Theory of thin proximity-effect sandwiches

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A theory for N-S sandwiches is developed for clean metals in perfect contact, where the thickness of N is much less than that of S. Assuming spatially constant pair potentials in N and S, the exact double-layer Green's function is obtained. From this, we calculate the local density of states at the interface between N and an oxide tunneling barrier. This tunneling density of states is examined in detail and compared with experimental results. We find that at energies far above Δ_N and Δ_S, the local density of states contains a BCS-like term depending on Δ_N, as well as types of oscillatory terms. The pair potential Δ_N also leads to an energy gap, but produces no BCS behavior at Δ_N. A large peak in the local density of states is found at the energy corresponding to a one-dimensional bound state in N. Between this bound state and the pair potential in S, no states exist. Qualitative agreement with experiment is demonstrated over wide energy regions, but quantitative agreement is unsatisfactory below Δ_S; sharp structure appearing near Δ_S in the experimental second harmonic signal (d^2V/dI^2) is also inadequately explained by the present theory. We make further use of the double-layer Green's function in obtaining the self-consistency conditions for the two pair potentials. Considering the possibility of extracting detailed information on the electron-phonon interaction in N from existing experiments, we conclude that the present theory must be modified in several respects, most notably by including normal scattering at the N-S interface.

I. INTRODUCTION

There has been much theoretical work on proximity-effect sandwiches in the Ginzburg-Landau regime. It is our intention to investigate these sandwiches where the Ginzburg-Landau theory *cannot* be applied, i.e., where at least one of the order parameters is large. We choose to consider a thin clean N metal in perfect contact with a thick clean S metal. The thickness of the S metal is taken to be greater than its bulk coherence length. Assuming the Fermi velocities of N and S to be identical, we therefore require the thickness of N to be at least an order of magnitude *less* than this length. For simplicity, we assume that when both N and S are normal, the transmission coefficient of the N-S interface is unity.

This paper is based on the approach presented by McMillan.[1] We have modified his work by allowing for the possibility of a pair potential in N, and restricting the N layer to be of finite thickness d. Reference 1 was primarily concerned with the magnitude of interference-effect oscillations found by Tomasch[2] and Rowell[3] in the tunneling density of states of N-S sandwiches. This work is designed to describe the tunneling density of states of N-S sandwiches, where the tunneling barrier is placed against N, which is backed by S, rather than vice versa.

We consider three phenomena in N-S sandwiches: (i) the pair potential induced by N; (ii) interference phenomena for energies above the pair-potential difference at the N-S interface; and (iii) bound states in N below the pair potential in S.

As pointed out in Ref. 1, for a superconductor, the excited states are mixtures of "quasielectron" and "quasihole" states described by a two-component wave function (we suppress the spin variable)

$$\begin{bmatrix} u(x) \\ v(x) \end{bmatrix}, \tag{1.1}$$

$u(x)$ being the electron and $v(x)$ being the hole amplitude. The quasiparticle obeys the strong coupling analog of the Bogolyubov equations[1]

$$[(-\hbar^2/2m)\nabla^2 - \mu]u(x) + \Sigma_{11}(x)u(x) + \Sigma_{12}(x)v(x) = Eu(x), \tag{1.2}$$

$$-[(-\hbar^2/2m)\nabla^2 - \mu]v(x) + \Sigma_{22}(x)v(x) + \Sigma_{21}(x)u(x) = Ev(x), \tag{1.3}$$

where $\Sigma(x)$ is the symmetric two-by-two matrix self-energy for the quasiparticle, assumed to be local in space. Note that when $\Sigma_{12}(x)$ and $\Sigma_{21}(x)$ vanish, these equations reduce to two separate equations: one for quasielectrons and the other for quasiholes. The crucial ingredient of superconductivity is the mixing of the quasielectrons and the quasiholes. As pointed out in Ref. 1, this mixing is understood to be a consequence of the possibility of the pairing of a quasiparticle above the Fermi sea with one below, leaving a holelike excitation. The quasiparticle in a superconductor is therefore an admixture of electronlike and holelike wave functions.

As is well known, the interaction which produces superconductivity arises from a difference of an attractive electron-phonon interaction at low ener-

gies and a repulsive Coulomb pseudopotential interaction. In a normal metal, there is no mixing between quasielectrons and quasiholes. Hence the self-energy is diagonal. In a superconductor, however, a quasielectron-quasihole mixing occurs. This in turn leads to $\Sigma_{12}(x)$ and $\Sigma_{21}(x)$. The theory is thus by nature a self-consistent one.

With these remarks, one can explain the genesis of a pair potential in N. Assume initially that there is a pair potential in $S(\Delta_S)$, but none in N. By assumption, this means that $\Sigma_{12}(x)$ and $\Sigma_{21}(x)$ vanish in N. As Andreev[4] has pointed out, a normal quasielectron incident on an interface between N and S will be reflected from this interface as a quasihole. That is to say, the incoming quasielectron is paired by the pair potential *at the interface* (Δ_S) with a quasielectron beneath the Fermi sea, leaving behind a reflected quasihole.

This local scattering potential at the N-S interface thus provides a means by which quasielectrons in N may mix with quasiholes in N. One may picture a quasielectron emitting a phonon in N, for example, and reflecting off Δ_S as a quasihole, which then absorbs that phonon. This mechanism provides the necessary quasielectron-quasihole admixture even when N would otherwise by normal. Therefore, *the presence of a pair potential at the N-S interface necessarily tends to induce a pair potential in N.* Full self-consistency for the pair potential in the N-S double layer must be maintained, however, so that while S influences N, we have N also influencing S, leading to a smaller pair potential in S at the interface. If N is thin compared to S, however, the effect of N on S is very small.

The manner in which quasiparticles in N are reflected from the difference in pair potential at the N-S interface, $\Delta_S - \Delta_N$, for energies $E > \Delta_S$ leads to two types of interference in the tunneling density of states. McMillan and Anderson[5] showed that a change in the pair potential of a superconductor leads to the interference phenomena observed by Tomasch[2] and Rowell.[3] A quasielectron in N is reflected from $\delta\Delta_N = \Delta_S - \Delta_N$ as a quasihole, and the two interact by means of Δ_N. In Ref. 1, McMillan finds (for $\Delta_S = 0$, i.e., when region S in Fig. 1 is a normal metal and region N is a superconducting metal) that the change in the tunneling density of states due to a change $\delta\Delta_N = -\Delta_N$ in Δ_N is (for $E \gg \Delta_N$):

$$\delta N_T(E) = \mathrm{Re}[(\Delta_N \delta\Delta_N / E^2) I(2Z_N \Omega_N d/\hbar v_F)], \quad (1.4)$$

where $I(y)$ is an oscillatory function of y with decaying amplitude as $\Omega_N = (E^2 - \Delta_N^2)^{1/2}$ increases [see Eq. (4.16)]. The renormalization function $Z_N(E)$ is energy dependent. It depends on the electron-phonon interaction in N [see Eq. (4.17)]. The occurrence of $2d$ in the argument is easy to understand,

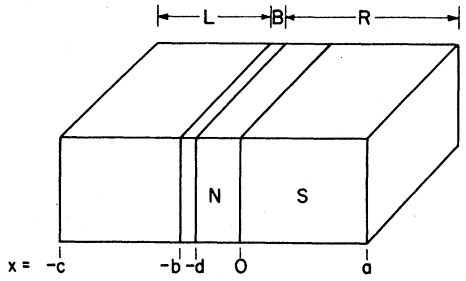

FIG. 1. Tunneling geometry.

since a quasielectron injected at $x = -d$ in N must travel the length of N, reflect as a quasihole at the N-S interface ($x = 0$), and then return to produce the interference via Δ_N. For nonzero Δ_S, with $E \gg \Delta_S$ and Δ_N, we obtain the above result, with $\delta\Delta_N = \Delta_S - \Delta_N$.

Another type of interference phenomenon was described by McMillan and Rowell.[6] A quasielectron injected at $x = -d$ travels to the N-S interface at $x = 0$, reflects as a quasihole, returning to the tunneling interface at $x = -d$. It then reflects normally from this surface as a quasihole, propagates to $x = 0$ again, reflects as a quasielectron, and returns to $x = -d$, producing the interference. A total distance of $4d$ is involved, and two reflections off the pair-potential difference at the N-S interface are required. Note that no quasielectron-quasihole coupling is necessary here. Thus for $E \gg \Delta_S, \Delta_N$, this interference changes the observed tunneling density of states by the factor

$$\delta N_T(E) = \mathrm{Re}\{\tfrac{1}{2}[(\Delta_S - \Delta_N)^2/E^2] I(4Z_N \Omega_N d/\hbar v_F)\}. \quad (1.5)$$

In Ref. 6, it is assumed that $\Delta_N = 0$, and $Z_N = 1$. Otherwise, this expression is identical to Eq. 8 of that work.

Quasiparticles with energies between Δ_N and Δ_S are in a quasi-one-dimensional "potential well" of depth $\Delta_S - \Delta_N$. de Gennes and Saint-James[7] showed that there exists at least one bound state in this potential well (they chose $\Delta_N = 0$). Since the problem is truly three dimensional, the quasiparticle states with wave vectors which are not normal to the N-S interface are also bound, but with effectively larger values of d, hence lower bound-state energies, since the length relevant for quantization of waves traveling off the normal direction is greater. Thus the density of bound states averaged over all angles shows a large peak at each value of the one-dimensional bound-state energies. Below each peak the density of states decreases rapidly until the next one-dimensional bound-state energy is reached. Reference 7 incorrectly indicates that between the highest-energy one-dimensional bound state and Δ_S, some states exist. This is not true,

as we will demonstrate in Sec. IV.

One can now sketch the general shape of the tunneling density of states $N_T(E)$ for a thin N metal backed by a semi-infinite S metal. Suppose that only one bound state exists (thin N metal). If the system were truly one dimensional, $N_T(E)$ would have a δ-function spike at the bound-state energy E_0. As argued above, however, the three dimensionality leads to a peak of finite height at E_0, from which $N_T(E)$ rapidly decreases with decreasing energy. Certainly no states exist below Δ_N, so $N_T(E)$ vanishes below Δ_N. In fact we show in Sec. IV that $N_T(E)$ vanishes below $(\Delta_S\Delta_N)^{1/2}$. In addition, there is no BCS singularity at Δ_N, because the quantization induced on the quasiparticle wave function by the "pair potential well" does not allow a large (so certainly not an infinite) density of states at any energy below E_0. Between E_0 and Δ_S there are no states. At Δ_S there is no reason why the density of states should be infinite, since the tunneling density of states is the local density of states at the tunneling interface (in N). In fact we find that the local density of states vanishes at Δ_S, rising rapidly (with infinite slope at Δ_S) to a peak at an energy slightly above Δ_S. For energies such that $E \gg \Delta_S, \Delta_N$, the local density of states is approximated by unity plus the sum of (1.4) and (1.5). In addition, we find that there is a BCS-like term

$$\mathrm{Re}[\tfrac{1}{2}\Delta_N(E)^2/E^2],$$

due to the pair potential in N. This is exactly what is obtained from an expansion of the bulk strong-coupling density of states when $E \gg \Delta_N(E)$. Far above the "pair potential well," near phonon energies in N, the density of states may be entirely of the bulk strong-coupling form because $Z_N(E)$ may have a substantial positive imaginary part there due to increased phonon scattering. This causes the oscillatory terms to become very small, leaving only the N metal dependence. This fact is propitious for the determination of the energy dependence of $\Delta_N(E)$ near phonon energies in N. Given the correct self-consistent equation for $\Delta_N(E)$, α^2F for N might be obtained by "inverting" this equation, using a technique developed by McMillan and Rowell and applied by them to tunneling into a single S layer.[8]

We have calculated the exact Green's function for the N-S double layer. Assuming that N has thickness d, and S is semi-infinite, we have solved the Bogolyubov equations (1.2) and (1.3). The pair potentials Δ_N and Δ_S, in N and S, respectively, are taken to be spatially independent. The technique by which the double layer Green's function is obtained is outlined in Sec. II and Appendix A. In Sec. III the Green's function is obtained and the one-dimensional bound-state energies are determined for various values of d. In Sec. IV the normalized differential conductance (NDC) for the N-S sandwich is calculated for all energies, and some analytic approximations are employed to sketch the NDC near Δ_S. The next section consists of the results of a computer calculation of the NDC and its derivative for "specular" and "random" tunneling.[1] Some comparison is made with experiments. In Sec. VI the first corrections to the local self-energy are obtained, and agreement with Ref. 1 is demonstrated for $d \to \infty$. Approximations for Δ_N, which are appropriate for thin weak-coupling N metals, are made in Sec. VII, allowing analytic expressions to be obtained for Δ_N at low energies and near phonon energies in N. Consistency of certain approximations made for $\Delta_N(E)$ in this paper is also verified in Sec. VII. In Sec. VIII an approximate result for Δ_S is obtained, and it is shown that, for thin N metals, the spatially dependent correction to the ansatz Δ_S value is negligible. Finally, Sec. IX discusses refinements of the model and the possibility of using tunneling in N-S sandwiches to extract detailed information on the electron-phonon interaction in N (e.g., α^2F in N).

II. PROGRAM FOR THE CALCULATION OF GREEN'S FUNCTION

The Bogolyubov equations for a system which is invariant with respect to translation in the y and z directions may be Fourier transformed to

$$[E - H(x,E)]\begin{pmatrix} u(x,E) \\ v(x,E) \end{pmatrix} = 0, \tag{2.1}$$

where

$$H(x,E) = \left[\frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} - \mu_x\right)\right]\tau_3 + \Sigma(xE), \tag{2.2}$$

$$\Sigma(x,x',E) = \int dy \int dz \int dt\, e^{i\vec{k}_\parallel\cdot(\vec{r}-\vec{r}')+iEt/\hbar} \times \Sigma(x,x',y,z;t), \tag{2.3}$$

$$\vec{k}_\parallel = (0,k_y,k_z), \tag{2.4}$$

$$\mu_x = \mu - \hbar^2 k_\parallel^2/2m. \tag{2.5}$$

The two-by-two matrix self-energy for a quasiparticle $\Sigma(\vec{r},\vec{r}',t)$ is generally a nonlocal function. However, in a bulk system, it is found that the momentum dependence of the self-energy arising from the electron-phonon interaction is negligible near the Fermi momentum p_F.[9] Since the self-energy always is combined with functions which decrease rapidly as the energy deviates from the Fermi energy, only momenta near p_F are important. Therefore, in a translationally invariant system, it is an excellent approximation to treat the self-energy as momentum independent. One therefore has an

effective self-energy which is *local* in space.

Even in a system which lacks translational invariance in one direction, the effective locality of the self-energy should persist, since the momenta of interest are still near the Fermi momentum. We therefore assert that the approximation

$$\Sigma(x,x',E)=\Sigma(x,E)\delta(x-x')$$

is a reasonable one.[10]

In all cases the dependence of functions on k and E will not be indicated unless the possibility of confusion exists. The chemical potential will be denoted by μ, and the Pauli matrices are represented by τ_1, τ_2, and τ_3 in Nambu's notation.[11]

By choosing a particular phase in two-dimensional Nambu space,[11] we can write the matrix self-energy

$$\Sigma(x)=[1-Z(x)]E+X(x)\tau_3+\phi(x)\tau_1. \tag{2.6}$$

In Appendix A, using an approach based on that developed by Feuchtwang,[12] it is shown that the two-by-two matrix Green's function satisfying

$$[E-H(x)]G(x,x')=\delta(x-x') \tag{2.7}$$

for two systems (N and S) in perfect planar contact, can be obtained from the Green's functions for the two separate systems $G_N(x,x')$ and $G_S(x,x')$.

