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Interface Effects in Normal Metal Tunneling

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In this paper, two model tunneling junctions are studied. In the first model, a single magnetic impurity is assumed to be present near a sharp metal-barrier interface. In the second, phonons with a single Einstein frequency are assumed to exist throughout one electrode and into the barrier region. The effect of the electron-spin (phonon) interaction on the conductance has been calculated. It is found that the zero-bias conductance anomaly produced by the magnetic impurity in model I is a sensitive function of the magnetic-impurity position, being of one sign in the barrier and oscillating in the electrode. In model II, we find, contrary to what had been believed that, when the phonons are strictly confined to the metal electrode and a local electron-phonon coupling is assumed, the conductance *decreases* at the phonon emission threshold. This decrease quickly becomes an increase, however, if the phonons are allowed to penetrate significantly into the barrier.

I. INTRODUCTION

Tunneling has served as a powerful probe of the superconducting properties of metals, giving us direct information about the bulk spectral function of the superconductor.[1] It has been hoped that similar information about many-body interactions other than superconductivity could be obtained by studying normal metal tunneling.

There is, however, a crucial difference between superconductivity and other many-body effects, namely, the long coherence length of the superconductor, typically hundreds or thousands of Fermi wavelengths. We presently know that tunneling measures the spectral function of the electrode in the vicinity of the metal-barrier interface.[2] In the case where the metal is superconducting, this spectral function is determined by what goes on within a coherence length. Since this coherence length is many times larger than the range over which the metal-insulator boundary modifies the electronic wave functions, it is not at all surprising that the spectral function at the interface should still reflect what is going on in the bulk of the superconductor. It is this extremely nonlocal behavior which has made tunneling into superconductors such a remarkable tool.

In the case of normal metals, the effective range of the many-body interactions are typically Fermi wavelengths, quite comparable to the range of disturbance due to the metal-barrier interface, and the spectral function in the vicinity of this interface is greatly influenced by boundary effects. Another area where these boundary effects play a striking role is in the study of tunnel junctions whose insulating barrier has been doped, intentionally or otherwise, with impurities. It is the purpose of this paper to examine these interface effects by presenting two model calculations based on the recent theory of many-body tunneling proposed by the authors[2] and independently, by Zawadowski.[3]

The first model junction we will consider consists of an ideal symmetric tunnel junction, with a rectangular barrier, in which a magnetic impurity is assumed to be located in the vicinity of one of the electrode-barrier interfaces. While this problem has been considered by other authors,[4–6] the purpose of the present calculation, done in Sec. II, will be to study the dependence of the conductance on the position of the impurity. We will find that this dependence is rather dramatic, with the change in the conductance resulting from the impurity changing sign as it moves from the barrier into the electrode.

The second model junction, studied in Sec. III, is similar to that described above, except the magnetic impurity is replaced by a uniform distribution of Einstein phonons throughout one of the electrodes and extending into the barrier. The electrons are assumed coupled to the phonon via a deformation-type coupling and the dependence of the conductance on phonon penetration into the barrier is studied.

Section IV is devoted to a discussion of the models, and a number of possible experiments are suggested to reveal interface effects.

II. MAGNETICALLY DOPED TUNNELING JUNCTION

We consider a single magnetic impurity in a tunneling junction as shown in Fig. 1. The magnetic impurity is shown at position z_0 in the insulating barrier, but we also consider the case when it is present in the A electrode. Note that metal-barrier interface is assumed sharp.

The interaction between the electron and local

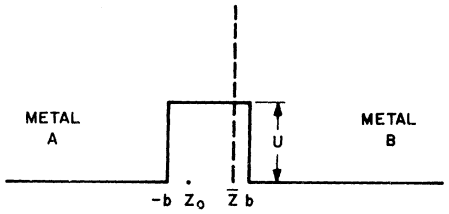

FIG. 1. The type barrier considered in text. The spin impurity is located at z_0. The surface on which the current is calculated is located at $\bar{z}$.

spin is taken to be of the form

$$-\tfrac{1}{2}J\delta(\vec{r}-\vec{r}_0)\vec{S}\cdot\vec{\sigma}; \quad \vec{r}_0=(0,0,z_0) \ , \tag{2.1}$$

where J is the exchange coupling constant for local spins $\vec{S}$ and $\vec{\sigma}$ the electron Pauli matrix.

The formula for the current,[2,3] generalized to finite temperature, is given by (in units where $\hbar=1$, $2m=1$, with m the electron mass)

$$\begin{aligned} I=+8\pi e\int_{-\infty}^{\infty} & d\omega\, d\omega'[f(\omega)-f(\omega')]\delta(\omega+eV-\omega') \\ & \times\int d^3r\int d^3r'\,\delta(z-\bar{z})\delta(z'-\bar{z}) \\ & \times\Big(\operatorname{Im}G^R(r',r;\omega)\frac{\partial^2}{\partial z\partial z'}\operatorname{Im}G^L(r;r';\omega') \\ & +\frac{\partial^2}{\partial z\partial z'}\operatorname{Im}G^R(r',r;\omega)\operatorname{Im}G^L(r,r';\omega) \\ & -\frac{\partial}{\partial z}\operatorname{Im}G^R(r',r;\omega)\frac{\partial}{\partial z'}\operatorname{Im}G^L(r,r';\omega) \\ & -\frac{\partial}{\partial z'}\operatorname{Im}G^R(r',r;\omega)\frac{\partial}{\partial z}\operatorname{Im}G^L(r,r';\omega) \ , \end{aligned} \tag{2.2}$$

where $G^{(R,L)}(r,r';\omega)$ are the Green's function for the left- and right-hand problems.[7,8] Current is defined as positive when a voltage V is applied to the left electrode. Equation (2.2) is also the starting point of the work of Sólyom and Zawadowski[6] on this problem. However, our subsequent approximations are quite different and lead to qualitatively different results.

