for the double layer. We find[9]

$$(E/|E|)k_{FX}^RcA=(E/\Omega_N)[iF(E)\cos(\Delta K^Nd)+\sin(\Delta K^Nd)]+iG(E)(\Delta_N/\Omega_N)\ , \tag{5.18}$$

$$(E/|E|)k_{FX}^RcB=(\Delta_N/\Omega_N)[iF(E)\cos(\Delta K^Nd)+\sin(\Delta K^Nd)]+iG(E)(E/\Omega_N)\ ,$$

$$C=0,\quad c=iF(E)\sin(\Delta K^Nd)-\cos(\Delta K^Nd)\ ,$$

where

$$F(E)\equiv(E^2-\Delta_S\Delta_N)/\Omega_S\Omega_N\ ,\quad G(E)\equiv E(\Delta_S-\Delta_N)/\Omega_S\Omega_N\ ,\quad \Delta K^Nd\equiv(K_+^N-K_-^N)d\ . \tag{5.19}$$

By simply evaluating $A^2-B^2-(1/K)^2$, one verifies (5.16) in this case.

One might hope that the simple tunneling Hamiltonian result would hold in *all* cases in which only one

of the three metallic layers of Fig. 1 is superconducting. However, a simple extension of the calculation of the *N-S* double-layer Green's function in the above example shows that this hope is *not* realized.

We find that when $k_F^N \neq k_F^S$, i.e., there exists a step potential barrier at the *NS* interface, then the $F(E)$ and $G(E)$ of (5.19) are multiplied by

$$(1-R^2)/(1+R^2) = 2k_F^N k_F^S/[(k_F^N)^2 + (k_F^S)^2] \ , \qquad (5.20)$$

where $1-R^2$ is the transmission coefficient of the step barrier

$$1-R^2 = 4k_F^N k_F^S/(k_F^N + k_F^S)^2 \ . \qquad (5.21)$$

We also have $k_{FY}^R = k_{FY}^N$. Thus, we find that

$$A^2 - B^2 - (1/K)^2 = [4R^2/(1+R^2)^2 - c^2] \times (k_{FX}^N c)^{-2} + (1/K)^2 \ . \qquad (5.22)$$

Even in the normal state, this leads to a "nonstandard" form for the tunneling current. We emphasize that this is *not* a density-of-states effect, but rather an effect arising in the *total transmission coefficient*, involving the interference between waves scattered from two potential barriers: the tunneling barrier *B* and the step potential at the *N-S* interface. The formalism we have developed here has enabled us to treat a problem to which the standard theory could not be applied.

Since, even in a perfect *N-S* contact, there will always exist a step potential barrier, the proximity-effect configuration will in general require use of the general expression (5.15) unless

$$\{K^2/[K^2 + (k_{FX}^N)^2]\} 4R^2/[c(1+R^2)]^2 << 1 \ ,$$

in which case (5.22) reduces to yield the standard result for the tunneling current.

In Fig. 2 we have illustrated a possible configuration for a proximity-effect tunneling sandwich. Using (5.18), (5.19) with the modifications described in (5.20), and (5.22), we have calculated the first and second derivatives of (5.15) normalized by their values in the normal state. In doing, we assumed that T^2 was a very sharply decreasing function of $k_\parallel^2$, so that a good approximation to the $k_\parallel^2$ integral could be obtained by simply evaluating the integrand at $k_\parallel = 0$.

The *S* metal was chosen to be Pb and, for simplicity, we chose $\Delta_N = 0$. The combined effects of finite temperature and modulation voltage smearing were simulated by averaging the results over 1 meV. The energy dependence of $\Delta_S(E)$ was obtained from the experimental results of Rowell and McMillan[7] for tunneling into Pb. We chose to compare the results obtained from the standard tunneling theory with those obtained from the present theory for two values of the reflection coefficient R^2. The ratio