We find that for $x,x'<0$ (in N, see Fig. 1),

$$G(x,x')=G_N(x,x')-G_N(x,0)\times[G_N(0,0)+G_S(0,0)]^{-1}G_N(0,x'). \tag{2.8}$$

The plane of contact is chosen to be at $x=0$. For $x,x'>0$ (in S) we have

$$G(x,x')=G_S(x,x')-G_S(x,0)\times[G_N(0,0)+G_S(0,0)]^{-1}G_S(0,x') \tag{2.9}$$

These equations are strictly correct only when the value of the self-energy chosen for N and S is close to the value of the actual (*self-consistently* determined) self-energy *at the N-S interface* (see Appendix A). We shall rely on making an accurate initial guess for the self-energy in N and S, leaving the deviation from the true self-consistent value (which depends on $G(x,x')$, and therefore on Σ_N and Σ_S) as a small correction. The accuracy of this procedure will be judged by obtaining the first correction to $\Sigma(x)$ in terms of Σ_N and Σ_S, and comparing with the initial guess.

The Green's functions $G_{N,S}(x,x')$ satisfy

$$[E-H_{N,S}(x)]G_{N,S}(x,x')=\delta(x-x'). \tag{2.10}$$

The Hamiltonian in Eq. (2.7) has been separated into two parts

$$H(x)=\begin{cases}H_N(x), & x<0,\\ H_S(x), & x>0.\end{cases} \tag{2.11}$$

The Green's functions G_N and G_S are then obtained for the *isolated* layers N and S, respectively. The boundary conditions on these functions at the N-S interface are chosen to be

$$\left.\frac{dG_{N,S}(x,x')}{dx}\right|_{x=0}=0=\left.\frac{dG_{N,S}(x,x')}{dx'}\right|_{x'=0} \tag{2.12}$$

Feuchtwang has shown[13] that the interface boundary conditions may be chosen in whatever way is convenient. We find that (2.12) is a convenient choice for our problem. At *free* surfaces, the Green's functions must vanish.

As usual, the temporal boundary conditions on the Green's function $G(x,t,x',t')$ may take two forms. If we require the function to vanish for $t<t'$, we obtain the retarded function. In order to define the Fourier transform $G(x,x',E)$, we assume that E possesses a *positive* infinitesimal imaginary part, making the transform regular only in the upper-half complex E plane. Likewise, the Fourier transform of the advanced Green's function (nonvanishing only for $t>t'$) is regular only in the lower-half E plane, since E has a *negative* infinitesimal imaginary part.

III. DOUBLE-LAYER GREEN'S FUNCTION AND BOUND STATES

In Fig. 1 the tunneling geometry is sketched. The metal electrode L is in the normal state throughout the experiment. The metal oxide barrier B separates L from the double layer R. In this geometry one observes the local density of states in the metal N at the interface between B and N (Ref. 8). The metal electrode S is in the superconducting state throughout the experiment. The metal N has a bulk critical temperature less than that of S. All contacts are perfectly planar.

In this section, we will obtain Green's function for the double layer (R). According to Feuchtwang's prescription, we must obtain Green's functions for the separate layers, with appropriate boundary conditions, and then use expressions like Eqs. (2.8) and (2.9) to obtain the Green's function for R.

The most general form for Green's matrix function is[1]

$$G(x,x')=\sum_g d_g\Psi_g(x_>)\Phi_g^\dagger(x_<). \tag{3.1}$$

Here $x_>$ ($x_<$) is the larger (smaller) of the two variables x and x'. The two-dimensional vector wave functions $\Psi_g(x_>)$ and $\Phi_g(x_<)$ satisfy the Bogolyubov equations with the boundary conditions appropriate for, respectively, the right boundary and left boundary of the domain of the equation. The index

g allows for degeneracy in the solutions. The constants d_g are uniquely determined by requiring the satisfaction of the "jump condition" on the first derivative of $G(x,x')$:

$$\tau_3 \frac{dG(x,x')}{dx}\bigg|_{x=x'-\delta}^{x=x'+\delta} = \frac{2m}{\hbar^2} = \tau_3 \frac{dG(x,x')}{dx'}\bigg|_{x'=x-\delta}^{x'=x+\delta}. \tag{3.2}$$

Here, as throughout this paper, δ is a positive infinitesimal.

The initial guess for the self-energy is

$$\Sigma(x) = \begin{cases} (1-Z_N)E + \phi_N \tau_1, & -d < x < 0, \\ (1-Z_S)E + \phi_S \tau_1, & 0 < x < a. \end{cases} \tag{3.3}$$

Since we are interested in the retarded Green's function, E contains a positive infinitesimal imaginary part. With this guess for the self-energy, the Bogolyubov equations in N or S take the form

$$\left[Z_{N,S}E + \left(\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \mu_x\right)\tau_3 - \phi_{N,S}\tau_1\right]\Psi_{N,S}(x) = 0. \tag{3.4}$$

There are two solutions for each energy. The general solutions are

$$\Psi_{N,S}(x) = \begin{bmatrix} u_\pm(x)_{N,S} \\ v_\pm(x)_{N,S} \end{bmatrix} = \begin{bmatrix} [(E \pm \Omega_{N,S})/\Omega_{N,S}]^{1/2} \\ [(E \mp \Omega_{N,S})/\Omega_{N,S}]^{1/2} \end{bmatrix} \times [A\cos(K_\pm^{N,S}x) + B\sin(K_\pm^{N,S}x)], \tag{3.5}$$

where

$$\Omega_{N,S} = (E^2 - \Delta_{N,S}^2)^{1/2}, \tag{3.6}$$

$$K_\pm^{N,S} = (k_{Fx}^2 \pm 2m/\hbar^2 Z_{N,S}\Omega_{N,S})^{1/2}, \tag{3.7}$$

$$k_{Fx}^2 = 2m\mu_x/\hbar^2. \tag{3.8}$$

The boundary conditions on $G_N(x,x')$ are that it have a vanishing derivative with respect to x (or x') at $-d$ and 0. The conditions on $G_S(x,x')$ require a vanishing derivative with respect to x (or x') at 0, but at the free surface (x or $x' = a$) $G_S(x,x')$ vanishes. The two Green's functions are now readily constructed (using the "jump condition")

$$G_N(x,x') = \sum_\pm \frac{\pm m}{\hbar^2 K_\pm^N \sin(K_\pm^N d)} \times \begin{bmatrix} (E \pm \Omega_N)/\Omega_N & \Delta_N/\Omega_N \\ \Delta_N/\Omega_N & (E \mp \Omega_N)/\Omega_N \end{bmatrix} \times \cos(K_\pm^N x_>)\cos[K_\pm^N(x_< + d)], \tag{3.9}$$

$$G_S(x,x') = \sum_\pm \frac{\pm m}{\hbar^2 K_\pm^S \cos(K_\pm^S a)} \times \begin{bmatrix} (E \pm \Omega_S)/\Omega_S & \Delta_S/\Omega_S \\ \Delta_S/\Omega_S & (E \mp \Omega_S)/\Omega_S \end{bmatrix} \times \cos(K_\pm^S x_<)\sin[K_\pm^S(x_> - a)]. \tag{3.10}$$

The calculation of these Green's functions and the calculation of the double-layer Green's function [using Eqs. (2.8) and (2.9)] are sketched in Appendix A.

Throughout this paper we will assume that what occurs at $-c$ and a (see Fig. 1), the free surfaces, has no effect on the observed current, so that the finite-sized sample may be regarded as effectively infinite in extent. Thus the limits $-c \to -\infty$ and $a \to +\infty$ are to be taken. In these limits, the temporal boundary condition on the Green's functions (retarded) automatically leads to the outgoing-wave behavior which is essential for a current-carrying state. For example, the positive infinitesimal imaginary part in E allows one to obtain the limit[14]

$$\lim_{a\to\infty} \sin[K_\pm^S(x_> - a)]/\cos(K_\pm^S a) = \mp i e^{\pm i K_\pm^S x_>}. \tag{3.11}$$

If these limits were not taken, the Dirichlet boundary conditions which were chosen for the Green's functions at the free surfaces would lead to no net current. Also, the case in which the S layer is much thicker than the N layer, corresponds to the experiments with which we will make comparisons in Sec. V.[15]

The results for the double-layer Green's function in this limit are, for $(x,x') < 0$ and $(x,x') > -d$,

$$G_R(x,x') = \sum_\pm \frac{m}{\hbar^2 k_{Fx}} \begin{bmatrix} (E \pm \Omega_N)/\Omega_N & \Delta_N/\Omega_N \\ \Delta_N/\Omega_N & (E \mp \Omega_N)/\Omega_N \end{bmatrix} \begin{bmatrix} A_{N\pm}(x_>) & B_{N\pm}(x_>) \\ B_{N\pm}(x_>) & A_{N\pm}(x_>) \end{bmatrix} \times \cos[K_\pm^N(x_< + d)]/[iF(E)\sin(\Delta K^N d) - \cos(\Delta K^N d)], \tag{3.12}$$

where

$$\Delta K^N = K_+^N - K_-^N; \quad F(E) = \frac{E^2 - \Delta_S\Delta_N}{\Omega_S\Omega_N}, \quad G(E) = \frac{E(\Delta_S - \Delta_N)}{\Omega_S\Omega_N}, \tag{3.13}$$

$$A_{N\pm}(x_>) = iF(E)\cos(K_\pm^N x_> + K_\mp^N d) \mp \sin(K_\pm^N x_> + K_\mp^N d), \tag{3.14}$$

$$B_{N\pm}(x_>) = iG(E)\cos[K_{\mp}^{N}(x_> + d)]; \tag{3.15}$$

for $(x, x') > 0$,

$$G_R(x,x') = \sum_{\pm} \frac{im}{2\hbar^2 k_{Fx}} \begin{bmatrix} (E \pm \Omega_S)/\Omega_S & \Delta_S/\Omega_S \\ \Delta_S/\Omega_S & (E \mp \Omega_S)/\Omega_S \end{bmatrix} \begin{bmatrix} A_{S\pm}(x_<) & B_{S\pm}(x_<) \\ B_{S\pm}(x_<) & A_{S\pm}(x_<) \end{bmatrix} \frac{e^{\pm iK_{\pm}^{S}(x_> - x_<)}}{iF(E)\sin(\Delta K^N d) - \cos(\Delta K^N d)}, \tag{3.16}$$

where

$$\Delta K^S = K_+^S - K_-^S, \tag{3.17}$$

$$A_{S\pm}(x_<) = \cos(\Delta K^N d) + \exp\{\pm[2iK_{\pm}^{S}x_< + i(K_+^N + K_-^N)d]\} - iF(E)\sin(\Delta K^N d), \tag{3.18}$$

$$B_{S\pm}(x_<) = iG(E)\sin(\Delta K^N d)\exp(i\Delta K^S x_<). \tag{3.19}$$

The off-diagonal terms (mixing electronlike and holelike wave functions) in the second matrices of Eqs. (3.12) and (3.16) arise from scattering off the pair-potential difference at the N-S interface.

As a quick check on the result for $(x, x') > 0$, one can take the limit $d \to 0$. It is a straightforward matter to verify that this indeed reduces to $G_S(x, x')$ in the limit $a \to \infty$ [see Eqs. (3.10) and (3.11)].

For $(x, x') < 0$ the denominator of the double layer Green's function exhibits zeros for real energies in the interval $(\Delta_S \Delta_N)^{1/2} < E < \Delta_S$. If we consider only particles moving in the x direction, so that in Eq. (3.7) we can replace k_{FX} by k_F, then this pole of the Green's function occurs when

$$\tan(\Delta K^N d) = \frac{\bar{\Omega}_S \Omega_N}{E^2 - \Delta_S \Delta_N} \approx \tan\left(\frac{2Z_N d\Omega_N}{\hbar v_F}\right), \tag{3.20}$$

where

$$\bar{\Omega}_S = (\Delta_S^2 - E^2)^{1/2}. \tag{3.21}$$

This pole indicates a bound state. For $(x, x') > 0$ (in S), the denominator also vanishes but the bound states decay exponentially as x or x' increases, whereas the states do not decay in N. This can be seen by noting that for $E < \Delta_S$ we can write $K_{\pm}^S = a \pm ib$ where a and b are real, and b is positive. Using (3.16), (3.10) one finds that $G_R(x, x')$ decays exponentially for $E < \Delta_S$. No such decay is found for $G_R(x, x')$ in N at these energies, as long as $E > \Delta_N$.

Because of the gap in the density of states on the S side, particles from the N side with energies less than Δ_S cannot travel very far into the S side. Thus particles in N see an effective one-dimensional potential well of depth $\Delta_S - \Delta_N$. At least one bound state will always be found in N. de Gennes and Saint James[7] have studied these bound states and their contribution to the *total* density of states of an N-S double layer for $\Delta_N = 0$ and $E < \Delta_S$. In Sec. IV the effect of these states on the tunneling density of states (which is a *local* density of states) will be investigated.

Setting $\Delta_N = 0$, it is easy to show by graphical arguments that the number of bound states is given by

$$M = 1 + [R\Delta_S/\pi]. \tag{3.22}$$

Here, we have defined

$$2Z_N dE/\hbar v_F = RE. \tag{3.23}$$

The symbol $[A]$ represents the greatest integer less than A. Thus the relevant parameter for determining the number of bound states is the ratio

$$\frac{R\Delta_S}{\pi} = \frac{2d\Delta_S}{\pi\hbar v_F/Z_N} = \frac{2d}{(\pi^2\xi_S)(Z_N/Z_S)},$$

where ξ_S is the zero-temperature BCS coherence length in S (based on the value of the pair potential at the $N-S$ boundary), and Z_N/Z_S is approximately (for low energies) equal to $(1+\lambda_N)/(1+\lambda_S)$, $\lambda_{S,N}$ being the McMillan parameter for S or N.

A graph of the bound-state energy versus R is given in Fig. 2 with $\Delta_S = 1.4$ mV (roughly the value for bulk Pb) and R ranging from 0.1 to 4.0 mV^{-1}. There is only one bound state for this case, as long as R is less than about 2.24 mV^{-1}. When $1/R$ is more than an order of magnitude greater than

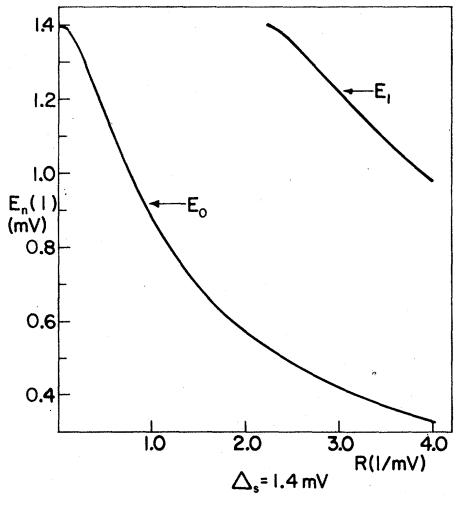

FIG. 2. Dependence of bound-state energies $E_n(1)$ on $R = 2Z_N d/\hbar v_F$.

Δ_S, the bound state is located so close to Δ_S that it cannot be distinguished from Δ_S on the graph.

IV. NORMALIZED DIFFERENTIAL CONDUCTANCE

For normal metals, it is known[8,12] that the tunneling current is proportional to the *local* density of states at the tunneling interface (in our case, at $x=-d$). In Ref. 1, McMillan finds that the NDC is proportional to

$$-\frac{1}{\pi}\,\mathrm{Im}[G_R(-d-d)_{11}] = -\frac{1}{\pi}\,\mathrm{Im}\left(\sum_{E'}\frac{\Psi_{E'}(-d)\Psi^*_{E'}(-d)}{E-E'+i\delta}\right), \quad (4.1)$$

which is the local density of states of the double layer at $x=-d$. Only the 11 component of the Green's function in R is needed. The wave function is the exact normalized wave function for the double layer evaluated at $x=-d$, and the formal sum over E' includes bound states as well as states in the continuum above Δ_S. We will demonstrate in the following that the local density of states exhibits structure arising from bound states below Δ_S as well as from the interference of waves scattering off the pair potential difference at $x=0$, for energies above Δ_S.

Following McMillan in Ref. 1, Eqs. 33 and 37, we assert that the tunneling density of states is given in terms of the imaginary part of the 11 component of G_R at the tunneling interface by

$$N_T(E)=\int_0^1 d(\cos\theta)\,\frac{-1}{\pi}\,\mathrm{Im}G_R(-d-d)_{11} \times D(\cos\theta)(\tfrac{1}{2}\pi\hbar v_{Fx}). \quad (4.2)$$

McMillan defines $D(\cos\theta)$ as "the normalized probability distribution of the tunneling electrons." Since

$$\cos\theta=(1-k_\parallel^2/k_F^2)^{1/2}, \quad (4.3)$$

one may interpret θ as the angle made by the electron k vector in R relative to the normal to the tunneling interface.