The decomposition of the tunnel junction into left- and right-hand problems, as discussed previously by the authors,[2] is shown in Fig. 2. In the decomposition we have assumed that the magnetic impurity is always much closer to the left electrode than the right, so that its interaction with the right electrode could be ignored. This means that $\bar{z}$, the point at which the Green's functions in Eq. (2.2) are evaluated, should be taken to the right of z_0, the site of the magnetic impurity.

The Hamiltonian for the left-hand problem is

$$\mathcal{H}_L=P^2+V_L(z)-\tfrac{1}{2}J\vec{S}\cdot\vec{\sigma}\,\delta(\vec{r}-\vec{r}_0) \ , \tag{2.3}$$

where
$$\begin{aligned} V_L(z)&=0, \quad z<-b \\ V_L(z)&=U, \quad z\geq -b \ ; \end{aligned} \tag{2.4}$$

while
$$\mathcal{H}_R=P^2+V_R(z) \ , \tag{2.5}$$

$$\begin{aligned} V_R(z)&=U, \quad z<b \\ V_R(z)&=0, \quad z>b \ . \end{aligned} \tag{2.6}$$

The Green's function, $G^R(\vec{r}',\vec{r};\omega)$, for the right-hand problem is a solution of equation

$$[\omega-p^2-V_R(z')]\,G^R(\vec{r}',\vec{r};\omega)=\delta(\vec{r}'-\vec{r})/2\pi \ . \tag{2.7}$$

By writing $G^R(\vec{r}',\vec{r};\omega)$ as

$$\begin{aligned} G^R(\vec{r}',\vec{r};\omega)&=[1/(2\pi)^2] \\ &\times\int e^{i\vec{k}_\perp\cdot(\vec{r}_\perp-\vec{r}'_\perp)}G^R(z',z;\vec{k}_\perp;\omega)\,d^2k_\perp \ , \end{aligned} \tag{2.8}$$

the equation for $G^R(z',z;\vec{k}_\perp;\omega)$ becomes

$$\left(\omega-\epsilon_{\vec{k}_\perp}+\frac{d^2}{dz'^2}-V_R(z')\right)G^R(z',z;\vec{k}_\perp;\omega)=\frac{\delta(z-z')}{2\pi} \ . \tag{2.9}$$

Equation (2.9) is easily solved, and one finds

$$\begin{aligned} G^R(z',z;\vec{k}_\perp;\omega)&=(1/4\pi\kappa) \\ &\times[e^{-\kappa|z-z'|}+((\kappa+ik)/(\kappa-ik))\,e^{\kappa(z+z'-2b)}] \end{aligned} \tag{2.10}$$

for $(z,z'<b)$, where

$$\kappa=(U-\omega+\epsilon_{\vec{k}_\perp})^{1/2}; \quad k=(\omega-\epsilon_{\vec{k}_\perp})^{1/2} \ . \tag{2.11}$$

The Green's function $G^L(\vec{r},\vec{r}';\omega)$ for the right-hand side, needless to say, is not so easily obtained. We will be interested in G^L only to third order in J, in which case

$$\begin{aligned} G^L(\vec{r},\vec{r}';\omega)&=G_0^L(\vec{r},\vec{r}';\omega) \\ &+G_0^L(\vec{r},\vec{r}_0;\omega)\,t(\vec{r}_0;\omega)G^L(\vec{r}_0,\vec{r}';\omega) \ , \end{aligned} \tag{2.12}$$

where
$$t(\vec{r}_0,\omega)=-(\pi J)^2B(\vec{r}_0;\omega)[1-\pi JA(\vec{r}_0;\omega)], \tag{2.13}$$

$$A(\vec{r}_0;\omega)=\int d\vec{x}\cdot G_0^L(\vec{r}_0,\vec{x};\omega)$$

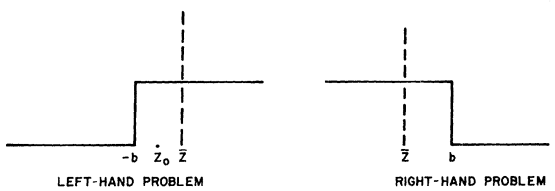

FIG. 2. Breakup of the problem into left- and right-hand problems. The impurity at z_0 is considered only in the left-hand problem.

$$\times[\langle\Psi_u^\dagger(\vec{r}_0)\Psi_u(\vec{\bar{x}})\rangle_0-\delta(\vec{\bar{x}}-\vec{r}_0)]\ , \tag{2.14}$$

$$B(\vec{r}_0;\omega)=\int d\vec{\bar{x}}\cdot G_0^L(\vec{r}_0,\vec{\bar{x}};\omega)$$

$$\times[\langle\vec{\sigma}_{uu'}\vec{S}\Psi_u^\dagger(\vec{r}_0)\Psi_{u'}(\vec{\bar{x}})\rangle_0-S(S+1)\delta(\vec{r}_0-\vec{\bar{x}})]\ . \tag{2.15}$$

In the above, the subscript 0 indicates the quantity is evaluated to lowest nonvanishing order in J. The spin labels u, u' are assumed summed over.