$$(\Delta K^N d/E) \approx (2d/\hbar v_F)$$

was fixed at 0.1 meV^{-1}. For a metal with a Fermi

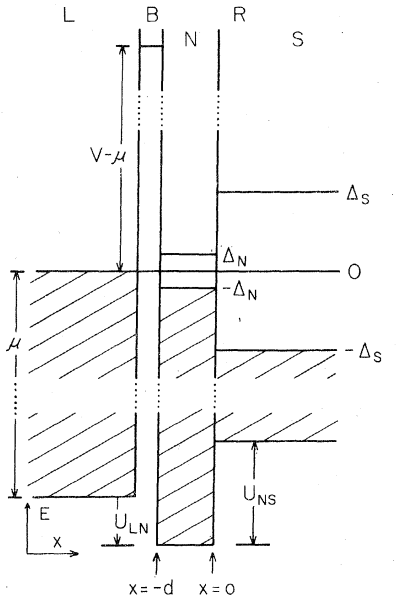

FIG. 2. Proximity-effect tunneling configuration considered in the text. U_{LN} and U_{NS} are the energy differences between the bottom of the conduction band in *N* and the bottom of the conduction band in *L* and *S*, respectively.

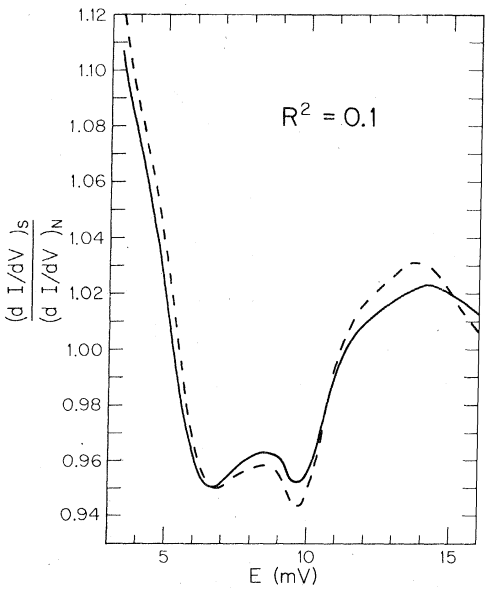

FIG. 3. Normalized first derivative of tunneling current for a reflection coefficient of 0.1. The dashed line is the result of the standard tunneling theory, the solid line the result obtained from Eq. (5.23).

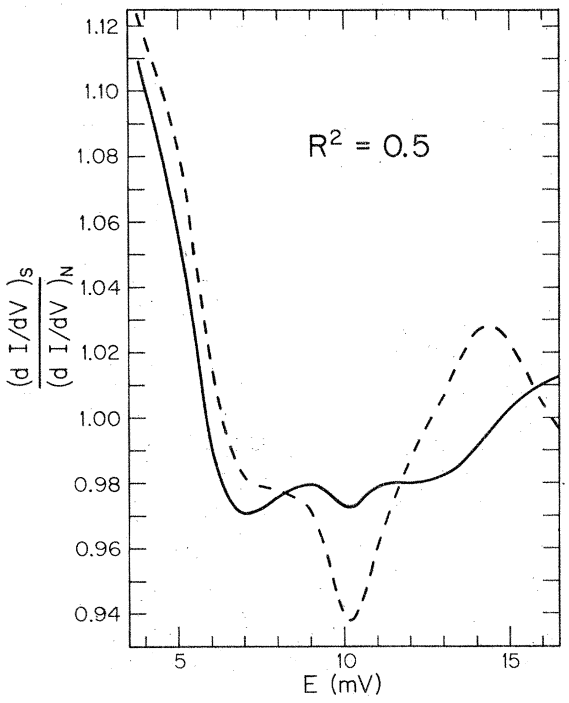

FIG. 4. Normalized first derivative with $R^2=0.5$, comparing result of the present work (solid line) with standard result.

velocity of 10^8 cm/sec, this corresponds to an N layer thickness (d) of about 300 Å. The parameter $(K/k_F^N)^2=(V-\mu)/(\mu+U_{LN})$ (see Fig. 2) was set at 0.5.

In Figs. 3 and 4 we show the results of our calculation of the normalized first derivative with a reflection coefficient of 0.1 and 0.5, respectively. For the smaller coefficient, the deviation of the standard result (dashed line) from the correct result is slight. At the higher coefficient, however, the deviation is pronounced.

In Figs. 5 and 6 we have graphed the normalized second derivative, for completeness, since this is also measured in experiments. Here we observe, more clearly than in the first derivative results, that the deviation of the standard result (dashed line) from the correct result increases with increasing energy, and tends to damp the phonon structure arising from the energy dependence of $\Delta_S(E)$.