It is difficult to give an explicit form of the function $D(1/x)$ $(1/x\equiv\cos\theta)$ since it involves details of the tunneling interface which are not known. Phenomenologically, McMillan has defined this function in two limits: (i) Random tunneling: In this case, all electrons of the same energy have the same probability of penetrating the tunneling barrier, regardless of the angle at which they approach the barrier. McMillan, therefore, chose $D(1/x)=1$ for this case. (ii) Specular tunneling: Because the tunneling interface is assumed to be perfect for this case and the barrier is taken to be a simple rectangular potential barrier, the transmission of electrons with k-vectors normal to the barrier is strongly favored. In this case, McMillan chose $D(1/x)$ $=\beta\exp[\beta(1-x)]$, where β is a large number (~40).

The differential conductance devided by its value when all layers of the sandwich are normal is given by[16]

$$g(V)=\left(\frac{dI}{dV}\right)_S\Big/\left(\frac{dI}{dV}\right)_N = \int_{-\infty}^{\infty} dE\,N_T(E)\,\frac{d}{d(eV)}[f(E)-f(E+eV)] = \int_0^{\infty} dE\,N_T(E)\left(\frac{-df(E-eV)}{dE}-\frac{df(E+eV)}{dE}\right) \quad (4.4)$$

at finite temperature.[17] The magnitude of the electronic charge is e, and V is the applied voltage.

Using Eq. (3.12) we find that

$$(-1/\pi)\,\mathrm{Im}G_R(-d-d)_{11} = (-2/\pi\hbar v_{Fx})\,\mathrm{Im}\{[(E/\Omega_N)[iF(E)\cos(\Delta K^N d)+\sin(\Delta K^N d)]+i(\Delta_N/\Omega_N)G(E)\}/[iF(E)\sin(\Delta K^N d)-\cos(\Delta K^N d)]\}. \quad (4.5)$$

Note that if $\Delta_S=\Delta_N$, then $G(E)$ vanishes, $F(E)$ is unity, and the above result reduces to

$$(2/\pi h v_{FX})\,\mathrm{Re}(E/\Omega_N). \quad (4.6)$$

This must occur because the entire region R is a homogeneous superconductor with order parameter Δ_N.

There are five regions of interest.

(i) $E<\Delta_N$—Here Ω_N and $\Delta K^N d$ are purely imaginary, $F(E)>0$ and real, and $G(E)<0$ and real, so that the denominator has no zeros for real E. Thus the right-hand side of (4.5) vanishes.

(ii) $\Delta_N<E<(\Delta_N\Delta_S)^{1/2}$—Here Ω_N and $\Delta K^N d$ are real, $F(E)$ and $G(E)$ are positive and negative imaginary, respectively, and the denominator in (4.5) has no zeros because $\Delta K^N d$ is positive. Thus the right-hand side of (4.5) vanishes in this case also.

It is interesting to note that there is *no BCS-like singularity* at $E=\Delta_N$ because of the quantization of

quasiparticle energy levels induced by the presence of a larger pair potential Δ_S at the N-S interface. As will be shown below, the density of states shows its first sharp peak at the value of the first bound state in the pair-potential well of depth $\Delta_S - \Delta_N$, and decreases rapidly below this. Thus even though there is a finite pair potential in N, there is no BCS behavior at Δ_N.

(iii) $(\Delta_S\Delta_N)^{1/2} \leq E < \Delta_S$—In this regime, Ω_N and $\Delta K^N d$ are real, and $F(E)$ and $G(E)$ are imaginary. The denominator of (4.5) diverges when

$$\tan(\Delta K^N d) \approx \tan\left(\frac{2Z_N d\Omega_N}{\hbar v_{FX}}\right) = \frac{\bar{\Omega}_S\Omega_N}{E^2 - \Delta_S\Delta_N}. \quad (4.7)$$

Expanding the denominator about the energies which satisfy this relation $[E_m = E_m(\cos\theta)]$, we obtain (see Appendix C for details of the calculation):

$$\frac{-2}{\pi\hbar v_{FX}} \sum_{m=0}^{M} (E_m + \Delta_N) \Big/ \left(\frac{2Z_N d}{\hbar v_{FX}} E_m + \frac{E_m^2 + \Delta_S\Delta_N}{E_m\bar{\Omega}_S}\right) \times \mathrm{Im}(E - E_m + i\delta)^{-1}. \quad (4.8)$$

The integer M is the index of the bound state of maximum energy. In the above expression the energy variations of Z_N, Δ_S, and Δ_N have been neglected. The imaginary parts of these quantities have also been assumed to vanish. These assumptions are correct as long as the metal N is assumed to be clean, because the energies of interest here are far below typical phonon energies in N and S, at which the neglected features should be prominent.

The imaginary part of the denominator in (4.8) is $-\pi\delta(E - E_m(\cos\theta))$. The $\cos\theta$ dependence of the bound-state energies can be used to convert the integration over $\cos\theta$ in (4.2) to an integral over $E_m(\cos\theta)$ using

$$\cos\theta = \frac{R\Omega_N}{m\pi + \arctan[\bar{\Omega}_S\Omega_N/(E_m^2 - \Delta_S\Delta_N)]} \equiv \frac{R\Omega_N}{m\pi + \phi(E_m)} \quad (4.9)$$

[the $m\pi$ in this equation arises from the possibility of multiple solutions for $\Delta K^N d$ in (4.7)], and

$$\frac{d\cos\theta}{dE_m} = R\left(\frac{E_m}{\Omega_N}[m\pi + \phi(E_m)] + \frac{(E_m^2 + \Delta_S\Delta_N)}{E_m\bar{\Omega}_S}\right) \Big/ [m\pi + \phi(E_m)]^2, \quad (4.10)$$

where $\bar{\Omega}_S$ and Ω_N are evaluated at $E = E_m$. We thus obtain, using the δ function

$$N_T(E) = \pi R \sum_{m=0}^{M} \left(\frac{E + \Delta_N}{[m\pi + \phi(E)]^2}\right) \times D\left(\frac{R\Omega_N}{m\pi + \phi(E)}\right) \Theta(E_m(1) - E). \quad (4.11)$$

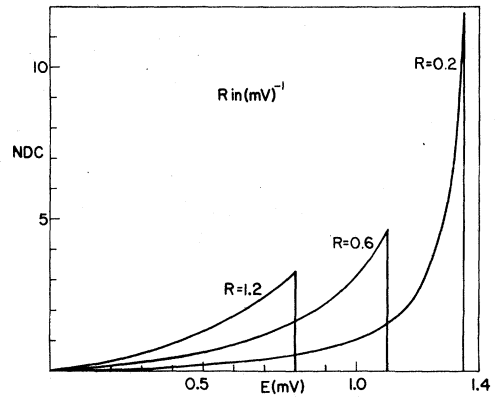

FIG. 3. NDC as a function of energy for $E < \Delta_S = 1.4$mV in the random tunneling model for three values of R.

The energies $E_m(1)$ are the solutions to equation (2.20), which is just equation (3.7) with $v_{FX} = v_F\cos\theta = v_F$. The unit step function $\Theta(E_m(1) - E)$ vanishes for $E > E_m(1)$.

This result differs from that of de Gennes and Saint-James[7] who have (for $\Delta_N = 0$) an extra factor $1 + \bar{\Omega}_S/[m\pi + \phi(E)]$ and implicitly take $D(\cos\theta) = 1$ for all θ. The difference can be traced to the fact that we calculate a *local* density of states at the tunneling interface, whereas Ref. 7 calculates a *total* density of states.

In Fig. 3 we show the local density of bound states for $\Delta_N = 0$, $R = 0.6$ and 1.2. We have set the function $D(\cos\theta)$ equal to unity. This corresponds to McMillan's "random tunneling" approximation. In the "specular tunneling" case, where $D(\cos\theta)$ is sharply peaked at $\cos\theta = 1$, one expects to see a steeper rise in $N_T(E)$ as the bound state energy is approached from below; below $E_0(1)$, $D(R\Omega_N/[m\pi + \phi(E)])$ becomes exponentially small. In the random tunneling case, the only thickness-dependent quantities are R and $E_0(1)$. Thus graphs for other values of R may easily be constructed from those shown once the bound state energy is determined.

Equation (4.10) may be used to determine the value of $E_0(1)$ as $R \to 0$ since $E_0(1)$ satisfies

$$\arctan\left(\frac{[\Delta_S^2 - E_0^2(1)]^{1/2}[E_0(1)^2 - \Delta_N^2]^{1/2}}{E_0(1)^2 - \Delta_S\Delta_N}\right) = R[E_0(1)^2 - \Delta_N^2]^{1/2}.$$

Since we know that as $R \to 0$, $E_0(1) \to \Delta_S$, we write

$$E_0(1) = \Delta_S(1 - \epsilon), \epsilon \ll 1.$$

Thus we have

$$(2\epsilon)^{1/2} = R(\Delta_S - \Delta_N),$$

which yields

$$E_0(1) = \Delta_S[1 - \tfrac{1}{2}R^2(\Delta_S - \Delta_N)^2]. \quad (4.12)$$

Near $E_0(1)$, the variation of $N_T(E)$ can be obtained by letting $E = E_0(1)(1-y)$, where $y \ll 1$. Then

$$\phi(E) \approx \frac{[R^2(\Delta_S - \Delta_N)^2 + 2y]^{1/2}(\Delta_S^2 - \Delta_N^2)^{1/2}}{\Delta_S - \Delta_N},$$

so that, near $E_0(1)$,

$$N_T(E) \approx \pi D(1)[R(\Delta_S - \Delta_N)]/[R^2(\Delta_S - \Delta_N)^2 + 2y].$$

Thus the value of $N_T(E_0(1))$ for $R(\Delta_S - \Delta_N) \ll 1$ (i.e., for thin N metals) is

$$N_T(E_0(1)) = \pi D(1)/R(\Delta_S - \Delta_N). \tag{4.13}$$

As d approaches zero, therefore, $N_T(E)$ shows an increasingly sharp maximum at $E_m(1)$, which is very near Δ_S. Experimentallly, as the N metal is made thinner, one should rapidly attain the point at which the density of states due to the bound state in N (where $\Delta_N = 0$) cannot be distinguished from the onset of the density of states, due to a BCS superconductor of energy gap $\sim\Delta_S$ in the presence of thermal smearing. To show this, we must also calculate the density of states for energies at and above Δ_S.

(iv) $\Delta_S \leq E$—Above Δ_S, a continuum of energies contributes to the tunneling density of states. Far below typical phonon energies in N and S, the imaginary parts of Z_N, Δ_N, and Δ_S are negligible, so that Eq. (4.5) reduces to

$$\frac{-1}{\pi}\,\mathrm{Im}G_R(-d-d)_{11} = \frac{(2E\Omega_S/\pi\hbar v_{FX})[E^2 - \Delta_S\Delta_N + \Delta_N(\Delta_S - \Delta_N)\cos(\Delta K^N d)]}{\Omega_S^2\,\Omega_N^2 + E^2(\Delta_S - \Delta_N)^2\sin^2(\Delta K^N d)}. \tag{4.14}$$

The most striking fact about this result is that it *vanishes* for $E = \Delta_S$ ($\Omega_S = 0$). However, for small $\Delta K^N d$, one observes a sharp peak just above Δ_S. The vanishing at Δ_S is due to our assumption that the N and S metals are perfectly coupled, meaning that, in the normal state of S, the transmission coefficient at the interface is unity. For strongly coupled N and S layers, at finite temperature, we expect [on the basis of (4.14)] that the NDC will exhibit a "dip" near Δ_S, and a maximum at the bound state in N, as well as at an energy just above Δ_S.

Consider the value of (4.14) near $E = \Delta_S$ for $\Delta K^N d = R(\Delta_S^2 - \Delta_N^2)^{1/2}/\cos\theta \ll 1$. Letting

$$E = \Delta_S(1+\epsilon),$$

where $\epsilon \ll 1$, we find, upon substitution of (4.14) into (4.2), that

$$N_T(\Delta_S(1+\epsilon)) \cong \int_0^1 \frac{d(\cos\theta)D(\cos\theta)(2\epsilon)^{1/2}}{2\epsilon(1+C/\cos^2\theta) + \Gamma^2(1+C)/\cos^2\theta},$$

where

$$C = [(2\Delta_S^2 - \Delta_N^2)/(\Delta_S^2 - \Delta_N^2)]R^2(\Delta_S - \Delta_N)^2 \ll 1,$$

assuming that Δ_N is much less than Δ_S. Also, we define

$$\Gamma^2(1+C) = R^2(\Delta_S - \Delta_N)^2.$$

In expanding the trigonometric functions, we have assumed that the dominant contributions to the $\cos\theta$ integral occur near $\cos\theta = 1$. This amounts to taking $D(\cos\theta)$ to be a very rapidly-decreasing function as $\cos\theta$ varies from 1 to 0 (specular tunneling). The integral may be evaluated approximately by replacing $\cos\theta$ by unity. We find

$$N_T(\Delta_S(1+\epsilon)) \approx D(1)(2\epsilon)^{1/2}/(2\epsilon + \Gamma^2).$$

This is a maximum at

$$\epsilon = \Gamma^2/2 \ll 1,$$

where it has the value

$$D(1)/2R(\Delta_S - \Delta_N).$$

The ratio of the tunneling density of states at $E_0(1)$ [Eq. (4.13)] to this value at the maximum just above Δ_S is equal to 2π. For specular tunneling, therefore, when $R(\Delta_S^2 - \Delta_N^2)^{1/2} \ll 1$ (thin N metals), the maximum at the first bound state is more than *six* times the maximum located just above Δ_S. Clearly, for random tunneling, the ratio would be even larger.

For thin N metals we conclude that, slightly above Δ_S, there is a peak in $N_T(E)$ of width $\Gamma \approx R(\Delta_S - \Delta_N) \ll 1$. The shape of $N_T(E)$ for a thin N metal near $E = \Delta_S$ is illustrated in Fig. 4 (note the scale of the abscissas) for $R = 0.02$, $\Delta_S = 1.40$, $\Delta_N = 0$, and random tunneling. The slope of $N_T(E)$ at Δ_S is infinite [this may be shown using (4.14)].

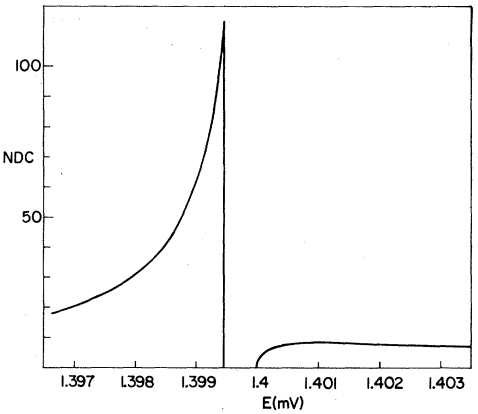

FIG. 4. NDC near $\Delta_S = 1.4$ mV for $R = 0.02$ mV^{-1}. (Note horizontal scale.)

(v) $\Delta_S \ll E$—At energies far above Δ_S, Eq. (4.5) may be evaluated very generally by retaining only the lowest-order nontrivial dependence on Δ_S and Δ_N. Insertion of this approximation into Eq. (4.2) yields the following form for $N_T(E)$:

$$N_T(E) \approx 1 + \tfrac{1}{2}\,\mathrm{Re}(\Delta_N^2/E^2) + \tfrac{1}{2}\,\mathrm{Re}\{[(\Delta_S - \Delta_N)^2/E^2]I(2R\Omega_N)\} + \mathrm{Re}\{[\Delta_N(\Delta_S - \Delta_N)/E^2]I(R\Omega_N)\}. \quad (4.15)$$

The second factor in this equation is exactly what one would obtain for tunneling into a bulk superconductor with pair potential $\Delta_N(E)$, i.e., the first term in the expansion of the bulk strong-coupling density of states for $E \gg \Delta_N$. This is remarkable because, as observed above, there is no BCS-like singularity at Δ_N. The explanation for this is that, far above the step-like pair-potential difference, the N metal behaves more like a bulk superconductor since, at these energies, the step potential can be treated as a perturbation.