$G_0^L(\vec{r},\vec{r}';\omega)$ satisfies the equation

$$[\omega-p^2-V_L(z)]\,G_0^L(\vec{r},\vec{r}';\omega)=\delta(\vec{r}-\vec{r}')/2\pi, \tag{2.16}$$

from which one obtains

$$G_0^L(\vec{r},\vec{r}';\omega)=[1/(2\pi)^2]\int d^2\vec{k}_\perp e^{-i\vec{k}_\perp\cdot(\vec{r}-\vec{r}')}G_0^L(z,z';\vec{k}_\perp;\omega) \tag{2.17}$$

with

$$G_0^L(z,z';k_\perp;\omega)=-(1/4\pi\kappa)$$

$$\times[e^{-\kappa|z-z'|}+(\kappa+ik)/(\kappa-ik)e^{-\kappa(z+z'+2b)}]\ , \tag{2.18}$$

for $z, z'>-b$ with κ and k defined by Eq. (2.11).

If Eqs. (2.12) and (2.8) are substituted into Eq. (2.2), and the integral over $\vec{r}_\perp$ and $\vec{r}_\perp'$ performed, one finds

$$\bar{I}=8\pi e\int_{-\infty}^{\infty}\int d\omega\,d\omega'[f(\omega)-f(\omega')]\,\delta(\omega+eV-\omega')$$
$$\times\int[d^2k_\perp/(2\pi)^2]\Big[\,\mathrm{Im}G_0^R(\bar{z},\bar{z};\vec{k}_\perp;\omega)$$
$$\times\frac{\partial^2}{\partial z\partial z'}\,\mathrm{Im}G^L(\bar{z},\bar{z};\vec{k}_\perp;\omega')$$
$$+\text{permutations of }\left(\frac{\partial}{\partial z},\frac{\partial}{\partial z'}\right)\Big]\ , \tag{2.19}$$

where $\bar{I}$ is the current density flowing in the tunnel junction. Substituting for G^L, the unperturbed Green's function leads to the usual expression for the current density in the absence of any interactions.

We proceed now to calculate $\Delta\bar{I}$, the change in the current due to the magnetic impurity. Using Eqs. (2.10), (2.12), and (2.18), and taking the spatial derivatives, one finds

$$\Delta\bar{I}=8\pi e\int_{-\infty}^{\infty}\int d\omega d\omega'[f(\omega)-f(\omega')]\delta(\omega+eV-\omega')$$
$$\times\int[d^2k_\perp/(2\pi)^2](\kappa_L+\kappa_R)^2\{\mathrm{Im}G_0^R(\bar{z},\bar{z};\omega-\epsilon_{\vec{k}_\perp})$$
$$\times\mathrm{Im}[G_0^L(\bar{z},z_0;\omega'-\epsilon_{\vec{k}_\perp})G_0^L(z_0,\bar{z};\omega'-\epsilon_{\vec{k}_\perp})t(\vec{r}_0,\omega')]\}\ , \tag{2.20}$$

where
$$\kappa_L=(U+\tfrac{1}{2}eV-\omega'+\epsilon_{\vec{k}_\perp})^{1/2};$$
$$\kappa_R=(U+\tfrac{1}{2}eV-\omega+\epsilon_{\vec{k}_\perp})^{1/2}\ . \tag{2.21}$$

Note that we have included in $\kappa_{(L,R)}$ the change in the average barrier height with voltage. This is necessary to ensure that $\kappa_L=\kappa_R$.

We now need to perform the $\vec{k}_\perp$ integration in Eq. (2.20). The dominant variation of the integrand with respect to $\vec{k}_\perp$ is contained in the factor $\exp[-4b(U-\frac{1}{2}eV-\omega'+\epsilon_{\vec{k}_\perp})^{1/2}]$, so that to a high degree of accuracy we can set $\epsilon_{\vec{k}_\perp}=0$ everywhere in the integrand except the exponent.[9] Doing this one finds

$$\Delta\bar{I}=\frac{4e}{b}\int_{-\infty}^{\infty}\int d\omega d\omega'[f(\omega)-f(\omega')]\delta(\omega+eV-\omega')\kappa^3$$
$$\times\{\mathrm{Im}G_0^R(\bar{z},\bar{z};\omega)\mathrm{Im}[G_0^{L^2}(z,z_0;\omega')t(\vec{r}_0;\omega')]\}\ . \tag{2.22}$$

The conductance due to the magnetic impurity $\Delta G(V)=\partial\Delta\bar{I}/\partial V$ is easily shown to be

$$\Delta G(V)=(4e^2/b)\,\kappa^3\mathrm{Im}G_0^R(\bar{z},\bar{z};\epsilon_F)$$
$$\times\mathrm{Im}[G_0^{L^2}(\bar{z},z_0;\epsilon_F+eV)t(\vec{r}_0,eV+\epsilon_F)]\ . \tag{2.23}$$

Having arrived at Eq. (2.23), we now need an expression for $t(\vec{r}_0,\omega)$. It is a simple matter to verify that to order J^3

$$t(\vec{r}_0;\omega)=(\pi J)^2S(S+1)G_0^L(\vec{r}_0,\vec{r}_0;\omega)$$
$$-(\pi J)^3S(S+1)G_0^L(\vec{r}_0,\vec{r}_0;\omega)\,(2/\pi)$$
$$\times\int\{d\omega'[2f(\omega')-\tfrac{1}{2}]$$
$$\times\mathrm{Im}G_0^L(\vec{r}_0,\vec{r}_0;\omega'+i\delta)/(\omega'-\omega-i\delta)\}$$
$$+(\pi J)^3S(S+1)(2/\pi)$$
$$\times\int[d\omega' f(\omega')/(\omega'-\omega-i\delta)]$$
$$\times\mathrm{Im}G_0^2(\vec{r}_0,\vec{r}_0;\omega'+i\delta). \tag{2.24}$$

As it stands, $G_0^L(\vec{r}_0,\vec{r}_0;\omega)$ is not defined, since the $\vec{k}_\perp$ integration in Eq. (2.17) does not converge. This results from our use of a δ-function exchange interaction and necessitates the introduction of an energy cutoff on the $\vec{k}_\perp$ integration in Eq. (2.8). In the calculations to be presented we set the cutoff at the Fermi energy. The essential features of the results will be insensitive to this cutoff.

