Theory of Many-Body Effects in Tunneling

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A general expression for the current voltage relation in a metal-oxide-metal tunnel junction is derived on the assumption of many-body interactions in the metals as well as the oxide. In the absence of many-body effects in the barrier, the expression for the conductance we derive is similar to that obtained from the tunneling-Hamiltonian approach in that it depends on the convolution of the product of the two spectral functions of the metals with a quantity analogous to the tunneling coupling constant. The coupling or transfer matrix element here is frequency-dependent as well as momentum-dependent, and does not suffer from the high-energy divergences characteristic of the tunneling Hamiltonian. The effect of the local variation of the self-energy on the tunneling conductance is examined, and is shown to be capable of producing structure in the conductance proportional to both the real and imaginary parts of the frequency-dependent self-energy. Finally, the method is shown to be capable of describing the usual barrier-excitation-assisted tunneling current.

I. INTRODUCTION

IN the past, many-body effects in metal-insulator-metal junctions have been almost exclusively derived using the tunneling Hamiltonian approach proposed by Cohen, Falicov, and Phillips.[1] In this approach it is assumed that the electron tunneling can be described by introducing into the Hamiltonian for the two metals a term which transfers bare electrons from one metal to the other. Until recently, it was adequate to treat these matrix elements as constants.

Refinement of experimental techniques during the past few years has led to the observation of fine structure whose understanding requires more detailed knowledge of these matrix elements. Several authors[2] have derived expressions for the transfer matrix elements, but as has been pointed out by Appelbaum and Brinkman[3] and independently by Davis and Duke,[4] these expressions lead to unphysical behavior. This unphysical behavior results from calculating the matrix element assuming the electron energy in the barrier is the bare energy ϵ_k. When many-body interactions mix the one-particle states the use of this matrix element greatly overestimates tunneling via high-energy bare states.

It is the purpose of this paper to derive an expression for the tunneling current which does not suffer this defect and which we believe to be exact when the coupling between the two metal electrodes is weak. Our derivation of the tunneling current is based on a similar calculation due to Bardeen.[5] We adopt from this work the following points: (1) The electron current is determined by the rate of transfer of electrons from appropriately chosen states of one electrode to those of the other. (2) These states are defined by suitably extending the oxide barrier thickness to infinity. (3) The transfer matrix elements between the two electrodes, determined from a solution to the time-dependent Schrödinger equation, is related to the expectation value of the current operator between left and right states. Our calculation differs, however, from Bardeen's in two significant ways: (a) We do not speak in terms of quasiparticles but rather of electrons being transferred between exact many-body states of the two electrodes; and (b) we have included explicitly the possibility of assisted tunneling via barrier excitations.

Using this transfer matrix element procedure, we derive an expression for the current in terms of the spectral functions of the two metals evaluated in the barrier region. By calculating these spectral functions using the WKB approximation the current is related to the bulk spectral functions. In this expression the quantity analogous to the transfer matrix element of the tunneling Hamiltonian approach is frequency-dependent and does not suffer from nonphysical divergences.[3] The tunneling Hamiltonian is thus more correctly regarded as a pseudo-Hamiltonian whose matrix elements are energy-dependent.

As an electron approaches the barrier, its self-energy changes from one characteristic of the metal electrode to that characteristic of the barrier region. This change in the self-energy which we will call local self-energy effects can lead to corrections to the tunneling conductance which are proportional to the frequency-dependent part of the self-energy. Within the WKB approximation only a small correction due to the dissipative or imaginary part of the self-energy appears. The local self-energy effects can, however, give rise to a contribution to the current which depends on both the real and imaginary parts of the self-energy. The magnitude of this current depends on the detailed variation of the self-energy near the barrier.