When performing calculations in the preceding, we have chosen to set $\Delta_N = 0$ in all cases, for simplicity. Our motivation for this arises from the implicit assumption that N is a relatively weak coupling material. As we will show below, for such a material, $\Delta_N(E)$ is negligible at energies far below the typical phonon energies of N. Near phonon energies in N, however, $\Delta_N(E)$ exhibits structure due to the rapid onset of virtual phonon emission.[18] Thus the appearance of the second term in (4.15) is encouraging to one who might wish to extract information on the phonon density of states and the electron-phonon interaction in N from proximity effect tunneling. We shall discuss this possibility in Sec. IX.

The integral $I(y)$, which occurs in the third and fourth terms of (4.15), was considered by McMillan in Ref. 1:

$$I(y) = \int_1^\infty \frac{dx}{x^2}\, D\!\left(\frac{1}{x}\right) e^{iyx} \quad (4.16)$$

For either form of the angular distribution probability, $D(1/x)$, $I(y)$ is an oscillatory function of its argument. Even for real y, the amplitude of these oscillations decays. If y has an imaginary component, the decay becomes quite rapid.

Recalling that $R = 2Z_N d/\hbar v_F$, one observes that the third term in (4.15) arises from the "4d oscillations" of McMillan and Rowell.[6] As discussed in Sec. I, these require two reflections off the pair-potential difference $\Delta_S - \Delta_N$ at the N-S interface [hence $(\Delta_S - \Delta_N)^2$] and arise from the interference of an incoming particlelike wave with its thrice-reflected outgoing particlelike wave. The fourth term in (4.15) arises from the "2d oscillations" of Tomasch[2] and Rowell,[3] which require only one reflection from $\Delta_S - \Delta_N$. The incoming particle-like wave may interfere with the outgoing holelike wave in this case, because Δ_N couples the two and allows them to interfere.

The renormalization parameter Z_N also shows structure at the phonon energies of N. This parameter has the form

$$Z_N(E) = 1 - (1/E)[M_N(E) - i\Gamma_N(E)], \quad (4.17)$$

where $M_N(E)$ is the modification of the quasiparticle energy due to electron-phonon interaction, and $\Gamma_N(E)$ is the damping of the quasiparticle excitation due to this interaction. Thus from the period and decay of the 2d and 4d oscillations, one may be able to extract further information on the electron-phonon interaction in N.

There are inherent difficulties in such an extraction, however, because of the presence of the angular distribution probability $D(1/x)$ in the oscillatory terms. As we stated above, this function is not known. If the tunneling barrier is regarded as structureless, i.e., a simple potential barrier of height V_B, then the "specular tunneling" case definitely holds, and electrons with $\vec{k}$ vectors normal to the tunneling interface ($\cos\theta = 1/x = 1$) will be the dominant ones selected by the tunneling process.

However, as Dowman, MacVicar, and Waldram[19] point out, the real case may be more complicated. The $\vec{k}$ vectors selected by $D(1/x)$ depend on selection rules which, even for perfect insulator-metal interfaces, may select groups of electrons with $\vec{k}$ vectors having significant components *parallel* to the interface. Since

$$k_{FX} = (2m\mu_x/\hbar^2)^{1/2} = [2m(\mu - \hbar^2 k_\parallel^2/2m)/\hbar^2]^{1/2},$$

the observed period and damping of the oscillations, which are inversely proportional to k_{FX}, may be considerably *increased* by selection rules at the tunneling interface which favor electrons with nonzero $k_\parallel$ values over electrons with $k_\parallel = 0$. The extraction of information from the oscillations is affected by these occurrences.[20] It is encouraging to note that no such difficulties appear in the extraction of information from the second term in (4.15).

Finally, in this section we wish to make contact with McMillan's results in Ref. 1, specifically, Eq. (40). Since he chose to treat two semi-infinite regions with $\Delta_S = 0$,[21] we must evaluate Eq. (4.5) in the limit $d \to \infty$. Since E contains a positive infinitesimal imaginary part, ΔK^N contains such a part, so that, as $d \to \infty$, we keep only the $\exp(-i\,\Delta K^N d)$ in each sine or cosine. One readily finds

$$\frac{-1}{\pi}\,\mathrm{Im}G_R(-d-d)_{11} = \frac{2}{\pi\hbar v_{FX}}\,\mathrm{Re}\left(\frac{E}{\Omega_N}-\frac{\Delta_N e^{i\Delta K^N d}}{(E+\Omega_N)}\right).$$

Since $\Delta_N/(E+\Omega_N) = (E-\Omega_N)/\Delta_N$, we have obtained Eq. (40) of Ref. 1, as required.

V. COMPUTER RESULTS FOR NDC WITH THIN WEAK-COUPLING N METALS

A compact expression[22] for the quantity in Eq. (4.5) is obtained by defining

$$\tan(i\zeta) = i\Omega_S\Omega_N/(E^2-\Delta_S\Delta_N) = -(iF)^{-1}, \tag{5.1}$$

and hence also

$$\sin(i\zeta) = -(iG)^{-1}.$$

Then we have

$$\frac{-1}{\pi}\,\mathrm{Im}G(-d-d)_{11} = \frac{-2}{\pi\hbar v_{FX}}\,\mathrm{Im}\left(\frac{E}{\Omega_N}\cot(\Delta K^N d+i\zeta) + \frac{\Delta_N}{\Omega_N}\csc(\Delta K^N d+i\zeta)\right) \tag{5.2}$$

and $N_T(E)$ is

$$N_T(E) = \int_0^1 d(\cos\theta)D(\cos\theta)\left[-\mathrm{Im}\left(\frac{E}{\Omega_N}\cot(\Delta K^N d+i\zeta) + \frac{\Delta_N}{\Omega_N}\csc(\Delta K^N d+i\zeta)\right)\right]. \tag{5.3}$$

For simplicity, we will assume that $\Delta_N(E) \ll \Delta_S(E)$ at the energies of interest in this section. These energies are from 1.4 to about 20 mV, where $\Delta_S(E)$ shows significant structure (we take Pb as the S metal). In Sec. VII we will show that for thin weak-coupling N metals, the assumption that $\Delta_N(E) \ll \Delta_S(E)$ for the chosen energy range is reasonable. In the following, therefore, we shall set $\Delta_N(E)$ equal to zero. In addition, we will always use the approximation for $\Delta K^N d$ indicated in Eq. (4.7).

For the random tunneling model, after making the above-described approximations, we transform the integral in Eq. (5.3) by changing integration variable to $y = (RE/2\pi)(1-\cos\theta)/\cos\theta$:

$$N_T(E) = \int_0^1 dy\,\frac{RE}{2\pi}\psi^{(1)}\left(\frac{RE}{2\pi}+y\right)\left[-\mathrm{Im}\cot(2\pi y + RE + i\zeta)\right]. \tag{5.4}$$

The trigamma function $\psi^{(1)}(x)$ is defined by[23]

$$\psi^{(1)}(x) = \sum_{n=0}^{\infty}(n+x)^{-2}. \tag{5.5}$$

Using the tabulated values of this function, we evaluate (5.4) numerically.

In the case of specular tunneling, we have simply evaluated the integral in (5.3) at $\cos\theta = 1$. This corresponds to allowing only those electrons with k vectors normal to the tunneling interface to be transmitted.

At zero temperature, the NDC is equal to $N_T(E = \mathrm{eV})$. Experimentally, one also measures the second derivative $(d^2I/dV^2)_S$, and divides by the value in the normal state $(d^2I/dV^2)_N$. This is proportional to the first derivative of $N_T(E)$. Below, we examine results for $N_T(E)$ and its derivative $N_T'(E)$ in the specular and random tunneling models for various values of $R = 2Z_N d/\hbar v_F$.

A. Specular tunneling

In Fig. 5 is displayed a comparison of the extra structure produced by the energy variation of $\Delta_S(E)$ in $N_T(E)$ for a proximity effect sandwich with $R = 0.02$ (solid lines) and for the bulk strong-coupling density of states (dashed lines). The featureless curves are the results for $\Delta_S(E) = 1.4$ mV at all energies.

As $d \to 0$, Eq. (4.5) reduces to $(2/\pi\hbar v_{FX})\,\mathrm{Re}(E/\Omega_S)$. This gives the bulk result for $N_T(E)$. Thus the dashed curves may be regarded as the $R = 0$ limits of the solid curves.

Note that the featureless curves are rather insensitive to the value of R, compared to the curves

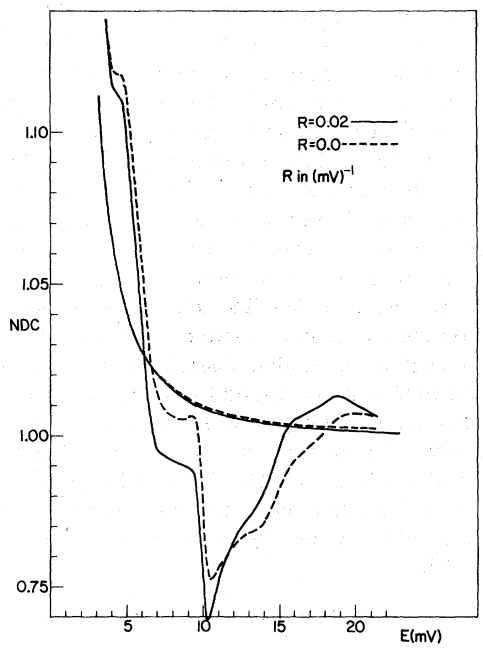

FIG. 5. Comparison of NDC curves with and without structure due to energy dependence of $\Delta_S(E)$ (S = Pb) for two values of R in the specular tunneling model.

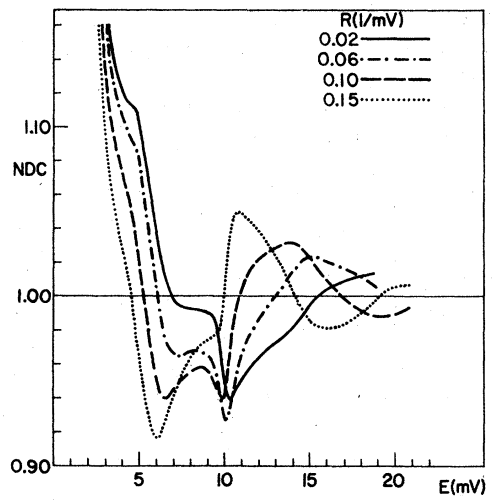

FIG. 6. Change in the structure of NDC curves with increasing R for specular tunneling.

with structure. The structure has shifted to slightly lower energies in going from $R = 0$ to $R = 0.02$. Further evidence of the extreme sensitivity to R is presented in Fig. 6 (note scale change). The structure continually shifts to lower energies as R increases, and the shape of the curve alters radically.

The curves for $N'_T(E)$ when $R = 0$ exhibit minima at the dominant phonon energies of Pb shifted upward by the Pb energy gap (~1.4 mV).[18] These energies are 4.5 and 8.5 mV for the transverse- and longitudinal-acoustical Pb phonons, respectively. The curves of Fig. 7 show that for $R = 0.02$, the minima are nearly at the values expected for $R = 0$ with a gap of 1.4 mV. For $R = 0.06$, the position of the upper minimum has decreased by about 0.3 mV, while the lower minimum has dropped by 1 mV. Succeeding values of R do not produce any appreciable lowering of the position of the lowest minimum, while the position of the higher minimum continues to decrease.

Experiments (see Ref. 15) indicate that the three peaks do shift to lower positions, but that the very narrow peak at the higher energy gradually decreases in height compared to the central peak, while the lower energy peak *increases*. These experimental observations do *not* agree with the results in Figs. 5–7. We therefore believe that the strict selection rule on k vectors implied by the specular model is not applicable to the experiments in Ref. 15.

B. Random tunneling

This case represents the other extreme, as far as tunneling selection rules are concerned, since it corresponds to the complete absence of *any* selection rule.

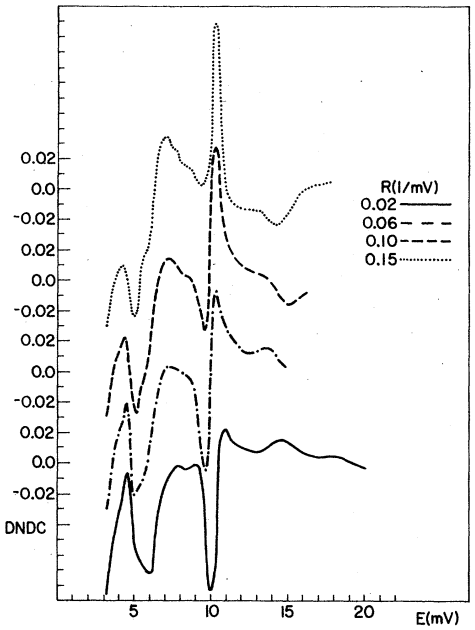

FIG. 7. First derivative of the NDC (DNDC) for various values of R with specular tunneling.

In Fig. 8 one observes that even the structureless curve is significantly modified in the random tunneling case. Again, we also observe the sensitivity to R of the shape and position of the structure in

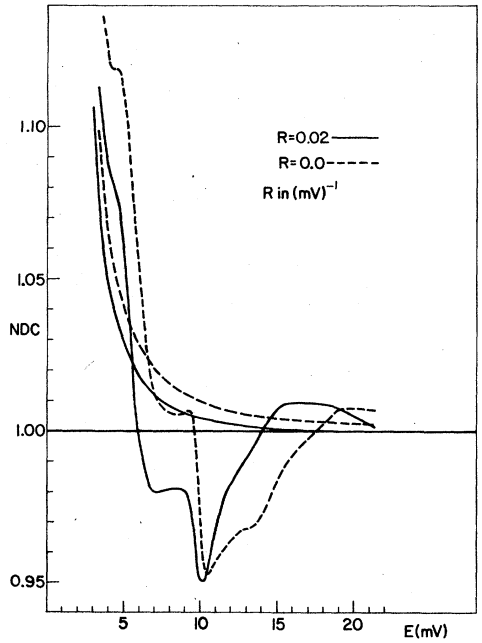

FIG. 8. Comparison of NDC curve with and without structure due to energy dependence of $\Delta_S(E)$ (S = Pb) for two values of R in the random tunneling model.

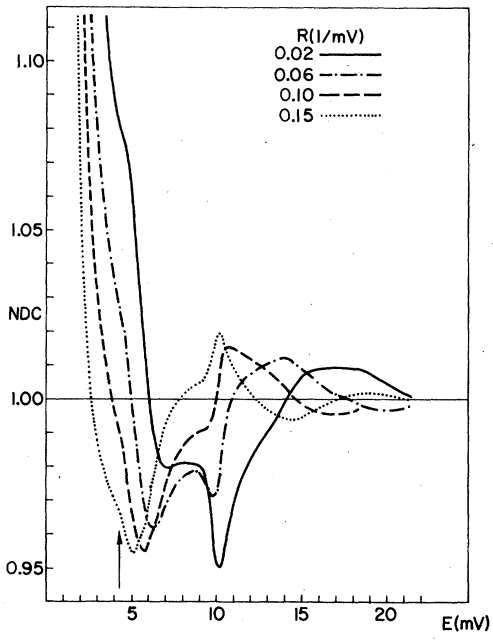

FIG. 9. Change in the structure of NDC curves with increasing R for random tunneling.

the curves which include the energy variation of $\Delta_S(E)$. In Fig. 9, $N_T(E)$ is plotted for various values of R. Note that the scale is twice magnified above that of Fig. 6. The trend of the variation of the structure is just that of Fig. 6.