Now the largest contribution to $\Delta G(V)$ comes from the J^2 term in $t(\vec{r}_0,\omega)$. This term is insensitive to temperature and voltage and has the effect of shifting the background conductance. Its importance, as Appelbaum[4] has shown, stems from the fact that in a magnetic field it becomes strongly temperature and voltage dependent, and thereby, easily identified.

Our interest here in the term will be to study its dependence on the position of the magnetic impurity in the junction.

The local Green's function at $\vec{r}_0$ is easily shown to be

$$G^L(\vec{r}_0, \vec{r}_0; \omega) = \frac{1}{4\pi} \int_0^{\epsilon_F} d\epsilon \, \frac{1}{4\pi i k} \left(1 + e^{-Ak} \frac{ik + \kappa}{ik - \kappa} \right), \quad A < 0 \quad (2.25a)$$

$$G^L(\vec{r}_0, \vec{r}_0; \omega) = \frac{1}{4\pi} \int_0^{\epsilon_F} d\epsilon \, \frac{-1}{4\pi \kappa} \left(1 + \frac{\kappa + ik}{\kappa - ik} e^{-2\kappa A} \right), \quad A > 0 \; ; \quad (2.25b)$$

where

$$\kappa = (1 - \omega + \epsilon)^{1/2}, \quad k = (\omega - \epsilon)^{1/2}, \quad A = 2(b + z_0) \; .$$

We have set $U = 1$. In addition we need

$$\mathrm{Im}G_0^R(\bar{z}, \omega)\mathrm{Re}G_0^{L^2}(\bar{z}, z_0; \omega) = [\tilde{k} e^{-4\tilde{\kappa} b}/(2\pi)^3]$$

$$[(\tilde{\kappa}^2 - \tilde{k}^2)\cos \tilde{k} A + 2\tilde{k}\tilde{\kappa} \sin \tilde{k} A], \quad A < 0 \quad (2.26a)$$

$$\mathrm{Im}G_0^R(\bar{z}, \omega)\mathrm{Re}G_0^{L^2}(\bar{z}, z_0; \omega) = -\frac{2\tilde{k} e^{-4\tilde{\kappa} b}}{(4\pi)^3 \tilde{\kappa}} \{ e^{2\tilde{\kappa} A} + (\tilde{\kappa}^2 - \tilde{k}^2) e^{2\tilde{\kappa} A}]^2 - 4\tilde{k}^2 \tilde{\kappa}^2 e^{-\tilde{\kappa} A} \}, \; A > 0 \quad (2.26b)$$

$$\mathrm{Im}G_0^R(\bar{z}; \omega)\mathrm{Im}G_0^{L^2}(\bar{z}, z_0; \omega) = -[\tilde{k} e^{-4\tilde{\kappa} b}/(2\pi)^3]$$

$$\times [2\tilde{k}\tilde{\kappa} \cos \tilde{k} A + (\tilde{k}^2 - \tilde{\kappa}^2) \sin \tilde{k} A], \; A < 0 \quad (2.27a)$$

$$\mathrm{Im}G_0^R(\bar{z}; \omega)\mathrm{Im}G_0^{L^2}(\bar{z}, z_0; \omega) = -[\tilde{k}^2 e^{-4\tilde{\kappa} b}/(2\pi)^3 \tilde{\kappa}]$$

$$\times [1 + (\tilde{\kappa}^2 - \tilde{k}^2) e^{-\tilde{\kappa} A}], \quad A > 0 \quad (2.27b)$$

where $\tilde{\kappa} = (1 - \omega)^{1/2}$; $\tilde{k} = \omega^{1/2}$.

It becomes immediately clear that ΔG will be an oscillating function of position when present in the electrode and of one sign when in the barrier. (It is in fact possible for ΔG to change sign in the barrier, when this occurs, however, it does so very close to the electrode-barrier interface.)

In Fig. 3 we have plotted $\Delta G(V = 0)$ as a function of A, confirming the behavior implied by Eqs. (2.26) and (2.27).

Turning now to the third-order contributions, we isolate the term containing the dominant voltage and temperature dependence:

$$\mathrm{Im}t^3(r_0, \omega) = (2\pi J)^3 \tfrac{1}{4} S(S+1) \mathrm{Im}G_0^L(r_0, \omega)$$
$$\times \int [f(\omega') - \tfrac{1}{2}] \mathrm{Im}G_0^L(\vec{r}_0, \omega') \, d\omega' / (\omega' - \omega) .$$

This term[4] accounts for the zero-bias conductance anomalies found in certain magnetically doped tunnel junctions. The voltage and temperature dependence of the conductance resulting from this term is $\ln[(eV)^2 + (k_B T)^2]/E_0^2$, where E_0 is a cutoff parameter.

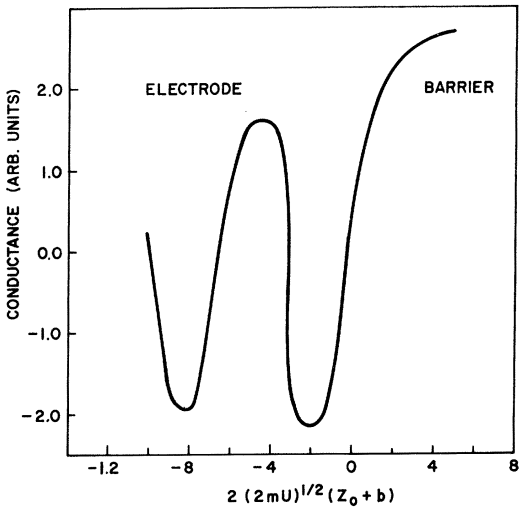

FIG. 3. Excess conductance at zero bias resulting from the magnetic impurity calculated to order $J^2\rho$ and plotted versus the impurity position.