We thus conclude that for a significant amount of reflection, the effective transmission coefficient tends to damp the structure which appears in the local density of states at the barrier–N-layer interface. Since the result of the standard theory is that the normalized first derivative is equal to this local density of states,[7] we find that the standard theory result is incorrect when applied in this situation.

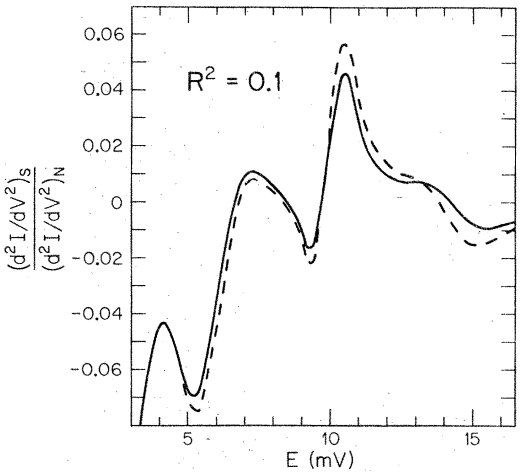

FIG. 5. Normalized second derivative comparison derived from the curves in Fig. 3.

The purpose for introducing the situation pictured in Fig. 2 was to indicate that there is at least one tunneling situation in which the standard tunneling Hamiltonian theory cannot be applied. Further details on the nature of tunneling into NS double layers with a potential barrier at the N-S interface will be deferred to a more complete treatment of proximity-effect tunneling.

VI. CONCLUSION

The Feuchtwang approach for calculating Green's functions for metals in perfectly planar contact has been extended to the superconducting state. The effect of interactions has been accounted for by making a local approximation for the self-energies.

Feuchtwang's approach for calculating the current through a tunnel junction in the normal state has been extended to the superconducting state. We have

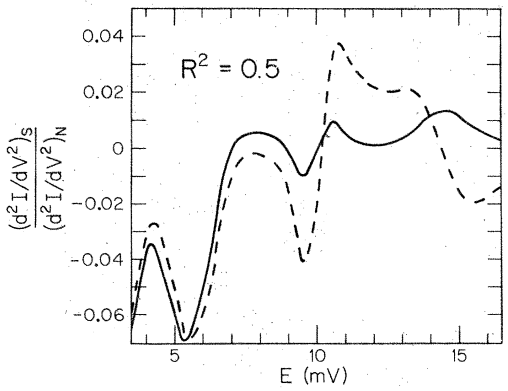

FIG. 6. Normalized second derivative comparison derived from the curves in Fig. 4.

thereby rigorously verified the standard tunneling Hamiltonian expression for the relationship between tunneling current and the local density of states in two cases: metal–insulator–superconductor and metal–insulator–N-S double-layer junctions. In the latter case, we have found that the presence of a step potential at the N-S interface, due to a difference in the height of the common Fermi level above the bottom of the band for the N and S metals, alters the standard result by modifying the effective total transmission coefficient for the whole junction. We conclude, therefore, that future work on proximity-effect tunneling may have to account for this alteration.

ACKNOWLEDGMENT

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[1]T. E. Feuchtwang, (a) Phys. Rev. B 10, 4121 (1974); (b) 10, 4135 (1974); (c) 12, 3979 (1975). In the first of these papers, Feuchtwang gives an illuminating discussion of the standard theory.

[2]G. B. Arnold (unpublished).

[3]L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Benjamin, New York, 1962). See especially Chap. 8.

[4]Y. Nambu, Phys. Rev. 117, 648 (1960).

[5]In Sec. IV, we present details on how these Green's functions are to be calculated.

[6]Two useful references on Green's functions are Ref. 3 above, and A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971).

[7]See, for example, the article by W. L. McMillan and J. M. Rowell, in *Superconductivity*, edited by R. Parks (Marcel Dekker, New York, 1969), Chap. 11, p. 578ff.

[8]Below, when we treat metal–insulator–superconductor tunneling, it will be seen that the factor $2k_{FN}^{R}$ is necessary.

[9]More detail on the calculation of this Green's function is presented in Ref. 2.