In Fig. 10, one begins to see the effects of the

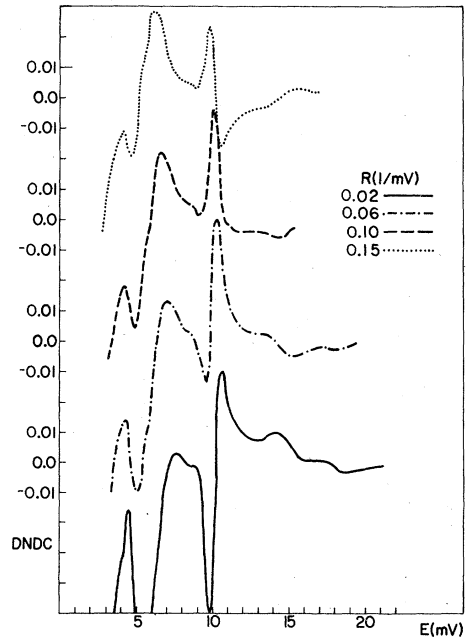

FIG. 10. First derivative of the NDC (DNDC) for various values of R with random tunneling.

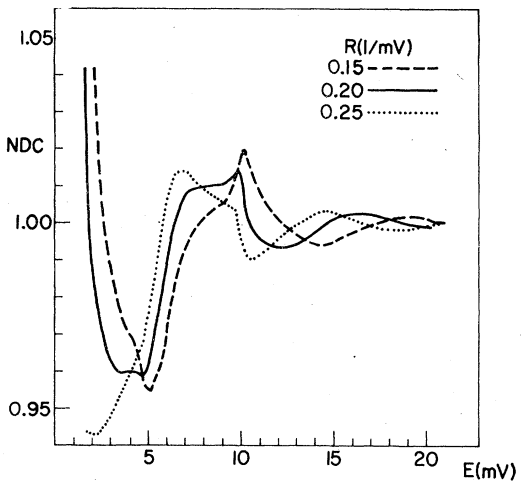

FIG. 11. NDC for higher values of R and random tunneling, showing the movement of the first local minimum to lower energies.

absence of selection rules in the more sensitive $N'_T(E)$ results. The two higher-energy peaks are varying in accordance with the experimental[15] observations: the highest-energy peak is decreasing in size compared to the central peak. The lowest-energy peak is also increasing in magnitude, though it is becoming less sharp.

From Fig. 9 one observes that the lower-energy peak for $R = 0.15$ in Fig. 10 arises from a "kink" in $N_T(E)$ at about 4.2 mV (see arrow). As R increases, this kink approaches the position of the first local minimum in $N_T(E)$ (at about 5 mV for $R = 0.15$). It is interesting to see what happens to this kink as R continues to increase. In Figs. 11 and 12, therefore, we have displayed $N_T(E)$ and its first derivative for larger values of R, ranging from $R = 0.15$ to $R = 0.25$. At $R = 0.2$, the kink coincides with the first minimum. Note in Fig. 12 that the first peak in $dN_T(E)/dE$ is now *positive*. At $R = 0.25$, the kink has progressed beyond the first minimum, making $N'_T(E)$ even more positive. Also note in Fig. 12 that the highest-energy peak continues to decrease as k increases, while the central peak varies little in height, but shifts slightly to lower energies.

In the experimental case, the curves in Fig. 10 would be smeared out somewhat due to finite temperature and modulation-voltage effects. The modulation voltage used in Ref. 15 is ~1 mV rms. A reasonably good approximation of the smearing effects is obtained by averaging the curves over an interval of about 2 mV. An interval of this size roughly accounts for both thermal- and modulation-voltage effects (see Ref. 15). In addition to these modifications, one must account for the fact that the experiments actually measure d^2V/dI^2. As

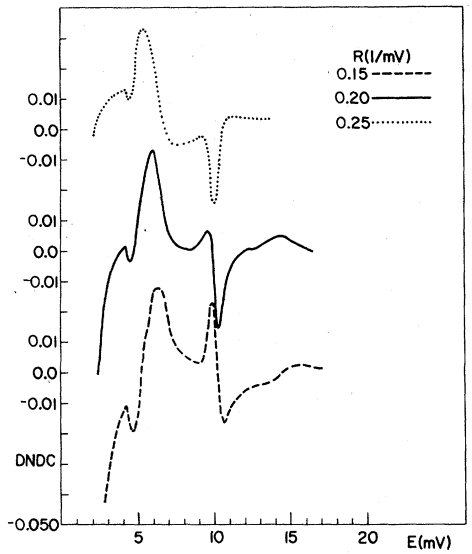

FIG. 12. First derivative of the NDC (DNDC) for higher values of R and random tunneling.

shown in Ref. 15, to a good approximation this is given by

$$\frac{d^2V}{dI^2} \propto \frac{N_T'(eV)}{[N_T(eV)]^3}.$$

In Fig. 13, we have plotted the right-hand side of the above expression averaged over a 2 mV interval centered at eV. The two higher-energy peaks show the expected behavior as R increases, but the lowest-energy peak gradually disappears.

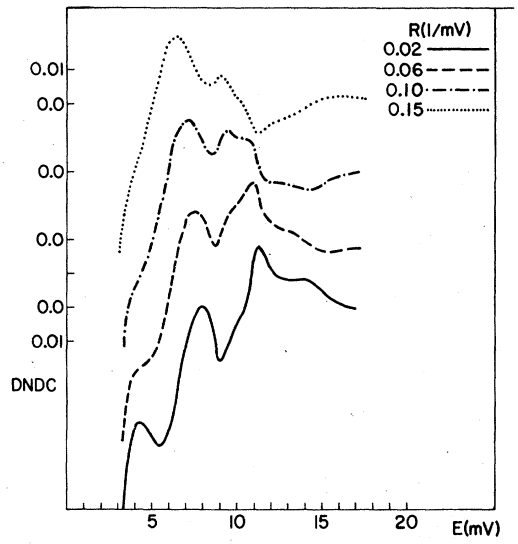

FIG. 13. First derivative of the NDC (DNDC) divided by the NDC cubed, and averaged over a 2-mV interval to give the experimentally measured d^2V/dI^2 for various values of R.

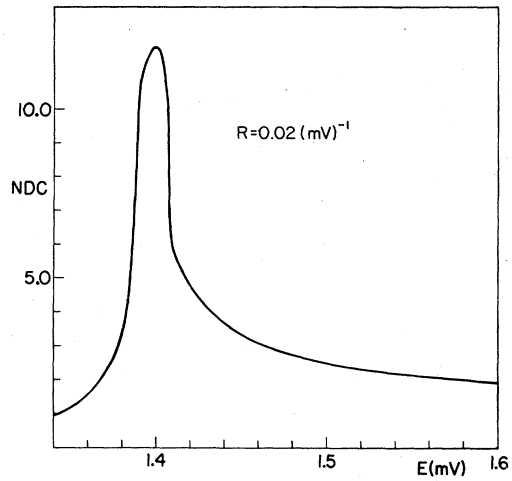

FIG. 14. NDC for $R = 0.02$ mV^{-1} averaged over an interval of 0.02 mV.

A comparison of these results with Figs. 2, 3, and 4 of Ref. 15 indicates that, while the theory can probably fit the central- and high-energy behavior, the lowest-energy peak cannot be fit. Necessary refinements of the model examined here will be discussed in Sec. IX.

To conclude this section, we compare our results for the NDC near Δ_S (=1.4 mV) with the experimental observations of Freake[24] on Cu-Pb proximity effect sandwiches at temperatures between 0.06 and 0.11 °K, Freake found that the NDC exhibited a dip between 1.1 and 1.4 mV before rising to a broad peak at lower energies. For a Cu sample of about 250 Å thickness, the dip did not appear, but at 540 Å thickness and more, the dip was pronounced (see Fig. 2 of Ref. 24).

We find that the qualitative features of the data can be explained by our results. In Figs. 14 and 15 we display the NDC, calculated from Eqs. (4.4) and (3.11) for random tunneling. We have averaged

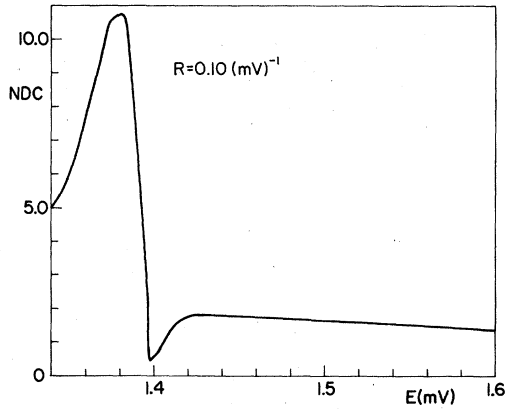

FIG. 15. NDC for $R = 0.10$ mV^{-1} averaged over an interval of 0.02 mV.

our results over an interval of 0.02 mV, which corresponds to the stated resolution of the experiments of Ref. 24. For $R = 0.02$, which corresponds to a Cu thickness of slightly less than 100 Å, we observe a fairly sharp peak near Δ_S, and no dip. For $R = 0.10$, a Cu thickness of about 500 Å, we observe the appearance of the dip just below Δ_S. Clearly, this dip arises from the absence of states between the bound state in N and Δ_S. For very thin N metals, the gap in the NDC cannot be resolved because the bound state is too close to Δ_S. As the N metal thickness increases, the bound-state energy decreases, and the gap widens until it surpasses the resolution. The peak of the NDC occurs slightly below the bound-state energy (allowing for resolution), and decreases in magnitude as R increases, in accordance with the results shown in Fig. 3.

Though we have obtained qualitative agreement with the results of Ref. 24, we are far from quantitative agreement. The structures we have derived in Figs. 14 and 15 are much sharper than the corresponding ones of the experiments, and the size of the peak at the bound-state energy is too great. However, we suspect that these features are sensitive to the degree of normal scattering at the N-S interface, which should decrease the amplitude of the bound-state peak, and smear out sharp structure. We have neglected such scattering in this work, although it is definitely present, even with perfect contact between N and S. In Sec. IX, we will speculate further on those factors which may bring our theory closer to quantitative agreement with experiment.

VI. FIRST CORRECTIONS TO THE LOCAL SELF-ENERGY

The local self-energy is determined via the equation

$$\Sigma(x) = [1 - Z(x)]E + \phi(x)\tau_1 = \int_0^\infty dE' \int_{-\infty}^{\infty} \frac{d^2k_\parallel}{(2\pi)^2} \left(\frac{-\operatorname{Im} G(x,x,E')}{\pi}\right) \times \frac{2(\pi\hbar)^2 K_\pm(E,E',x)}{mk_F} . \tag{6.1}$$

The kernels $K_\pm(E,E',x)$ are given by

$$\begin{aligned} K_\pm(E,E',x) = \int_0^\infty d\nu\, \alpha^2(\nu,x)F(\nu,x)\{&[N(\nu)+f(-E')][(E'+E+\nu)^{-1} \pm (E'-E+\nu)^{-1}] \\ &\mp [N(\nu)+f(E')][(-E'+\nu+E)^{-1} \pm (-E'+\nu-E)^{-1}]\} \\ &- \mu^*(x)\Theta(E_B(x)-E')[f(\mp E') - f(E')] . \end{aligned} \tag{6.2}$$

The plus sign applies to the off-diagonal, and the minus sign to the diagonal part of $\Sigma(x)$. This expression is semiphenomenological in nature, being based on the corresponding expression for bulk materials.[18] The local average electron-phonon interaction (squared) times the local phonon density of states is

$$\alpha^2(\nu,x)F(\nu,x) = \begin{cases} \alpha_N^2(\nu)F_N(\nu), & x \in N , \\ \alpha_S^2(\nu)F_S(\nu), & x \in S . \end{cases} \tag{6.3}$$

The local Coulomb pseudopotential is

$$\mu^*(x) = \begin{cases} \mu_N^*, & x \in N , \\ \mu_S^*, & x \in S . \end{cases} \tag{6.4}$$

The energy $E_B(x)$ is a local value of the cutoff energy for the local Coulomb pseudopotential equal to E_{BN} in N and E_{BS} in S. Both of these energies are presumed to be an order of magnitude greater than the Debye energies in N or S.[25]

The symmetry of the matrix quantity in large parentheses in Eq. (6.1) [cf. Eq. (3.12)] yields

$$Z(x) = 1 - \frac{1}{E}\int_0^\infty dE' \left[\frac{d^2k_\parallel}{(2\pi)^2}\right] \left(\frac{-\operatorname{Im} G(x,x,E')_{11}}{\pi}\right) \frac{2(\pi\hbar)^2 K_-(E,E',x)}{mk_F} , \tag{6.5}$$

$$\phi(x) = \int_0^\infty dE' \int \left(\frac{d^2k_\parallel}{(2\pi)^2}\right) \left(\frac{-\operatorname{Im} G(x,x,E')_{12}}{\pi}\right) \frac{2(\pi\hbar)^2 K_+(E,E',x)}{mk_F} . \tag{6.6}$$

In both equations, the Green's function contains terms which oscillate like $\exp(\pm 2ik_F x)$. These will introduce rapidly varying contributions to $\Delta(x) = \phi(x)/Z(x)$. Presumably, however, full self-consistency for $\Delta(x)$ with respect to its spatial dependence will suppress such rapid variations. If one considers the effect of these terms on the values of $Z(x)$ and $\phi(x)$ *averaged* over x in region N, the terms which rapidly oscillate are smaller than the other terms by a factor of E/E_F. These terms will accordingly be neglected. This

being done, one obtains from Eq. (3.12) (See Appendix B for details of the derivation)

$$Z_N(x)=1-\frac{1}{E}\int_0^\infty dE'\int_0^1 d(\cos\theta)\left[-\mathrm{Im}\left(\frac{E'}{\Omega_N}\cot(\Delta K^N d+i\zeta)\right)-\mathrm{Im}\left(\frac{\Delta_N}{\Omega_N}\cos[\Delta K^N(x+d)]\right.\right.$$
$$\left.\left.\times\csc(\Delta K^N d+i\zeta)\right)\right]K_-(E,E')_N, \tag{6.7}$$

$$\phi_N(x)=\int_0^\infty dE'\int_0^1 d(\cos\theta)\left[-\mathrm{Im}\left(\frac{\Delta_N}{\Omega_N}\cot(\Delta K^N d+i\zeta)\right)-\mathrm{Im}\left(\frac{E'}{\Omega_N}\cos[\Delta K^N(x+d)]\right.\right.$$
$$\left.\left.\times\csc(\Delta K^N d+i\zeta)\right)\right]K_+(E,E')_N \tag{6.8}$$

for the self-energy in N. The self-energy in S is obtained from Eq. (3.16) (see Appendix B)

$$Z_S(x)=1-\frac{1}{E}\int_0^\infty dE'\left[\mathrm{Re}\frac{E'}{\Omega_S}-\int_0^1 d(\cos\theta)\,\mathrm{Re}\left(\frac{\Delta_S\sin(\Delta K^N d)\,e^{i\Delta K^S x}}{[\Omega_S\sin(\Delta K^N d+i\zeta)]}\right)\right]K_-(E,E')_S, \tag{6.9}$$

$$\phi_S(x)=\int_0^\infty dE'\left[\mathrm{Re}\frac{\Delta_S}{\Omega_S}-\int_0^1 d(\cos\theta)\,\mathrm{Re}\left(\frac{(E'/\Omega_S)\sin(\Delta K^N d)\,e^{i\Delta K^S x}}{\sin(\Delta K^N d+i\zeta)}\right)\right]K_+(E,E')_S. \tag{6.10}$$

The quantity ζ is defined by Eq. (5.1).