In Fig. 4 we have plotted the position-dependent coefficient of the logarithmic term in ΔG. Note once again the oscillatory behavior of ΔG in the electrode.

III. TUNNELING JUNCTION WITH EINSTEIN PHONONS

We now consider the model in which the electrons are coupled to a set of phonons all of the same frequency ω_E. Calculations are performed for two situations: (i) The phonons exist and are coupled to the electrons in metal A (Fig. 1) and do not extend into the barrier; and (ii) the phonons exist and are coupled to the electrons throughout metal A and through barrier up to metal B. This latter case is certainly pathological as there are large changes in the phonon spectrum from a metal to an oxide. However, comparing these two calculations illustrates the essential difference between the effects of inelastic scattering off excitations in the bulk of an electrode and that of inelastic scattering off excitations in the barrier itself. The Hamiltonian describing the electron-phonon interaction is

$$g \int_{z < z_0} d^3r \, \varphi(\vec{r}) \Psi^\dagger(\vec{r}) \Psi(\vec{r}) \quad , \quad (3.1)$$

where z_0 is either $\pm b$ as discussed above and $\varphi(\vec{r})$ is the phonon field operator. We treat this interaction in second-order perturbation theory. This approximation was justified by Migdal even for strong coupling for situations where one is interested in the frequency dependences of various quantities. However, we are looking at effects

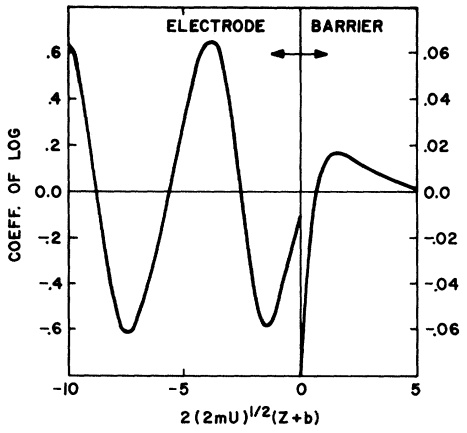

FIG. 4. The coefficient of the logarithmic singularity in the third-order contribution to the conductance due to the scattering from the spin impurity as a function of distance.

which are due to momentum dependences and Migdal's justification does not apply. Our results are therefore justified only for weak coupling. To this order,

$$G^L(\vec{r},\vec{r}';\omega)=G_0^L(\vec{r},\vec{r}';\omega)+\int_{z''<z_0} d^3r'' \times G_0^L(\vec{r},\vec{r}'';\omega)\Sigma(z'';\omega)G_0^L(\vec{r}'',\vec{r}';\omega), \tag{3.2}$$

with

$$\Sigma(z;\omega)=g^2\int \frac{d^3k}{(2\pi)^3}\left|\varphi_{k_z}(z)\right|^2 \times\left(\frac{1-f(\epsilon_{\vec{k}})}{\omega-\epsilon_{\vec{k}}-\omega_E}+\frac{f(\epsilon_{\vec{k}})}{\omega-\epsilon_{\vec{k}}+\omega_E}\right). \tag{3.3}$$

The $\varphi_{k_z}(z)$ are the solutions of the Schrödinger equation for the unperturbed left-hand problem (Fig. 2). The integrals over $\vec{k}_\perp$ can be performed and one finds the resulting expression to be essentially described by

$$\Sigma(z,\omega)\simeq g^2\rho(z,\epsilon_F)\ln[(\omega-\epsilon_F-\omega_E)/(\omega-\epsilon_F+\omega_E)], \tag{3.4}$$

where $$\rho(z,\epsilon_F)=\int_0^{k_F}[dk_z/(2\pi)^2]\,|\varphi_{k_z}(z)|^2 \tag{3.5}$$

is the local density of states at the Fermi surface. The form Eq. (3.2) is similar to Eq. (2.12) with the self-energy replacing the t matrix except for the integration over $\vec{r}''$. The reasoning that went into the derivation of Eq. (2.23) can be repeated so that the change in conductance can be written as

$$\Delta G(V)=(4e^2/b)\,\kappa^3\mathrm{Im}G_0^R(\bar{z},\bar{z};\epsilon_F) \times\mathrm{Im}\left[\int_{-\infty}^{z_0} dz\, G_0^{L^2}(\bar{z},z;\epsilon_F+eV)\Sigma(z,\epsilon_F+eV)\right]. \tag{3.6}$$

There is no significant voltage dependence in $G_0^{L^2}(\bar{z},z;\epsilon_F+eV)$ so that it can be set equal to its value at ϵ_F. The voltage dependence of $\Delta G(V)$ thus arises entirely from the self-energy. There are two contributions. The contribution from the $\mathrm{Im}\Sigma$ is even with respect to voltage and is simply a step at $\pm\omega_E$. The contribution from $\mathrm{Re}\Sigma$ is odd with respect to voltage and is logarithmically singular at $\pm\omega_E$. The two functions are illustrated in Fig. 5. We are interested in the magnitude and more importantly the sign of the coefficient of these functions for the two cases mentioned at the beginning of this section. Thus let ΔG_e denote the magnitude of the step in the conductance arising from $\mathrm{Im}\Sigma$ and ΔG_{odd} the coefficient of the logarithm.