For convenience, the paper is divided into three sections. In Sec. II the form of the transfer matrix element is derived for the electron-phonon coupled system using a heuristic approach. In this connection

[1] M. H. Cohen, L. M. Falicov, and J. C. Phillips, Phys. Rev. Letters **8**, 31 (1962).
[2] R. E. Prange, Phys. Rev. **131**, 1083 (1963); H. Hermann and A. Schmid, Z. Physik **211**, 313 (1968).
[3] J. A. Appelbaum and W. F. Brinkman, Phys. Rev. **183**, 553 (1969).
[4] L. C. Davis and C. B. Duke, Phys. Rev. (to be published).
[5] J. Bardeen, Phys. Rev. Letters **6**, 57 (1961).

the many-body wave functions are obtained by a variational technique. A more general formal derivation of the tunneling current is given in Sec. III. Included here will be a discussion of local self-energy effects and barrier excitations and a comparison of this work with previous tunneling theories.

II. HEURISTIC APPROACH

In this section we wish to present a derivation of an expression for the electron current in a tunnel junction making clear the physical content of the approach. The spirit of the section will therefore be intuitive and physical rather than formal. The formal justification and extension of the ideas to be presented now is reserved for Sec. III.

Essential to all previous tunneling theories and to the approach we take in this paper is the view that the electron tunnels between essentially independent many particle systems, i.e., the two electrodes. The small size of the electron current in the junction is a manifestation of the weak coupling between the two systems. This coupling depends crucially on the nature of the electron wave function in the barrier region.

An important prerequisite, therefore, for any correct theory of tunneling is that it must treat properly the behavior of the electronic wave functions in the barrier region. The fulfillment of this requirement is made difficult by the fact that even weak interactions in the bulk have a nonpertubative influence on the electron wave functions in the barrier. This means that the coupling between the two systems must be calculated in a representation which diagonalizes the Hamiltonians of both electrodes from the outset.

A convenient method of calculating the electron tunnel current is due to Bardeen.[5] He showed that if one has a set of states in which the electrons of each electrode are assumed to be distinguishable from those of the other electrode the matrix element for the transfer of an electron from one electrode to the other can be calculated by time-dependent perturbation theory. Bardeen's expression for this transfer matrix element is written in terms of the expectation value of the one electron current through a surface in the barrier region. The expectation value was assumed by Bardeen to be taken between two quasiparticle states, namely

$$M_{mn}=-\frac{1}{2m}\int \times\left[(\psi_m{}^Q)^*\frac{\partial\psi_n{}^Q}{\partial z}-\psi_n{}^Q\frac{\partial(\psi_m{}^Q)^*}{\partial z}\right]\delta(z-z_0)d^3r. \quad (2.1)$$

Here m and n label the quasiparticle states ψ^Q of the left- and right-hand side metals, respectively. It is our view that tunneling cannot be considered in terms of quasiparticles but rather must be thought of as the transfer of bare electrons between exact many-body states. Bardeen's expression can be retained, however, provided the quasiparticle wave functions are replaced by the probability amplitude of finding a many particle excitation in its bare electron configuration. As an example of this point of view we calculate the many-body wave functions for a junction in which the electrons interact with phonons in the left electrode only. In order to do this we divide the problem into left- and right-hand side problems by suitably extending the barrier to the left- or right-hand side so that the wave functions are localized in one or the other of the electrodes. The states of the right-hand-side electrode are taken to be independent particle states, while the left-hand states are eigenfunctions of the Hamiltonian

$$H_L=\int\psi^\dagger(\mathbf{r})\left(-\frac{\nabla^2}{2m}+V(\mathbf{r})\right)\psi(\mathbf{r})d^3r +\sum_{\mathbf{q}}\int g(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}}(b_{\mathbf{q}}{}^\dagger+b_{-\mathbf{q}})\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\theta(-z)d^3r +\sum_{\mathbf{q}}\omega_{\mathbf{q}}(b_{\mathbf{q}}{}^\dagger b_{\mathbf{q}}+\tfrac{1}{2}). \quad (2.2)$$