Now we will examine the limit as $d\to\infty$. This limit exists in virtue of the positive imaginary infinitesimal part of E (and therefore of ΔK^N, ΔK^S) as mentioned previously. One obtains

$$Z_N(x)=1-\frac{1}{E}\int_0^\infty dE'\left[\mathrm{Re}\frac{E'}{\Omega_N}-\int_0^1 d(\cos\theta)\,\mathrm{Re}\left(\frac{\Delta_N e^{-i\Delta K^N x-\zeta}}{\Omega_N}\right)\right]K_-(E,E')_N, \tag{6.11}$$

where

$$e^{-\zeta}=\exp\left[-\tfrac{1}{2}\ln\left(\frac{(E')^2-\Delta_S\Delta_N+\Omega_S\Omega_N}{(E')^2-\Delta_S\Delta_N-\Omega_S\Omega_N}\right)\right]=\frac{E'(\Delta_S-\Delta_N)}{(E')^2-\Delta_S\Delta_N+\Omega_S\Omega_N},$$

$$\phi_N(x)=\int_0^\infty dE'\left[\mathrm{Re}\frac{\Delta_N}{\Omega_N}+\int_0^1 d(\cos\theta)\,\mathrm{Re}\left(\frac{E'e^{-i\Delta K^N x-\zeta}}{\Omega_N}\right)\right]K_+(E,E')_N, \tag{6.12}$$

$$Z_S(x)=1-\frac{1}{E}\int_0^\infty dE'\left[\mathrm{Re}\frac{E'}{\Omega_S}-\int_0^1 d(\cos\theta)\,\mathrm{Re}\left(\frac{\Delta_S e^{i\Delta K^S x-\zeta}}{\Omega_S}\right)\right]K_-(E,E')_S, \tag{6.13}$$

$$\phi_S(x)=\int_0^\infty dE'\left[\mathrm{Re}\frac{\Delta_S}{\Omega_S}-\int_0^1 d(\cos\theta)\,\mathrm{Re}\left(\frac{E'e^{i\Delta K^S x-\zeta}}{\Omega_S}\right)\right]K_+(E,E')_S. \tag{6.14}$$

In McMillan's (zero-temperature) theory (Ref. 1), Δ_N is chosen to be zero *at all energies* as an initial ansatz, and d is taken to be infinite. Since the theory was not concerned with describing phonon structure arising from the energy dependence of the kernel near typical phonon energies, McMillan used the fact that the dominant contributions to all the energy integrals occur at low energy. For this reason, he set E and E' equal to zero in the kernels, and introduced a cutoff E_{co} on the E' integrals (assuming the cutoff to be the same in N as in S). In this way he obtained the equations (the energy dependence of the self-energy functions is explicitly indicated, for clarity)

$$\Delta_S(x,E=0)=\frac{\phi_S(x,E=0)}{Z_S(x,E=0)}=\lambda_S^*(x)\int_0^{E_{co}}dE'\int_0^1 d(\cos\theta)\,\mathrm{Re}\left[\frac{\Delta_S}{\Omega_S}-\frac{E'\Delta_S}{\Omega_S(E'+\Omega_S)}\exp\left(\frac{-2i\Omega_S x}{\hbar v_F\cos\theta}\right)\right], \tag{6.15}$$

$$\Delta_N(x,E=0)=\lambda_N^*(x)\int_0^{E_{co}}dE'\int_0^1 d(\cos\theta)\,\mathrm{Re}\left[\frac{E'-\Omega_S}{\Delta_S}\exp\left(\frac{2iE'x}{\hbar v_F\cos\theta}\right)\right]. \tag{6.16}$$

Here

$$\lambda_{S,N}^*(x)=K_+(0,0)_{S,N}/Z_{S,N}(x,0).$$

is a dimensionless coupling parameter. The above equations correspond respectively to Eqs. (51) and (53) in Ref. 1. Taking $x\to -x$ in Eqs. (6.12) and (6.14) (our geometry is the reverse of McMillan's) with $\Delta_N=0$, and employing McMillan's approximations for the kernels, one finds agreement with (6.15) and (6.16) since, under these operations

$$(E'/\Omega_N)e^{-i\Delta K^N x-\zeta} \to [\Delta_S/(E'+\Omega_S)]\exp(+2iE'x/\hbar v_F\cos\theta),$$

with $\Delta_S/(E'+\Omega_S)=(E'-\Omega_S)/\Delta_S$ in (6.12), yielding (6.16), while in (6.14):

$$(E'/\Omega_S)e^{i\Delta K^S x-\zeta} \to [E'\Delta_S/\Omega_S(E'+\Omega_S)]\exp(-2i\Omega_S x/\hbar v_F\cos\theta),$$

yielding (6.15). Note that the $E=0$ limit of $Z_{S,N}$ is well-defined because the kernel $K_-(E,E')_{S,N}$ approaches zero linearly in E as E goes to zero [see (6.2)].

VII. PAIR POTENTIAL IN N FOR THIN WEAK-COUPLING N METALS

We have already shown above (Sec. IV) that a pair potential Δ_N may exist in N without giving rise to any density of states for $\Delta_N<E<(\Delta_{S0}\Delta_N)^{1/2}$, where Δ_{S0} is the value of $\Delta_S(E)$ at $E=\Delta_S(E)$. This novel feature of proximity-effect tunneling is a consequence of the quantization of quasiparticle energy levels which is forced on the N layer by the existence of a positive pair-potential difference at the N-S interface. There is an energy gap between $E=0$ and $E=(\Delta_{S0}\Delta_N)^{1/2}$, but there is no BCS singularity at the gap edge. Instead, the density of states rises from zero at $(\Delta_{S0}\Delta_N)^{1/2}$ to a maximum at the bound-state energy $E_0(1)$, as shown in Fig. 3.

We shall consider only thin[26] weak-coupling N metals. In the integrals of (6.7) and (6.8), the most important energies are low energies (near Δ_{S0}), where the density of states exhibits sharp peaks. For weak-coupling materials, it is reasonable to assume that energies of the order of Δ_{S0} are far below typical phonon energies. Since the maximum values of $\Delta_N(E)$ will occur near the phonon energies in N, and since N is a weak coupling material, we therefore expect that for low energies $\Delta_N(E)$ will be negligible compared to $\Delta_S(E)$. At *higher energies* (phonon energies in N) we expect that this will *not* be true, but these energies have little weight in the E' integral. Neglecting $\Delta_N(E')$ in the integrals of (6.7) and (6.8) leaves

$$Z_N(x)=Z_N=1-\frac{1}{E}\int_0^\infty dE'\int_0^1 d(\cos\theta)\,[-\mathrm{Im}\cot(\Delta K^N d+i\zeta)]K_-(E,E')_N\ , \tag{7.1}$$

$$\phi_N(x)=\int_0^\infty dE'\int_0^1 d(\cos\theta)\left[-\mathrm{Im}\left(\frac{\cos[\Delta K^N(x+d)]}{\sin(\Delta K^N d+i\zeta)}\right)K_+(E,E')_N\right]. \tag{7.2}$$

The order parameter in N is given by

$$\Delta_N(x)=\phi_N(x)/Z_N(x). \tag{7.3}$$

The spatial variation of $\phi_N(x)$, which predicts that $\phi_N(x)$ *increases* as x approaches the tunneling interface ($x=-d$), is spurious. It arises from the fact that we have not solved for the Green's function of the *entire* tunneling geometry (including the L region and the B region in Fig. 2). Certainly, were we to take into account the influence of the other regions, we would find that $\Delta_N(x)$ near $x=-d$ would be depressed from its value at $x=0$, just as we will find that $\Delta_S(x)$ is depressed from the ansatz (bulk) value Δ_S at $x=0$. For thin N metals, however, any spatial variation of $\Delta_N(x)$ is suppressed, because such a variation over a small distance would lead to a large free-energy contribution. Since we wish to treat thin N metals, where $\Delta_N(x)$ is not expected to vary much, we shall therefore calculate an *average* of $\Delta_N(x)$ over the width of N.

Averaging the ratio of (7.2) and (7.1):

$$\Delta_N=\frac{1}{d}\int_{-d}^0\Delta_N(x)\,dx=\frac{1}{Z_N}\int_0^\infty dE'\int_0^1 d(\cos\theta)\left[-\mathrm{Im}\left(\frac{\sin(\Delta K^N d)}{(\Delta K^N d)\sin(\Delta K^N d+i\zeta)}\right)K_+(E,E')_N\right]. \tag{7.4}$$

Unless $\cos\theta\lesssim R\Delta_{S0}\ll 1$, we may approximate $\sin(\Delta K^N d)/\Delta K^N d$ by unity ($\Delta K^N d\approx RE'/\cos\theta$) since the dominant values of E' are near Δ_{S0} and $R\Delta_{S0}\ll 1$. The values of $\cos\theta\lesssim R\Delta_{S0}$ account for a negligible fraction of the total integration range of $\cos\theta$. Furthermore, over most of these values of $\cos\theta$, $\sin(\Delta K^N d)/\Delta K^N d$ oscillates rapidly, giving a small total contribution. We may therefore safely neglect the region where $\sin(\Delta K^N d)/\Delta K^N d$ is not equal to unity in (7.4). Again, there are two regimes for the energy integration

(i) $E'<\Delta_{S0}$—Here we find the bound state $E_0(\cos\theta)$. (We assume that the N metal is thin enough that only one exists.) Expanding about the

bound-state energy $[E_0 = E_0(\cos\theta)]$:

$$-\mathrm{Im}[\csc(\Delta K^N d + i\zeta)] = \frac{\pi\delta(E' - E_0)E_0}{\arctan(\bar{\Omega}_{S0}/E_0) + E_0/\bar{\Omega}_{S0}}, \tag{7.5}$$

where $\bar{\Omega}_{S0} = [\Delta_{S0}^2 - (E')^2]^{1/2}$, implicitly evaluated here at $E' = E_0$. One obtains this equation by using (C.4) and (C.7) of Appendix C in Eq. (B.4) of Appendix B, setting $\Delta_N = 0$, and recognizing that $\arctan(\bar{\Omega}_{S0}/E_0) = 2Z_N dE_0/\hbar v_{FX}$.

Changing the integration variable from $\cos\theta$ to $E_0(\cos\theta)$ using Eqs. (4.9) and (4.10) for $\Delta_N = 0$, we obtain the bound state contribution

$$\frac{1}{Z_N}\int_0^{E_0} dE' \frac{\pi R E' K_+(E,E')_N}{[\arctan(\bar{\Omega}_{S0}/E')]^2}. \tag{7.6}$$

In order to check the accuracy of our guess for $\Delta_N(E)$ at low E, we calculate $\Delta_N(0)$. Since the important E' variations of the kernels $K_\pm(0E')_N$ are only in the vicinity of $E' = \hbar\omega_N$, where $\hbar\omega_N$ is a typical phonon energy in N, and since the dominant contributions to the integral are at low energies, $E' \approx \Delta_{S0} \ll \hbar\omega_N$, we set (following McMillan)[25]

$$K_+(0,E')_N \approx \lambda_N^* \tanh(\tfrac{1}{2}\beta E')\Theta(E_{CN} - E') \quad K_-(0,E')_N \approx 0, \tag{7.7}$$

where λ_N^* is defined by Eq. (6.17). Thus at $E = 0$, we have $Z_N \approx 1$.

Changing the variable in (7.6) from E' to $y = \arctan(\bar{\Omega}_{S0}/E')$, we obtain [with (7.7)]:

$$\tfrac{1}{2}\pi\lambda_N^* R\Delta_{S0}^2 \int_{RE_0}^{\pi/2} \frac{dy(\sin 2y)\tanh[(\cos y)\tfrac{1}{2}\beta\Delta_{S0}]}{y^2}. \tag{7.8}$$

In the limit $RE_0(1) \ll 1$, this is approximately

$$\lambda_N^* \pi R \Delta_{S0}^2 \ln[1/RE_0(1)]. \tag{7.9}$$

Assuming that $\lambda_N^* \lesssim 0.05$ (λ^* for Pb is about 0.48) and that $RE_0(1) = R\Delta_{S0} \lesssim 0.1$, we find that this is less than or equal to about $0.04\Delta_{S0}$. Thus for thin metals ($RE_0(1) \approx R\Delta_{S0} \ll 1$) the assumption that $\Delta_N \ll \Delta_{S0}$ is correct as far as the contribution from bound states is concerned. The remaining contribution will be considered next. (ii) $\Delta_{S0} \lesssim E'$— Since the most important contributions to the E' integral in (6.4) are at low energies, we will neglect the energy dependence of $\Delta_S(E)$, setting $\Delta_S(E) = \Delta_{S0}$ and $\Delta_N = 0$. Using

$$\csc(\Delta K^N d + i\zeta) = \frac{\Delta_{S0}}{E' \sin(\Delta K^N d) + i\bar{\Omega}_{S0}\cos(\Delta K^N d)} \tag{7.10}$$

we obtain

$$\frac{1}{Z_N}\int_{\Delta S0}^{\infty} dE' \int_0^1 d(\cos\theta)\left(\frac{\Delta_{S0}\bar{\Omega}_{S0}\cos(\Delta K^N d)}{\bar{\Omega}_{S0}^2 + \Delta_{S0}^2\sin^2(\Delta K^N d)}\right) \times K_+(E,E')_N \tag{7.11}$$

for the contribution to $\Delta_N(E)$ in this regime. With the approximation in (7.7), this becomes

$$\lambda_N^*\Delta_{S0}\int_{\Delta_{S0}}^{E_{CN}} dE' \int_0^1 d(\cos\theta)\left(\frac{\Omega_{S0}\cos(\Delta K^N d)}{\bar{\Omega}_{S0}^2 + \Delta_{S0}^2\sin^2(\Delta K^N d)}\right) \times \tanh\tfrac{1}{2}\beta E'. \tag{7.12}$$

Choosing $k_B T \ll \Delta_{S0}$, the hyperbolic tangent may be replaced by unity. This integral is then less than or equal to

$$\lambda_N^*\Delta_{S0}\,\mathrm{arccosh}\left(\frac{E_{CN}}{\Delta_{S0}}\right) \cong \lambda_N^*\Delta_{S0}\ln\left(\frac{2E_{CN}}{\Delta_{S0}}\right), \tag{7.13}$$

which is the result in the limit $R \to 0$. Using the zero-temperature BCS value of Δ_{S0}:

$$\Delta_{S0} = 2E_{CS}e^{-1/\lambda_S^*}.$$

This can be written

$$\lambda_N^*[\ln(E_{CN}/E_{CS}) + 1/\lambda_S^*]\Delta_{S0}. \tag{7.14}$$

Since we expect E_{CN} and E_{CS} to be roughly comparable, this result is small compared to Δ_{S0} if $\lambda_N^* \ll \lambda_S^*$, as we have assumed.

Thus for $RE_0(1) \ll 1, \lambda_N^* \ll \lambda_S^*$, the initial assumption that $\Delta_N(E)$ is negligible [compared to $\Delta_S(E)$] at low energies is consistent.

Using arguments similar to those advanced above, we can obtain a rough picture of the behavior of $\Delta_N(E)$ when E is near a typical phonon energy ($\hbar\omega_N$) of N and $\Delta_S(E)$ is negligible. In Ref. 15, assuming that the phonon spectrum of N has one peak at $\hbar\omega_N$ of width $\sim b_N$, it was argued that a reasonable approximation for $K_+(E,E')_N$ near $\hbar\omega_N$ is (neglecting the Coulomb pseudopotential)

$$K_+(E,E')_N \approx \alpha_N^2(E' - E + \hbar\omega_N - ib_N)^{-1}. \tag{7.15}$$

For the integral over the bound-state region, the temperature dependence must be considered. The modification of (7.15) to include finite temperature simply involves a multiplication by $\tanh(\frac{1}{2}\beta E')$.

One may now proceed as before to obtain the bound-state contribution

$$\tfrac{1}{2}\left(\frac{1}{Z_N}\right)\alpha_N^2\pi R\Delta_{S0}^2\int_{RE_0}^{\pi/2} dy\left(\frac{\sin 2y}{y^2}\right)(\Delta_{S0}\cos y - E + \hbar\omega_N - ib_N)^{-1} \times \tanh(\tfrac{1}{2}\beta\Delta_{S0}\cos y). \tag{7.16}$$

For $b_N/\Delta_{S0} \gg RE_0$, the variation of the E-dependent term is slow compared to that of the other terms in the integrand for y near RE_0. In this

case, (7.16) may be approximated by

$$\left(\frac{1}{Z_N}\right)\alpha_N^2\pi R\Delta_{S0}^2\ln\left(\frac{1}{RE_0}\right)(\Delta_{S0}-E+\hbar\omega_N-ib_N)^{-1}. \quad (7.17)$$

An approximation for the contribution from states above Δ_{S0} may be obtained by taking the limit $R \to 0$, yielding [compare Eq. (24) of Ref. 15]

$$\frac{1}{Z_N}\alpha_N^2\left[\frac{\Delta_{S0}}{[(E-\hbar\omega_N+ib_N)^2-\Delta_{S0}^2]^{1/2}}\right] \times \ln\left(\frac{[(E-\hbar\omega_N+ib_N)^2-\Delta_{S0}^2]^{1/2}-E+\hbar\omega_N-ib_N}{\Delta_{S0}}\right). \quad (7.18)$$

At the peaks of the real and imaginary parts of the sum of (7.17) and (7.18), we find [setting $Z_N = 1+\lambda_N$ and neglecting the logarithm in (7.18)]

$$\mathrm{Re}\Delta_N(E), \mathrm{Im}\Delta_N(E) \approx \frac{\alpha_N^2}{1+\lambda_N}\left[\pi R\Delta_{S0}\ln\left(\frac{1}{RE_0}\right) \times\left(\frac{\Delta_{S0}}{b_N}\right)+\left(\frac{\Delta_{S0}}{b_N}\right)^{1/2}\right]. \quad (7.19)$$

In the limit $R\Delta_{S0}\to 0$, this reduces to the result in Eq. (25) of Ref. 15.