For case A when the phonons exist only in the left electrode we might to a first approximation assume that $\rho(z,\epsilon_F)$ is a constant up to the barrier equal to $\rho(-\infty,\epsilon_F)$. The integral over z can then be performed and one finds

$$\Delta G_e/G^0=-(g^2/4\pi)(1-k_F^2)^{1/2}, \tag{3.7}$$

$$\Delta G_{\mathrm{odd}}/G^0=-(g^2/8\pi^2k_F)(1-2k_F^2). \tag{3.8}$$

Here we have again set $U=1$. Note that the sign of ΔG_e is negative, that is, there is a drop in conductance. This result can be understood by realizing that for energies above ω_E the electrons

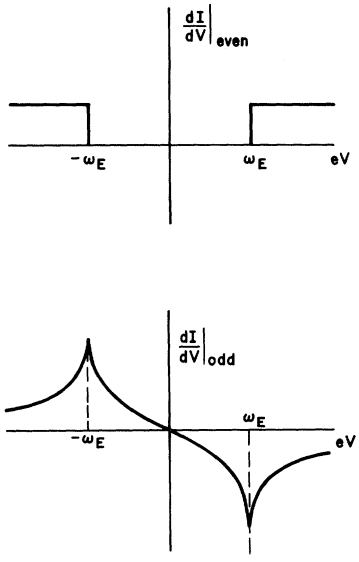

FIG. 5. The form of the contribution to the even and odd parts of the conductance due to the electron phonon interaction.

are tunneling into a dissipative medium (electrode A) so that the reflection coefficient at the electrode-barrier interface increases. The functions (3.7), (3.8) are plotted in Figs. 7 and 8, respectively, [curves (a)]. For this simple form of the self-energy, i.e., with $\rho(z,\epsilon_F)=\rho(-\infty,G_F)$ in (3.4), one can solve the Dyson equations exactly. Using the resulting Green's function an analytic expression can be obtained for the current and (3.7), (3.8) can be obtained by expanding in powers of Σ over K or k_z. The use of Eq. (3.2) is therefore a good approximation except for energies near the top or bottom of the barrier. The result obtained by not expanding G in powers of Σ has been previously obtained by Davis.[10] His approach to the problem does not include the imaginary part of the self-energy. An expansion of his result leads to Eq. (3.8) while Eq. (3.7) is omitted.

The actual density of states calculated in this model has Friedel oscillations near the surface of the metal and drops smoothly to zero in the barrier (Fig. 6). If we use this density in the above calculation the integrals become more complicated:

$$\Delta G_e/G_0=(g^2/2\pi k_F)\int_{-\infty}^{b} dz''\cos 2[k_F(z''+b)-\varphi_{k_F}] \times\int_0^{k_F}\sin^2[k(z+b)-\varphi_k]\,, \qquad (3.9)$$

$$\Delta G_{\text{odd}}/G_0=(g^2/2\pi^2 k_F)\int_{-\infty}^{b} dz''\sin 2[k_F(z''+b)-\varphi_{k_F}] \times\int_0^{k_F}\sin^2[k(z+b)-\varphi_k]\,dk\,. \qquad (3.10)$$

Here $e^{i\varphi_k}=(\kappa+ik)$. These integrals can be worked out analytically and the results are plotted in Figs. 7 and 8, curves (b). The integral (3.10) is actually logarithmically divergent because one is considering scattering off a potential, $\mathrm{Re}\Sigma(z,\omega)$, which oscillates with wave vector $2k_F$. It is easily seen that this divergence results from the simplications we have made in deriving Eq. (3.6) and that in a more correct treatment the logarithm is actually averaged over energies of the order of the width of allowed values of $\vec{k}_\perp$ and is also reduced by the fact that we are considering energies $\epsilon_F+\omega_E$ which we earlier set equal to ϵ_F. Both effects lead to comparable smearing of the singularity so we replace the singular term by $\ln(\omega_e/4\epsilon_F)\simeq 5$. Note that the coefficient ΔG_e of the step function at ω_E is still always negative.

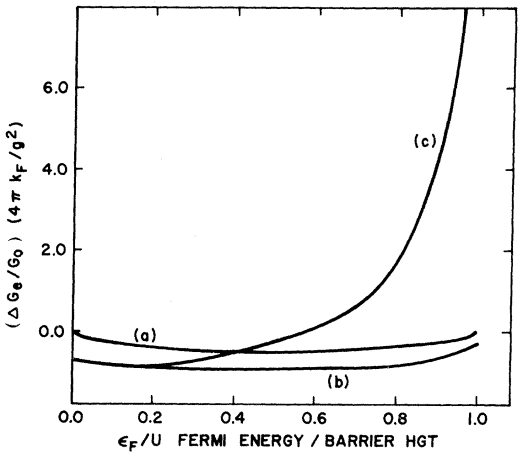

FIG. 7. The coefficient of the step in the even conductance for various approximations discussed in the text as a function of ϵ_F/U.

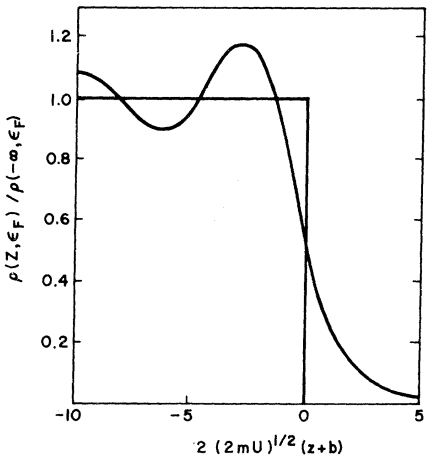

FIG. 6. The electron density near the barrier. We have taken $\epsilon_F/U=0.8$.