Here $V(\mathbf{r})$ is the self-consistent static potential which we take to be a step function $V(\mathbf{r})=V_0\theta(z)$. $\psi^\dagger(\mathbf{r})$ creates an electron at $\mathbf{r}$ while $b_{\mathbf{q}}{}^\dagger$ creates a phonon of momentum $\mathbf{q}$ and energy $\omega_{\mathbf{q}}$. The electron-phonon coupling is $g(\mathbf{q})$. For convenience, we assume a translationally invariant phonon system with the coupling to the electrons confined to the metal electrode. We approach the calculation of the wave functions from a variational principle[6] by adopting for the $(N+1)$ particle excited states the form

$$\left\{\int d^3r\ \varphi_m(\mathbf{r})\psi^\dagger(\mathbf{r})+\sum_{\mathbf{q}}\int d^3r[\varphi_m{}^1(\mathbf{q},\mathbf{r})\psi^\dagger(\mathbf{r})b_{\mathbf{q}}{}^\dagger +\varphi_m{}^2(\mathbf{q},\mathbf{r})\psi^\dagger(\mathbf{r})b_{-\mathbf{q}}]\right\}|0\rangle\equiv A_m{}^\dagger|0\rangle, \quad (2.3)$$

where $|0\rangle$ is the ground state of the N-particle system. The idea here is that the function $\varphi_m(\mathbf{r})$ is the one to be used in calculating the transfer matrix element. The choice of the above wave function is equivalent to the Migdal Approximation in the usual diagrammatic expansion. The most convenient variational scheme for obtaining the energies and wave functions is to vary

$$\langle 0|[A_m,[H,A_m{}^\dagger]_-]_+|0\rangle$$

subject to the normalization condition

$$\langle 0|[A_m,A_{m'}{}^\dagger]_+|0\rangle=\delta_{mm'}.$$

The variation of the anticommutator assures us that $A_m{}^\dagger$ creates an excited $(N+1)$ particle state and A_m creates an excited $(N-1)$ particle state and at the

[6] L. Roth, Phys. Rev. Letters **20**, 1431 (1968).

same time builds in particle-hole symmetry. Varying

$$\langle 0|[A_m,[H,A_m^\dagger]_-]_+|0\rangle$$

with respect to $\varphi_m^*(\mathbf{r})$, $\varphi_m^1(\mathbf{q},\mathbf{r})^*$, and $\varphi_m^2(\mathbf{q},\mathbf{r})^*$, we obtain

$$\left[-\frac{\nabla^2}{2m}+V(\mathbf{r})\right]\varphi_m(\mathbf{r})+\frac{1}{V}\sum_{\mathbf{q}} g(\mathbf{q})e^{-i\mathbf{q}_{||}\cdot\mathbf{r}}\cos q_z z \times\int d^3r'\varphi_m^1(\mathbf{q},\mathbf{r}')[\delta(\mathbf{r}-\mathbf{r}')-\langle\psi^\dagger(\mathbf{r}')\psi(\mathbf{r})\rangle] +\frac{1}{V}\sum_{\mathbf{q}} g(\mathbf{q})e^{-i\mathbf{q}_{||}\cdot\mathbf{r}}\cos q_z z \times\int d^3r'\varphi_m^2(\mathbf{q},\mathbf{r}')[\langle\psi^\dagger(\mathbf{r}')\psi(\mathbf{r})\rangle]=E_m\varphi_m(\mathbf{r}). \quad (2.4)$$

$$\left[E_m-\omega_{\mathbf{q}}-\left(-\frac{\nabla^2}{2m}+V(\mathbf{r})\right)\right]\varphi_m^1(\mathbf{q},\mathbf{r}) =+g(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}}\varphi_m^0(\mathbf{r}), \quad (2.5)$$

$$\left[E_m+\omega_{\mathbf{q}}-\left(-\frac{\nabla^2}{2m}+V(\mathbf{r})\right)\right]\varphi_m^2(\mathbf{q},\mathbf{r}) =-g(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}}\varphi_m^0(\mathbf{r}). \quad (2.6)$$

Using the translational invariance of the system parallel to the surface we write

$$\varphi_m(\mathbf{r})=e^{-i\mathbf{k}_{||}\cdot\mathbf{r}}\varphi_m(z)$$

and

$$\varphi_m^i(\mathbf{q},\mathbf{r})=e^{-i(\mathbf{k}_{||}-\mathbf{q}_{||})\cdot\mathbf{r}}\varphi_m^i(\mathbf{q},z).$$