Inspection of Eqs. (7.9), (7.13), and (7.19) indicates that, in the limit as $R\Delta_{S0}$ approaches zero, and for $\lambda_N^* \ll \lambda_S^*$ (so that Δ_N may be neglected relative to Δ_S), the induced pair potential may be determined by the equation

$$\Delta_N(E)=\frac{1}{Z_N(E)}\int_0^\infty dE'\left(\mathrm{Re}\frac{\Delta_S(E')}{[(E')^2-\Delta_S(E')^2]^{1/2}}\right) \times K_+(E,E')_N \quad (7.20)$$

where

$$Z_N(E)=1-\frac{1}{E}\int_0^\infty dE'\,\mathrm{Re}\left(\frac{E'}{[(E')^2-\Delta_S(E')^2]^{1/2}}\right) \times K_-(E,E')_N. \quad (7.21)$$

One may verify this exactly by evaluating (7.1) and (7.2) in the limit as $R\to 0$.

If it turns out that a calculation of $\Delta_N(E)$ from Eq. (7.20) yields a $\Delta_N(E)$ which is comparable to $\Delta_S(E)$ at low energies, then it is necessary to carry out a full self-consistent treatment, based on Eqs. (6.7)–(6.10). We will assume that the coupling strength in N is so small ($\lambda_N^* \ll \lambda_S^*$) that this is unnecessary.

VIII. PAIR POTENTIAL IN S FOR THIN WEAK-COUPLING N METALS

In Eqs. (6.9) and (6.10) we may again neglect $\Delta_N(E')$, since the energies contributing the most to the E' integrals are near $E'=\Delta_{S0}$, where $\Delta_N(E')$ is small. Using Eq. (7.10), neglecting the energy dependence of $\Delta_S(E)$, and taking the real parts, we find

$$Z_S(x)=1-\frac{1}{E}\int_{\Delta_{S0}}^\infty dE'\int_0^1 d(\cos\theta) \times\left(\frac{(E'/\Omega_{S0})\{\Omega_{S0}^2-\Delta_{S0}^2\sin^2(\Delta K^N d)[1-\cos(\Delta K^S x)]-\Delta_{S0}^2(\Omega_{S0}/E')^{\frac{1}{2}}\sin(2\Delta K^N d)\sin(\Delta K^S x)\}}{\Omega_{S0}^2+\Delta_{S0}^2\sin^2(\Delta K^N d)}\right) \times K_-(E,E')_S \quad (8.1)$$

$$\phi_S(x)=\int_{\Delta_S}^\infty dE'\int_0^1 d(\cos\theta) \times\left(\frac{(\Delta_{S0}/\Omega_{S0})[\Omega_{S0}^2+\Delta_{S0}^2\sin^2(\Delta K^N d)-(E')^2\sin^2(\Delta K^N d)\cos(\Delta K^S x)-\frac{1}{2}E'\Omega_{S0}\sin(2\Delta K^N d)\sin(\Delta K^S x)]}{\Omega_{S0}^2+\Delta_{S0}^2\sin^2(\Delta K^N d)}\right) \times K_+(E,E')_S. \quad (8.2)$$

We are particularly interested in the values of these functions at the N-S interface, where the deviation from their bulk values is maximal, so we set $x=0$. The $\cos\theta$ integral in (8.2) may then be approximately obtained in the limit of small $R\Delta_{S0}$:

$$\phi_S(E)=\int_{\Delta_{S0}}^\infty dE'\left(\frac{\Delta_{S0}}{\Omega_{S0}}\right)\left[1-\left(\frac{\Delta_{S0}RE'}{\Omega_{S0}}\arctan\frac{\Omega_{S0}}{\Delta_{S0}RE'}\right)\right]K_+(E,E')_S. \quad (8.3)$$

The energy integrals will be evaluated for $E=0$, which is assumed to be far enough from phonon frequencies in S that the approximations ($\Delta_{S0} \gg k_BT$),

$$K_+(0,E')_S=\lambda_S^*\Theta(E_{CS}-E'),$$

$$K_-(0,E')_S\approx 0$$

are appropriate. Taking $Z_S(0)=1$, we have $\phi_S(0)$

$= \Delta_{S0}$. The first term in (8.3) corresponds to the value of Δ_{S0} in the bulk. The second term is the modification of Δ_{S0} at the N-S interface due to the presence of the interface. The result of the first integral is

$$\lambda_S^* \Delta_{S0} \ln(2E_{CS}/\Delta_{S0}) . \tag{8.4}$$

One must compare this to the result of the second integral, which may be written

$$\lambda_S^* \Delta_{S0} R \Delta_{S0} \int_1^{E_{CS}/\Delta_{S0}} d\epsilon \left(\frac{\epsilon}{\epsilon^2 - 1}\right) \arctan\left[\frac{(\epsilon^2 - 1)^{1/2}}{\epsilon R \Delta_S}\right] . \tag{8.5}$$

This is *less* than or equal to

$$\lambda_S^* \Delta_{S0} \pi \; R\Delta_{S0} \left[\ln\left(\frac{E_{CS}}{\Delta_{S0}}\right) + \ln\left(\frac{1}{R\Delta_{S0}}\right) - 1/2 \ln 2\right] . \tag{8.6}$$

Thus if $R\Delta_{S0} \ll 1$, as is assumed throughout this paper, then the modification of Δ_{S0} at the N-S interface is negligible, and Δ_S is equal to the *bulk* pair potential in S.

IX. SUGGESTIONS FOR IMPROVEMENT OF THE MODEL AND CONCLUSIONS

In our opinion, a complete picture of proximity-effect tunneling has been obtained here for thin N metals in perfect contact with much thicker S metals, where both N and S are clean. An extension of our results to thicker N metals may make use of the Green's functions derived here, but we suspect that the spatial dependence of the pair potentials in N and S will require a different approach in order to achieve self-consistency. For this reason, we have restricted ourselves to thin N metals.

It may be possible, however, to extend our approach to the case of a thin N metal and a comparably thin S metal by keeping a (the thickness of S) finite in the Green's function of Eq. (3.10), and carrying out the calculation of $G(xx')$ for this case. The thicknesses of both S and N should be less than a coherence length, in order that the pair potentials remain spatially constant. In this event, Δ_S would correspond not to the bulk value of the pair potential in S, but to the final self-consistently-determined value, which will be less than the bulk value because of the influence of the N layer. We also expect that Δ_N will be smaller for this case because the Δ_S potential, which induces the Δ_N, is smaller.

If the contact between S and N is not perfect, i.e., if there is an effective potential barrier at the N-S interface, as is probably the case in experiments, the approach must be modified. The behavior of the NDC at energies near and below Δ_S should be most affected since the existence of normal scattering (scattering present when both N and S are in the normal state) will decrease the height of the peak due to the bound states, allowing states to exist in the region between Δ_S and the highest-energy bound state. The weaker coupling of N and S will also cause the induced pair potential (Δ_N) to decrease.

Finally, it may be desirable to introduce a finite amount of elastic impurity scattering and diffuse surface scattering. In the bulk, there is a general theorem that elastic impurity scattering does not affect the energy gap. Hence no effects are observed on the NDC for one superconducting layer. As we have seen, however, proximity-effect tunneling is capable of measuring the renormalization parameter $Z(E)$ separately. Since elastic scattering does affect $Z(E)$, its effects on the oscillatory terms in the NDC may be observed.

At energies far above Δ_S, Eq. (4.15) indicates that the NDC behaves in a relatively simple way as a function of Δ_S and Δ_N. We believe that before one attempts to extract information on Δ_N from the NDC, however, the role of normal scattering at the N-S interface must be determined. Upon inclusion of this into the theory, one should be able to determine the energy dependence of $\Delta_N(E)$ from the NDC by knowing $\Delta_S(E)$ and the transmission coefficient at the N-S interface. A determination of $\alpha^2 F$ for the N metal might then be made, based on the "inversion" of an equation for $\Delta_N(E)$ like Eq. (6.4). A knowledge of tunneling selection rules for the tunneling interface would also allow one to obtain separate information on the renormalization parameter in N in the same experiment.

APPENDIX A: GENERAL EXPRESSION FOR THE DOUBLE-LAYER GREEN'S FUNCTION

The Feuchtwang technique involves the application of Green's theorem over the region in which it is desired that the exact Green's function $G(x,x')$ be known. First, consider the equations

$$EG_i(x,x') + \frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} - \mu_x\right) G_i(x,x')\tau_3 - G_i(x,x')\Sigma_i(x') = \delta(x - x') = G_i(x,x')[E - \vec{\vec{H}}_i(x')] , \tag{A1}$$

$$\left[E + \frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} - \mu_x\right)\tau_3 - \Sigma(x)\right] G(x,x') = \delta(x - x') = [E - \vec{\vec{H}}(x)]G(x,x') . \tag{A2}$$

The index i designates the layer occupying region D_i. $\Sigma_i(x')$ is the ansatz matrix self-energy in this region. The direction of the arrow indicates the

direction in which the second derivative operates. One now constructs the identity

$$\int_{X_{iL}}^{X_{iR}} \{G_i(x,x_1)[E-\vec{\mathrm{H}}_i(x_1)]G(x_1,x') - G_i(x,x_1)[E-\vec{\mathrm{H}}(x_1)]G(x_1,x')\}dx_1 = G(x,x')\Theta(x\in D_i) - G_i(x,x')\Theta(x'\in D_i)\,. \tag{A3}$$

The unit step function $\Theta(x\in E_i)$ vanishes unless x is in region D_i, which has a boundary on the left-hand side at x_{iL}, on the right-hand side at x_{iR}. The left-hand side may be partially integrated, yielding

$$\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial x_1}G_i(x,x_1)\tau_3 G(x_1,x') - G_i(x,x_1)\tau_3\frac{\partial}{\partial x_1}\right)G(x_1,x')\Big|_{x_{iL}}^{x_{iR}} + \int_{X_{iL}}^{X_{iR}} dx_1 G_i(x,x_1)[\Sigma(x_1)-\Sigma_i(x_1)]G(x_1,x')$$
$$= G(x,x')\Theta(x\in D_i) - G_i(x,x')\Theta(x'\in D_i)\,, \tag{A4}$$

since both Green's functions are solutions to a self-adjoint boundary value problem. A similar calculation using

$$\int_{X_{iL}}^{X_{iR}} dx_1\{G(x,x_1)[E-\vec{\mathrm{H}}_i(x_1)]G_i(x_1,x') - G(x,x_1)[E-\vec{\mathrm{H}}(x_1)]G_i(x_1,x')\} \tag{A5}$$

yields

$$\frac{\hbar^2}{2m}\left(G(x,x_1)\tau_3\frac{\partial}{\partial x_1}G_i(x_1,x') - \frac{\partial}{\partial x_1}G(x,x_1)\tau_3 G_i(x_1,x')\right)\Big|_{X_{iL}}^{X_{iR}} + \int_{X_{iL}}^{X_{iR}} G(x,x_1)[\Sigma(x_1)-\Sigma_i(x_1)]G_i(x_1,x')$$
$$= G(x,x')\Theta(x'\in D_i) - G_i(x,x')\Theta(x\in D_i)\,. \tag{A6}$$

It is convenient to assume that $\Sigma_i(x)$ can be chosen so that $\Sigma(x)-\Sigma_i(x)$ is negligible in the region D_i. An initial assumption of this type is justified only if, using $\Sigma_i(x)$ to calculate $G(x,x')$, it is found that the value of $\Sigma(x)$, which depends on $G(x,x')$, differs negligibly from $\Sigma_i(x)$ everywhere in D_i. In the following, we assume that such a $\Sigma_i(x)$ can be found. In the main text we verify how good our initial guess for the self-energy $\Sigma_i(x)$ is by calculating $\Sigma(x)$ with Green's functions depending on $\Sigma_i(x)$ and comparing with $\Sigma_i(x)$. If $\Sigma(x)$ is *spatially independent* in the region D_i, it is always possible to choose $\Sigma_i(x)$ to coincide exactly with $\Sigma(x)$.

The appropriate boundary conditions on Green's function at interfaces are

$$\frac{\partial}{\partial x}G_{N,S}(x,x')\Big|_{x=0} = 0 = \frac{\partial}{\partial x'}G_{N,S}(x,x')\Big|_{x'=0}\,. \tag{A7}$$

For the double layer function

$$G(x=a,x') = 0 = G(x,x'=a)\,, \tag{A8}$$

$$\frac{\partial}{\partial x}G(x,x')\Big|_{x=-d} = 0 = \frac{\partial}{\partial x'}G(x,x')\Big|_{x'=-d}\,, \tag{A9}$$

where a and $-d$ are defined in Fig. 1. Conditions (A8) and (A9) must also be obeyed by G_S and G_N, respectively.

The Dirichlet boundary condition (A8) at the free surface must be taken to include the implied limit $a\to+\infty$, as mentioned in the text after Eq. (3.10). Otherwise, the absence of outgoing-wave behavior at $x=a$ would lead to no net current. The combination of the $a\to\infty$ limit and the temporal boundary condition on the retarded Green's function automatically produces the necessary outgoing wave.

As Feuchtwang has shown,[13] one is free to choose whatever boundary conditions are convenient at the interfaces. He has also shown[12] that, in the normal state, the choice (A9) for Green's function for the right electrode (which is an N-S double layer in our case), and a similar choice for Green's function for the left electrode reproduces the tunneling Hamiltonian expression for the current, of which we make use in this work. This expression involves the product of the tunneling matrix element squared and the local density of states in the left electrode (assumed normal) at $-d$ times the local density of states in the right electrode at $-d$. We have shown that the same result holds in the superconducting state.[27]

With these boundary conditions, (A4) and (A6) reduce to single expressions depending only on the first derivative of the double layer Green's function at the N-S interface. One now may obtain the necessary first derivatives by differentiating (A4) and (A6) at the N-S interface, leaving an expression depending on the mixed *second* derivative

$$\frac{\partial^2}{\partial x\partial x'}G(x,x')\Big|_{x=x'=0}\,,$$

which is *continuous*.

Using the discontinuity of $G(xx')$ at the source point $x=x'$:

$$\frac{\partial G(x,x')}{\partial x}\Bigg|_{x=x'-}^{x=x'+} = \frac{2m}{\hbar^2}\tau_3 = \frac{\partial}{\partial x'}G(x,x')\Bigg|_{x'=x-}^{x'=x+},$$

one may easily solve for the mixed second derivative at $x=x'=0$. In this way, Eqs. (2.8) and (2.9) are obtained.

The calculation of $G(x,x')$ from (2.8) and (2.9) is a straightforward but algebraically complicated affair. The only approximation employed is the replacement

$$K_\pm^{N,S} \to k_{FX} = [(2m/\hbar^2)\mu - k_\parallel^2]^{1/2},$$

whenever $K_\pm^{N,S}$ is *not* involved in the argument of a trigonometric function in the Green's functions of (3.9) and (3.10). Corrections to this approximation are of order Δ/E_F. We also use (3.10) in the limit $a\to\infty$ [see Eq. (3.11)].