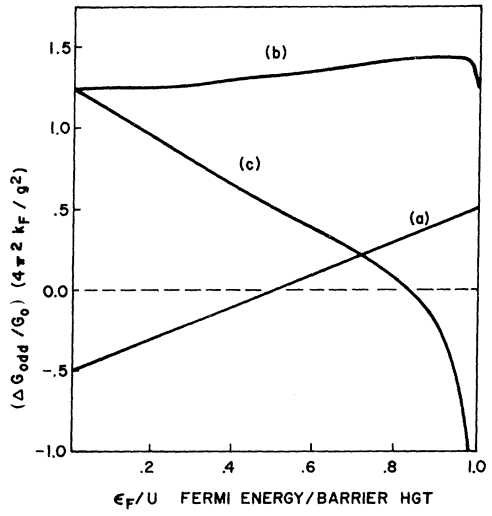

FIG. 8. The coefficient of the logarithmic singularity $\ln[(eV-\omega_E)/(eV+\omega_E)]$ for various approximations discussed in text.

From this result it seems quite unlikely that one obtains anything like assisted processes due to bulk metal phonons unless either the phonons extend into the barrier region itself or the coupling constant is sufficiently nonlocal so that the electrons see the metal ion motion in the barrier region. To illustrate the effect of the extension of the phonons into the barrier we consider the case where the phonons exist throughout the barrier as well as in metal A. The integration over z in Eq. (3.6) can be again carried out, however, the approximation of setting $\vec{k}_\perp = 0$ everywhere except in the exponent is no longer valid for calculating ΔG_e. It is true that the electron must have essentially all of its momentum perpendicular to the barrier to tunnel but since the phonons exist throughout the barrier it may admit a phonon before or after it tunnels. Setting $\vec{k}_\perp = 0$ does not allow for the former process, since in this case it is the final wave vector which must be perpendicular to the barrier. A closer examination of the integrals involved reveals that this effect can be taken into account by simply multiplying by 2 the term describing the process in which the electron goes directly through the barrier emitting a phonon without any reflections at the interfaces. One thus obtains for the contributions from the barrier region

$$\Delta G_e/G = (g^2/8\pi)(1/\kappa^2 k_F)\int_{-b}^{b} dz\{2e^{2\kappa(z+b)} + 2(\kappa^2 - k^2) + [(\kappa^2 - k^2)^2 - 4\kappa^2 k^2]e^{-2\kappa(z+b)}\} \times \int_0^{k_F} dk_z k_z^2 e^{-2k'(z+b)} , \quad (3.11)$$

$$\Delta G_{\text{odd}}/G = -(g^2/2\pi^2\kappa)\int_{-b}^{b} [1 + e^{-2\kappa(z+b)}(\kappa^2 - k^2)]\, dz \times \int_0^{k_F} dk' k'^2 e^{-2k'(z+b)} . \quad (3.12)$$

The results of doing these integrals have been added to the contributions from the bulk and the total coefficients are plotted against ϵ_F/U in Figs. 7 and 8, curves (c). As one can see the contribution from the barrier region dominates that from the bulk so that in this example the extra conductance will usually be predominantly of the assisted type.

IV. CONCLUSIONS

Several remarks regarding the relationship of the preceding calculations to experiment and previous calculations[1-6] are in order. We will consider first the magnetic impurity calculation. There have been a number of different theoretical calculations for this problem. Appelbaum,[4] using the tunneling Hamiltonian, calculated the current which flowed in the extra tunneling channel which he assumed was opened up by the magnetic impurity. This led to a conductance increase in order J^2, clearly independent of the sign of J, which manifested itself experimentally in a decrease[11,12] in conductance in the presence of an applied magnetic field. In third order Appelbaum (A) predicted a "zero-bias conductance peak" for $J > 0$, a dip for $J < 0$. This calculation was extended by Appelbaum, Phillips, and Tzoura[5] (APT) who showed, again using the tunneling Hamiltonian, that there are two contributions to the tunneling current, one which came from the extra channel opened by the impurity, as calculated by Appelbaum,[4] the second, identified as a local self-energy effect, led to a decrease in conductance to order J^2 and a "zero-bias conductance peak" for $J < 0$, a dip for $J > 0$. This second term was derived first using a Green's function formalism by Sólyom and Zawadowski. The method they used is the same as that used in this paper.

Sólyom and Zawadowski[6] drew a number of conclusions from their calculation. First, that to second order the conductance was always suppressed by a magnetic impurity. Second, they argued that the only way A and APT could obtain an enhanced conductance was from a nonlocal exchange interaction, one not assumed by A or APT. A third conclusion, really a consequence of the first, was that a conductance peak was obtained for $J > 0$, a dip for $J < 0$, which is opposite to that predicted by Appelbaum.

The results of the present calculation basically confirm those of Appelbaum. We find that when the magnetic impurity sits in the barrier region this leads to an enhancement of the tunneling current to order J^2, and a zero-bias conductance peak for $J < 0$. Sólyom and Zawadowski (SZ) obtain results opposite to those reported here because they failed to retain the real part of the unperturbed Green's function in their solution of Dyson's equation.

As the position of the impurity moves into the electrode region the forward and back scattering resulting from the impurity become comparable. This results in rapid (on the scale of $1/k_F$) spatial oscillation of the sign of the conductance change resulting from the magnetic scattering. The presence of spatial oscillations is contained in the work of SZ, but they erroneously argued that they are on a much longer scale than $1/k_F$, and therefore ignored them.