The solutions for the $\varphi_m^i(\mathbf{q},z)$ can be obtained using the Green's function for the noninteracting system

$$G_{k||}(z,z',\omega)=\sum_{k_z>0}\frac{\psi_{k_z}^*(z)\psi_{k_z}(z')}{(\omega-\epsilon_{\mathbf{k}})}, \quad (2.7)$$

where we have adopted box normalization so that the poles of the Green's function can be considered discrete. With the help of (2.7), (2.5) and (2.6) become

$$\varphi_m^i(\mathbf{q},z)=\sum_{k_z}\frac{\psi_{k_z}^*(z)\int dz'\psi_{k_z}(z')e^{iq_zz'}\varphi_m(z')}{[E_m+(-1)^i\omega_q-\epsilon_{(\mathbf{k}-\mathbf{q})||k_z}]} \quad (i=1,2). \quad (2.8)$$

Putting these expressions into the equation for $\varphi_m(z)$, we obtain

$$\left[E_m-\epsilon_{\mathbf{k}||}-\left(-\frac{1}{2m}\frac{\partial^2}{\partial z^2}\right)-V(z)\right]\varphi_m(z) -\int\Sigma_{\mathbf{k}||}(z,z',E_m)\varphi_m(z')dz'=0, \quad (2.9)$$

$$\Sigma_{\mathbf{k}||}(z,z',E_m)=\sum_{\mathbf{q}}\sum_{k_z}|g(\mathbf{q})|^2e^{iq_zz}\psi_{k_z}^*(z) \times\psi_{k_z}(z')e^{-iq_zz'}\left\{\frac{1-f_{(\mathbf{k}-\mathbf{q})||k_z}}{(E_m-\omega_{\mathbf{q}}-\epsilon_{(\mathbf{k}-\mathbf{q})||k_z})} +\frac{f_{(\mathbf{k}-\mathbf{q})||k_z}}{(E_m+\omega_{\mathbf{q}}-\epsilon_{(\mathbf{k}-\mathbf{q})||k_z})}\right\}. \quad (2.10)$$

Likewise, the normalization condition reduces to

$$\int dzdz'\left\{\varphi_m^*(z)\left[\delta(z-z') -\frac{\partial}{\partial E_m}\Sigma_{\mathbf{k}||}(z,z',E_m)\right]\varphi_m(z')\right\}=1. \quad (2.11)$$

In the bulk of the electrode the self-energy becomes translationally invariant and can be written as

$$\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\Sigma_{\mathbf{k}}(E_m)$$

so that except near the surface the amplitude $\varphi_m(z)$ is a sine wave of the form

$$A_{k_z}^m(2/L)^{1/2}\sin(k_zz-\chi). \quad (2.12)$$

Here χ is the phase shift determined by the boundary conditions and $A_{k_z}^n$ is a normalization constant determined from (2.11). Using (2.12) this normalization condition reduces to

$$|A_{k_z}^n|^2=[1-(\partial\Sigma_{\mathbf{k}}(E)/\partial E|_{E_m}]^{-1}. \quad (2.13)$$

In order to determine the secular equation for the allowed values of the energy E_m we insert (2.12) into (2.9) obtaining the equation

$$E_{\mathbf{k}}^n-\epsilon_{\mathbf{k}}-\sum_{\mathbf{q}}|g(\mathbf{q})|^2\left\{\frac{(1-f_{\mathbf{k}-\mathbf{q}})}{E_{\mathbf{k}}^n-\epsilon_{\mathbf{k}-\mathbf{q}}-\omega_{\mathbf{q}}}+\frac{f_{\mathbf{k}-\mathbf{q}}}{E_{\mathbf{k}}^n-\epsilon_{\mathbf{k}-\mathbf{q}}+\omega_{-\mathbf{q}}}\right\} =[E_{\mathbf{k}}^n-\epsilon_{\mathbf{k}}-\Sigma_{\mathbf{k}}(E_{\mathbf{k}}^n)]=0, \quad (2.14)$$

where the index m has been replaced by two indices, $\mathbf{k}$ indicating the total momentum of the excitation and n indicating the various solutions of the above equation for given $\mathbf{k}$.