We will illustrate the calculation of the Green's function for the double layer by using (3.9) and (3.10) in (2.8), then taking the limit $a\to+\infty$. First by defining

$$\begin{aligned}
&\chi_{N\pm}(x_>) = \cos(K_\pm^N x_>),\\
&\chi_{N\pm}(x_< + d) = \cos[K_\pm^N(x_< + d)],\\
&W_{N\pm} = \left(\frac{d}{dx_>} - \frac{d}{dx_<}\right)\chi_{N\pm}(x_>)\chi_{N\pm}(x_< + d)\Big|_{x_>=x_<},
\end{aligned} \tag{A10}$$

we may write (3.9) in the form

$$G_N(x,x') = \sum_\pm \frac{\pm m}{\hbar^2 W_{N\pm}}\begin{pmatrix}(E\pm\Omega_N)/\Omega_N & \Delta_N/\Omega_N\\ \Delta_N/\Omega_N & (E\mp\Omega_N)/\Omega_N\end{pmatrix} \times \chi_{N\pm}(x_>)\chi_{N\pm}(x_< + d). \tag{A11}$$

The term $W_{N\pm}$ is the Wronskian, and is therefore spatially independent. By first replacing N by S and then letting $x_< + d \to x_> - a + \pi/2K_\pm^S$ and $x_> \to x_<$, Eq. (3.10) may be obtained from (A11) and (A10). Using this device, the "symmetry" in N and S exhibited by (2.8) and (2.9) may be exploited, so that by finding (2.8) in terms of the functions in (A11), we may also determine (2.9).

For the matrix sum we find [using $\chi_{N\pm}(0)=1$]

$$\begin{aligned}
G_N(0,0) + G_S(0,0) &= \frac{m}{\hbar^2}\left[\frac{E}{\Omega_N}D_{N-} + \frac{E}{\Omega_S}D_{S-}\right.\\
&\left. + (D_{N+}+D_{S+})\tau_3 + \left(\frac{\Delta_N}{\Omega_N}D_{N-} + \frac{\Delta_S}{\Omega_S}D_{S-}\right)\tau_1\right],
\end{aligned} \tag{A12}$$

where

$$D_{N\pm} = \sum_\pm \pm\frac{\chi_{N\pm}(d)}{W_{N\pm}} \cong \frac{\sin[(K_-^N \pm K_+^N)d]}{k_{FX}\sin(K_+^N d)\sin(K_-^N d)} \tag{A13}$$

and

$$D_{S\pm} \cong \frac{-\sin[(K_+^S \pm K_-^S)a]}{k_{FX}\cos(K_+^S a)\cos(K_-^S a)} \tag{A14}$$

The approximate equality is due to the replacement $K_\pm^{N,S} \to k_{FX}$ discussed above. The matrices τ_1, τ_2, and τ_3 are the Pauli matrices in Nambu's notation. (The unit matrix is implied wherever necessary.)

The inverse of (A12) is easily obtained. Using

$$G_N(x,0) = G_N(0,x) \tag{A15}$$

and

$$G_N(x,0) = \frac{m}{\hbar^2}\sum_\pm \pm\left(\frac{E}{\Omega_N}\pm\tau_3 + \frac{\Delta_N}{\Omega_N}\tau_1\right)\alpha_{N\pm}, \tag{A16}$$

where

$$\alpha_{N\pm} = \frac{\chi_{N\pm}(x+d)}{W_{N\pm}} \cong \frac{\cos[K_\pm^N(x+d)]}{k_{FX}\sin(K_\pm^N d)} \tag{A17}$$

and

$$\alpha'_{N\pm} = \chi_{N\pm}(x'+d)/W_{N\pm},$$

with (choosing $x'>x$),

$$G_N(x,x') = \frac{m}{\hbar^2}\sum_\pm \pm\left(\frac{E}{\Omega_N}\pm\tau_3 + \frac{\Delta_N}{\Omega_N}\tau_1\right)\chi_{N\pm}(x')\alpha_{N\pm}, \tag{A18}$$

one may now obtain the right-hand side of (2.8) for $x'>x$. In the expression thus obtained one next rearranges terms so as to obtain the coefficients of α_{N+} and α_{N-}.

The result of these manipulations is, for $x'>x$:

$$\frac{m}{\hbar^2}\sum_\sigma \sigma\left[\left(\frac{E+\sigma\Omega_N\tau_3}{\Omega_N}\right)(a^2-b^2-c^2)\chi_{N\sigma}(x') - 2\left(\frac{E+\sigma\Omega_N\tau_3}{\Omega_N}\right)M_{N\sigma}\alpha'_{N\sigma} + 2\left(\frac{\Delta_N}{\Omega_N}\right)L_{N\sigma}\alpha'_{N-\sigma}\right.$$
$$\left. + \left(\frac{\Delta_N}{\Omega_N}\right)(a^2-b^2-c^2)\tau_1\chi_{N\sigma}(x') - 2\left(\frac{\Delta_N}{\Omega_N}\right)M_{N\sigma}\tau_1\alpha'_{N\sigma} + 2\left(\frac{E+\sigma\Omega_N\tau_3}{\Omega_N}\right)L_{N\sigma}\tau_1\alpha'_{N-\sigma}\right]\frac{\alpha_{N\sigma}}{a^2-b^2-c^2}, \tag{A19}$$

where

$$\begin{aligned}
a &= (E/\Omega_N)D_{N-} + (E/\Omega_S)D_{S-},\\
b &= D_{N+} + D_{S+},\\
c &= (\Delta_N/\Omega_N)D_{N-} + (\Delta_S/\Omega_S)D_{S-},
\end{aligned} \tag{A20}$$

and

$$\begin{aligned}
\sigma M_{N\sigma} &= a(E/\Omega_N) - b\sigma - c(\Delta_N/\Omega_N)\\
&= D_{N-} + F(E)D_{S-} - (D_{N+}+D_{S+})\sigma,
\end{aligned} \tag{A21}$$

$$\sigma L_{N\sigma} = a(\Delta_N/\Omega_N) - c(E/\Omega_N) = -G(E)D_{S-}. \tag{A22}$$

Both $F(E)$ and $G(E)$ are defined in (3.13), and $\sigma = \pm$. We also note that

$$a^2 - b^2 - c^2 = 2F(E)D_{N-}D_{S-} - 2D_{N+}D_{S+} + D_{N-}^2 - D_{N+}^2 + D_{S-}^2 - D_{S+}^2 . \quad \text{(A23)}$$

In the limit as $a \to \infty$ we have (approximating $1/K_\pm^S$ by $1/k_{FX}$):

$$D_{S+} \to 0$$

$$D_{S-} \to -2i/k_{FX} .$$

Using (A.13) this gives for (A.23) (approximating $1/K_\pm^N$ by $1/k_{FX}$ throughout)

$$a^2 - b^2 - c^2 \to \frac{4[iF(E)\sin(\Delta K^N d) - \cos(\Delta K^N d)]}{k_{FX}^2 \sin(K_+^N d)\sin(K_-^N d)} . \quad \text{(A24)}$$

Also in this limit we have

$$(a^2 - b^2 - c^2)\chi_{N\sigma}(x') - 2M_{N\sigma}\alpha'_{N\sigma} \to \frac{4\sigma A_{N\sigma}(x')}{k_{FX}^2 \sin(K_{-\sigma}^N d)} \quad \text{(A25)}$$

and

$$2L_{N\sigma}\alpha'_{N-\sigma} \to 4\sigma B_{N\sigma}(x')/k_{FX}^2 \sin(K_{-\sigma}^N d) , \quad \text{(A26)}$$

where $A_{N\sigma}(x')$ and $B_{N\sigma}(x')$ are defined by (3.14) and (3.15), respectively.

If $x > x'$, the only modification of the above results is the interchange of x and x'. Thus (A19)–(A26) remain valid when we replace x' by $x_>$ and x by $x_<$. One now readily observes that (A19) is equal to (3.12).

For $(x, x') > 0$ one performs the transformation described below (A11) on the results in (A19)–(A23). Using (3.11) one observes that

$$\lim_{a\to\infty} \alpha_{S\sigma} = -(i\sigma/k_{FX}) e^{i\sigma K_\sigma^S x_>} . \quad \text{(A27)}$$

The result (A24) is the same for this case [see (A23)]. However, for the other terms we have

$$\sigma M_{S\sigma} = D_{S-} + F(E)D_{N-} - (D_{N+} + D_{S+})\sigma ,$$

$$\sigma L_{S\sigma} = G(E)D_{N-} ,$$

$$(a^2 - b^2 - c^2)\chi_{S\sigma}(x_<) - 2M_{S\sigma}\alpha'_{S\sigma} \to \frac{-2e^{-i\sigma K_\sigma^S x_<} A_{S\sigma}(x_<)}{k_{FX}^2 \sin(K_+^N d)\sin(K_-^N d)} , \quad \text{(A28)}$$

and

$$2L_{S\sigma}\alpha'_{S-\sigma} \to \frac{-2e^{-i\sigma K_\sigma^S x_<} B_{S\sigma}(x_<)}{k_{FX}^2 \sin(K_+^N d)\sin(K_-^N d)} , \quad \text{(A29)}$$

where $A_{S\sigma}(x_<)$ and $B_{S\sigma}(x_<)$ are defined by (3.18) and (3.19), respectively. Thus is Eq. (3.16) obtained from (A19).

APPENDIX B: DERIVATION OF EQUATIONS FOR THE SELF-ENERGIES IN N AND S

The quantity relevant to the calculation of the self-energies is the matrix

$$-1/\pi \ \mathrm{Im}[G(x,x)] . \quad \text{(B1)}$$

This matrix may be obtained from (3.12) and (3.16) for x in the N layer and S layer, respectively. As mentioned below Eq. (6.6) in this paper, the elements of this matrix contain terms which oscillate rapidly as a function of x, going as $\exp(\pm 2ik_F x)$, both in the N layer and in the S layer.

For the N layer, the rapidly oscillating terms must be separated from the following products of trigonometric functions:

$$\cos(K_\pm^N x + K_\mp^N d)\cos[K_\pm^N(x+d)] = \tfrac{1}{2}\{\cos[2K_\pm^N x + (K_+^N + K_-^N)d] + \cos(\Delta K^N d)\} ,$$

$$\sin(K_\pm^N x + K_\mp^N d)\cos[K_\pm^N(x+d)] = \tfrac{1}{2}\{\sin[2K_\pm^N x + (K_+^N + K_-^N)d] \mp \sin(\Delta K^N d)\} ,$$

$$\cos[K_\mp^N(x+d)]\cos[K_\pm^N(x+d)] = \tfrac{1}{2}\{\cos[(K_+^N + K_-^N)(x+d)] + \cos[\Delta K^N(x+d)]\} .$$

When averaged over the width of the N layer, the first terms on the right-hand sides of the above equations give a relatively negligible contribution due to their rapid oscillation. We will therefore neglect these terms. Thus

$$A_{N\pm}(x)\cos[K_\pm^N(x+d)] \approx \tfrac{1}{2}[iF(E)\cos(\Delta K^N d) + \sin(\Delta K^N d)] \equiv \tfrac{1}{2}P_N ,$$

$$B_{N\pm}(x)\cos[K_\pm^N(x+d)] \approx \tfrac{1}{2}iG(E)\cos[\Delta K^N(x+d)] .$$

In a similar way, we find that the approximation

$$A_{S\pm}(x) \approx \cos(\Delta K^N d) - iF(E)\sin(\Delta K^N d)$$

is appropriate when considering (B1) for the S layer. As discussed below Eq. (6.6) in the text of the paper, we presume that in a fully self-consistent treatment, rapidly oscillating contributions to the self-energy will be suppressed, justifying the neglect of such terms.

With these approximations we find for the N layer [from (3.12)]:

$$-\frac{1}{\pi}[G(xx)_{11}] = \left(\frac{-1}{\pi\hbar v_{FX}}\right)\left(\frac{E}{\Omega_N}P_N + \frac{\Delta_N}{\Omega_N}iG(E) \times \cos[\Delta K^N(x+d)]\right)\Big/ S ,$$

$$-\frac{1}{\pi}[G(xx)_{12}] = \left(\frac{-1}{\pi\hbar v_{FX}}\right)\left(\frac{E}{\Omega_N}iG(E)\cos[\Delta K^N(x+d)] + \frac{\Delta_N}{\Omega_N}P_N\right)\Big/ S ,$$

where

$$S = iF(E)\sin(\Delta K^N d) - \cos(\Delta K^N d)\,. \tag{B2}$$

For the S layer, we obtain

$$-\frac{1}{\pi}[G(xx)_{11}] = \left(\frac{i}{\pi\hbar v_{FX}}\right)\left(\frac{E}{\Omega_S} - i\frac{\Delta_S}{\Omega_S}G(E) \times \sin(\Delta K^N d)e^{i\Delta K^S x}/S\right),$$

$$-\frac{1}{\pi}[G(xx)_{12}] = \left(\frac{i}{\pi\hbar v_{FX}}\right)\left(\frac{\Delta_S}{\Omega_S} - i\frac{E}{\Omega_S}G(E) \times \sin(\Delta K^N d)e^{i\Delta K^S x}/S\right).$$

By employing Eq. (5.1), one observes that

$$P_N/S = \cot(\Delta K^N d + i\zeta)\,, \tag{B3}$$

$$iG(E)/S = \csc(\Delta K^N d + i\zeta)\,. \tag{B4}$$

With the transformation of the $k_\parallel$ integrals to integrals over $\cos\theta = [1 - (k_\parallel/k_F)^2]^{1/2}$ the derivation of (6.7)–(6.10) is completed.

APPENDIX C: BOUND-STATE CALCULATIONS

From Eq. (4.7), at any of the bound-state energies E_m, we have

$$\sin(\Delta K^N d) = \bar{\Omega}_S\Omega_N/E(\Delta_S - \Delta_N) \equiv 1/\bar{G}\,, \tag{C1}$$

$$\cos(\Delta K^N d) = \bar{F}/\bar{G}\,, \tag{C2}$$

where

$$\bar{G} = iG(E)\,, \tag{C3}$$

$$\bar{F} = (E^2 - \Delta_S\Delta_N)/\bar{\Omega}_S\Omega_N = iF(E) \tag{C4}$$

(note: $\bar{F}^2 + 1 = \bar{G}^2$).

The expansion of the denominator of (4.5) about E_m is

$$S \equiv iF(E)\sin(\Delta K^N d) - \cos(\Delta K^N d) \cong \left([\bar{F}\cos(\Delta K^N d) + \sin(\Delta K^N d)]\frac{d(\Delta K^N d)}{dE} + \frac{d\bar{F}}{dE}\sin(\Delta K^N d)\right)_{E=E_m}(E - E_m)\,. \tag{C5}$$

Using (C1) and (C2), the right-hand side of (C5) becomes

$$S \approx \left(\bar{G}\frac{d(\Delta K^N d)}{dE} + \frac{1}{\bar{G}}\frac{d\bar{F}}{dE}\right)_{E=E_m}(E - E_m)\,. \tag{C6}$$

We neglect the possible energy dependence of Z_N and (Δ_N, Δ_S), as well as any imagninary part of these functions, near the bound-state energies [see discussion below Eq. (4.8) of main text]. The energy derivatives in (C6) thus yield

$$S \approx \bar{G}\left(\frac{2Z_N d}{\hbar v_{FX}}\frac{E}{\Omega_N} + \frac{E^2 + \Delta_S\Delta_N}{E\bar{\Omega}_S\Omega_N}\right)_{E=E_m}(E - E_m)\,. \tag{C7}$$

Evaluating the numerator of (4.5) at E_m using (C1) and (C2) we find:

$$\left(\frac{-2}{\pi\hbar v_{FX}}\right)\left(\frac{E}{\Omega_N}[iF(E)\cos(\Delta K^N d) + \sin(\Delta K^N d)] + \frac{\Delta_N}{\Omega_N}iG(E)\right) = \left(\frac{-2}{\pi\hbar v_{FX}}\right)\left(\frac{E}{\Omega_N}\bar{G} + \frac{\Delta_N}{\Omega_N}\bar{G}\right)_{E=E_m}. \tag{C8}$$

The ratio of (C8) and (C7), summed over all possible m, yields (4.8).

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