The implications of these results for experiment are as follows. With respect to the J^2 terms, magnetic impurities introduced into the barrier region result in an enhanced conductance manifested by a depression of conductance in a magnetic field.[11,12] For magnetic impurities intro-

duced into the electrode there may be a sizable reduction in the effect of these impurities on the conductance because of the cancellation among the impurities resulting from the spatial oscillations ΔG, the conductance charge due to a single impurity, as shown in Fig. 3. In those cases where the impurities are introduced randomly with respect to the oxide-metal interface the dominance of the barrier impurities in order J^2 will result in these tunnel junction exhibiting a characteristic negative magnetoresistance. If the impurities could be confined to the electrode region a rather novel positive magnetoresistance, as yet unobserved, could be expected.

The sign of the logarithmic conductance anomaly in third order is shown in Fig. 4. Once again, for impurities confined to the oxide barrier a conductance peak for $J<0$ is expected. For the case where the impurities are distributed randomly with respect to the interface, the sign of the effect is determined by a delicate balance between the barrier and electrode impurities. Unlike the J^2 term, the J^3 terms drop off rapidly with distance into the barrier, and therefore the barrier impurities do not exercise the dominant role in the logarithmic anomaly that they do in the magnetoresistance effect. This fact must be kept in mind when attempting to extract information about the size of J from the ratio of the logarithmic conductance anomaly to the magnetoresistance effect.

In the calculations of Sec. III for the electron-phonon coupled system it is clear that the exact nature of the metal-oxide interface plays an essential role in determining the characteristics of the many-body corrections to the tunneling current. However, the calculations do indicate that if the phonons exist only in the electrode and the electron-phonon interaction is local, one will obtain an increase in the even part of the resistance at the characteristic phonon frequencies of the bulk material. If, however, the phonons exist in the barrier, an increased even conductance is expected. Experimentally,[13–15] a number of junctions have been found in which the conductance anomalously increases at voltages equal to the positions of the peaks in the bulk metal phonon density of states. Assuming a local interaction we can only explain these results if the metal phonons extend into the barrier region. However, it is quite unlikely that the electron-phonon interaction can be considered to be local. In fact one might expect it to be particularly nonlocal near the metal barrier interface where screening by the conduction electrons becomes less effective. In this case we believe the assisted processes in the barrier will again dominate the current although we have not attempted to construct a model including the nonlocal character of the electron-phonon interaction. The model considered above is the same as that treated by Davis and Duke[16] for a semiconductor using the tunneling Hamiltonian approach and, more recently, by Davis.[10] They consider the effect of the bulk self-energy on the conductance. If we use the form for the tunneling matrix element, derived in the WKB approximation in Ref. 2 and include only the self-energy effects, we obtain Eqs. (3.7), (3.8). Davis, in his calculations, does not include the imaginary part of the self-energy and his result corresponds to Eq. (3.8). The Davis and Duke result is different in that they take the tunneling matrix element to be a constant. Their calculations, therefore, gives both the even and odd contributions to the current but the coefficients of these two terms differ considerably from Eqs. (3.7), (3.8). The ambiguities Davis and Duke discussed in using the tunneling Hamiltonian are not present in our calculations.

In conclusion, we believe that the calculations in Secs. III and IV clearly illustrate the usefulness of our approach to tunneling. In the case of the magnetic impurity it has allowed us to obtain a more fundamental picture of the effect and thereby eliminating a number of parameters in the original theory. For the magnetic impurity problem as well as for the electron-phonon interaction the approach exhibits clearly the spatial dependence of the various contributions to the current. Furthermore, it eliminates the necessity of dividing many-body effects into assisted processes and self-energy corrections as is done when the tunneling Hamiltonian approach is used. This division can still be made for interactions deep in the barrier but it is not useful for studying interface effects.

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Noninteracting Band Model for Dielectric Screening in Transition Metals: Application to Paramagnetic Nickel

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The static dielectric function is studied for a transition metal on the basis of a model band structure with noninteracting s and d bands. The free-electron approximation is used for electrons in the s band, while a simplified tight-binding scheme is used for the d electrons. Explicit expressions are obtained for the intraband and interband contributions to the dielectric function. The model is applied to calculate the static dielectric function for paramagnetic nickel for $(3d)^9\,(4s)^1$ and $(3d)^{9.4}\,(4s)^{0.6}$ configurations along the three principal symmetry directions [100], [110], and [111]. The contributions due to the intraband and interband transitions are compared: It is found that the major contribution to the dielectric function is due to the intraband transitions.

I. INTRODUCTION

The response of a many-electron system to an external perturbation can be discussed in terms of the frequency and wave-number–dependent dielectric function $\epsilon(\vec{q}, \omega)$.[1] Here $\vec{q}$ is the wave number and ω is the frequency. Nozières and Pines[2] and Ehrenreich and Cohen[3] deduced explicit expressions for the longitudinal component of the dielectric tensor within the random-phase approximation, and they did not consider the local field effects. Adler[4] deduced an integral equation for the generalized dielectric tensor, including local field effects, and discussed some limiting cases of the general expression. When we are dealing with a system of nearly free electrons, the complex expression for the dielectric function reduces to a simple form. There have been attempts at evaluation of the dielectric function for semiconductors,[5-7] but because of the difficulties introduced by the presence of d electrons, not much work has been done on the problem of dielectric screening in the transition metals. Recently, Hayashi and Shimizu[8] studied the dielectric screening in a transition metal. They considered two models, first a single-band model for d electrons and then a two-band model for s- and d-band electrons. They did not consider explicitely the contribution from the interband transitions.

In this paper, an explicit expression for the longitudinal component of the static dielectric tensor for a transition metal is deduced. The formalism, presented in Sec. II, is applied to the specific case of paramagnetic nickel in Sec. III. The results are discussed in Sec. IV.

II. THEORY

The general expression for the longitudinal static dielectric matrix in the random-phase approximation is[9]