While these results hold in the bulk of the electrode the expression for the matrix element involves the $\varphi_{\mathbf{k}n}(z)$ in the barrier region. The simplest way to determine the wave function in this region is to assume that one can take into account the variation of the potential *and* that of the self-energy using the WKB approximation. In this case whenever z is in the barrier region

$$\varphi_{\mathbf{k}n}(z)\approx[(k_z/K)(2/L)]^{1/2}A_{\mathbf{k}}^ne^{-Kz}, \quad (2.15)$$

where $K=\{2m[V_0-(E_m-\epsilon_{\mathbf{k}||})]\}^{1/2}$. We will discuss the effect of the variation of the self-energy near the barrier on the preexponential factor in (2.15) further in Sec. III.

Using (2.15) for the form of $\varphi_{\mathbf{k}n}$ in the barrier, the transfer matrix element for taking an electron from a single particle state χ_1 on the right-hand side to the many-body state $(\mathbf{k},n)$ is

$$|M_{(\mathbf{k},n)1}|^2=\delta_{\mathbf{k}_{||},l_{||}}e^{-2Ka}4k_zl_z|A_{\mathbf{k}n}|^2 \equiv\delta_{\mathbf{k}_{||}l_{||}}|T_{(\mathbf{k},n)1}|^2|A_{\mathbf{k}n}|^2. \quad (2.16)$$

The barrier thickness is denoted by a. The current can be obtained summing on $\mathbf{k}$, n, and $\mathbf{l}$, taking into account the Pauli exclusion principle and energy conservation

$$I=4\pi e\sum_{\substack{\mathbf{k}\mathbf{l}\\ n}}|T_{(\mathbf{k},n)1}|^2\delta_{\mathbf{k}_{||},l_{||}}[f(E_{\mathbf{k}}{}^n)-f(\epsilon_1)] \times\delta(E_{\mathbf{k}}{}^n-\epsilon_1+eV)|A_{\mathbf{k}n}|^2 \quad (2.17)$$

$$=4\pi e\sum_{\substack{\mathbf{k}\mathbf{l}\\ n}}\delta_{\mathbf{k}_{||},l_{||}}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi} \times[f(\omega)-f(\omega')]|T_{\mathbf{k}1}(\omega)|^2\delta(\omega-\omega'+eV) \times\pi\delta(\omega'-\epsilon_1)\pi\delta(\omega-E_{\mathbf{k}n})|A_{\mathbf{k}n}|^2. \quad (2.18)$$

The $T_{\mathbf{k}1}(\omega)$ is $T_{(\mathbf{k},n)1}$ with $E_{\mathbf{k}n}$ replaced by ω. The sum over n can be performed

$$\sum_n\pi\delta(\omega-E_{kn})|A_{kn}|^2=\sum_n\frac{\pi\delta(\omega-E_{kn})}{[1-\partial\Sigma_k(E)/\partial E|E_{kn}]} =\int_c\frac{d\omega'}{2i}\delta(\omega-\omega')G_{\mathbf{k}}{}^L(\omega'). \quad (2.19)$$

Here

$$G_{\mathbf{k}}{}^L(\omega')\equiv[\omega'-\epsilon_{\mathbf{k}}-\Sigma_{\mathbf{k}}(\omega')]^{-1} \quad (2.20)$$

and the contour c is one which encloses the poles of $G_{\mathbf{k}}$ on the real axis. Thus

$$\sum_n\pi\delta(\omega-E_{\mathbf{k}n})|A_{\mathbf{k}n}|^2=\mathrm{Im}G_{\mathbf{k}}{}^L(\omega-i\delta). \quad (2.21)$$

Since

$$\pi\delta(\omega'-\epsilon_1)=\mathrm{Im}G_1{}^R(\omega'-i\delta), \quad (2.22)$$

the final expression for the current is

$$I=4\pi e\sum_{\mathbf{k}\mathbf{l}}\delta_{k_{||},l_{||}}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{d\omega'}{\pi}|T_{\mathbf{k}1}(\omega)|^2[f(\omega)-f(\omega')] \times\delta(\omega-\omega'+eV)\,\mathrm{Im}G_{\mathbf{k}}{}^L(\omega-i\delta)\,\mathrm{Im}G_1{}^R(\omega'-i\delta). \quad (2.23)$$

In this expression, T depends on ω as well as the momentum $\mathbf{k}$. In particular, $K=\{2m[V_0-(\omega-\epsilon_{\mathbf{k}_{||}})]\}^{1/2}$ and the unphysical weighting of high-energy states is not present. Formula (2.23) is similar to that obtained from the tunneling Hamiltonian approach. However, T is energy-dependent so that the tunneling Hamiltonian must be viewed as a pseudo-Hamiltonian similar to the pseudopotential of band theory.

The fact that the many particle effects enter formula (2.23) through the spectral functions can be traced back to the assumption that the electron only tunnels when in the bare electron configuration. This is essentially the view that the tunneling Hamiltonian takes and therefore it is not surprising that both approaches lead to similar results. However, it must be borne in mind that the local self-energy effects to be considered in Sec. III are not contained in the tunneling Hamiltonian, and an explicit expression for T has been obtained which may lead to qualitatively different behavior for the conductance than forms previously used.[7]

III. FORMAL DERIVATION

In this section we give a more detailed and rigorous justification of our heuristic approach to tunneling.[8] We will try to make our arguments independent of the interactions present in the junction except to assume they are short ranged. Consider a junction with a voltage V applied to the left-hand-side electrode at a given time ($t=0$) at which there are $N_R{}^0$ electrons in the right-hand-side electrode (metal R) and $N_L{}^0$ in the left (metal L). The current is to be calculated by determining the rate of transfer of a single electron from right to left. We assume that all the states of the electrons in the two electrodes in this nonequilibrium configuration are obtained by solving so-called left- and right-hand-side problems. These two problems are defined by extending the barrier potential so that the wave functions of a given metal drop off exponentially outside that metal. The total wave function is taken to be an antisymmetrized product of the left- and right-hand-side functions. By using wave functions of this type the electrons are definitely assigned to one or the other of the electrodes. The unsymmetrized product wave functions have the advantage that for a given choice of the number of electrons in each metal, say (N_R,N_L), they are eigenfunctions of the total Hamiltonian whenever the N_L electron coordinates are restricted to the region to the left of metal R and the remaining N_R coordinates are restricted to the right-hand side of metal L. This statement is valid provided the interactions are sufficiently short ranged so that there are no interactions across the barrier.

We assume at $t=0$ that the state of the total junction Ψ_0 is a symmetrized product of the ground states of the two electrodes. At time t the wave function has the form

$$\Psi(t)=a(t)\Psi_0e^{-iW_0t}+\Sigma b_{mn}(t)\Psi_{mn}e^{-iW_{mn}t}, \quad (3.1)$$

where Ψ_{mn} is a symmetrized product wave function with a single electron transferred from the right- to the left-hand-side electrode. W_0 (W_{mn}) is the expectation value of the total Hamiltonian $\mathcal{H}$ in state Ψ_0 (Ψ_{mn}). The rate at which an electron tunnels from the ground state in

[7] See Refs. 3 and 4 for a detailed discussion of these points.

[8] The technique used here is quite similar to that discussed by C. Herring for the calculation of exchange between well-separated atoms. C. Herring, in *Magnetism*, edited by G. T. Rado and H. Suhl (Academic Press Inc., New York, 1966), Vol. IIB.

metal R to a state m in metal L leaving R in the excited state n is

$$\partial/\partial t|b_{mn}(t)|^2=2\pi|M_{mn}|^2\delta(W_{mn}-W_0), \quad (3.2)$$

where

$$M_{mn}=\int \Psi_{mn}^*(H-W_0)\Psi_0 d\tau \quad (3.3)$$

and $d\tau$ refers to the total number of electrons in the junction as well as any external coordinates, such as phonons, and the domain of integration is over the entire junction. Consider a particular term in the above integral in which an electron labeled r_i' has been transferred across the barrier

$$\int \Psi_m{}^{l*}(r_1\cdots r_{Nl},r_i')\Psi_n{}^{r*}(r_1'\cdots r_{N_r-1}')(H-W_0)\Psi_0{}^l \times(r_1\cdots r_{Nl})\Psi_0{}^r(r_1'\cdots r_{N_r}')d\tau, \quad (3.4)$$

where the coordinate r_i' in $\Psi_0{}^r$ is contained in the set $\{r_1'\cdots r_{N_r}'\}$.

First consider a situation where the coordinates $\{r_1\cdots r_{Nl}\}$, $\{r_1'\cdots r_{N_r}'\}$ are restricted to the left- and right-hand-side electrodes, respectively. Because of the choice of wave functions the integrand vanishes identically in this region. Now consider relaxing this restriction for one coordinate at a time. In particular, start with any coordinate $r_j(j\neq i')$. Then $|\Psi^{(l,r)}(\cdots r_j)|^2$ in the integrand is at most second order, i.e., is proportional to $|T|^2$, the magnitude squared of the exponential tail of a wave function at the far end of the barrier. For the ith primed coordinate, however, the integration over the region to the left-hand side of the barrier will give a first-order contribution, i.e., proportional to $|T|$, the magnitude of the exponential tail and not its square. Thus to first order we can take the r_i' variable to range from some surface in the barrier ($z_i'=z_0$) to infinity on the left-hand side. Allowing the other variables to be unrestricted introduces errors of order $|T|^3$. Over this restricted region of integration the expression

$$\int d\tau\Psi_0{}^l(r_1\cdots r_{Nl})\Psi_0{}^r(r_1'\cdots r_{N_r}')(H-W_{mn})\Psi_m{}^{l*} \times(r_1\cdots r_{Nl},r_i')\Psi_n{}^{r*}(r_1',\cdots,r_{N_r}'-1) \quad (3.5)$$

vanishes to first order so it may be substracted from (3.4). Then since $W_{mn}=W_0$ we are left with

$$\int_{z_i<z_0}[\Psi_m{}^{l*}(r_1\cdots r_{Nl},r_i')\Psi_n{}^{r*}(r_1'\cdots r_{N_r}'-1) \times H\Psi_0{}^l(r_1\cdots r_{Nl})\Psi_0{}^r(r_1'\cdots r_{N_r}') -\Psi_0{}^l(r_1,\cdots,r_{Nl})\Psi_0{}^r(r_1'\cdots r_{N_r}')H\Psi_m{}^{l*} \times(r_1\cdots r_{Nl},r_i')\Psi_n{}^{r*}(r_1'\cdots r_{N_r}'-1)]d\tau. \quad (3.6)$$

The potential energy terms cancel out of this expression along with all kinetic energy operators except the $\mathbf{r}_i$th. The x_i' and y_i' terms vanish and the z_i' term can be written as the expectation value of the current operator:

$$-\frac{1}{2m}\int\Big[\Psi_m{}^{l*}(r_1,\cdots r_{Nl},r_i')\Psi_n{}^{r*}(r_1'\cdots r_{Nl}'-1) \times\frac{\partial}{\partial z_i'}\Psi_0{}^r(r_1'\cdots r_{N_r}')\Psi_0{}^l(r_1\cdots r_{Nl}) -\frac{\partial\Psi_m{}^{l*}}{\partial z_i'}(r_1,\cdots,r_{Nl},r_i')\Psi_n{}^{r*}(r_1'\cdots r_{N_r-1}') \times\Psi_0{}^r(r_1'\cdots r_{N_r}')\Psi_0{}^l(r_1\cdots r_{Nl})\Big]\delta(z_i-z_0)d\tau. \quad (3.7)$$

Taking the symmetrized sum of this expression and using the fact that

$$\int\prod_j d^3r_j\,\Psi_m{}^{l*}(r_1\cdots r_{Nl},r_i)\Psi_0{}^l(r_1\cdots r_{Nl}) =\frac{1}{(N_l)^{1/2}}\langle m|\psi^\dagger(\mathbf{r}_i)|0\rangle_L, \quad (3.8)$$

we obtain

$$M_{mn}=J_{mn}\equiv-\frac{1}{2m}\int d^3r\,\delta(z-z_0) \times\Big[\langle m|\psi^\dagger(\mathbf{r})|0\rangle_L\frac{\partial}{\partial z}\langle n|\psi(\mathbf{r})|0\rangle_R -\langle n|\psi(\mathbf{r})|0\rangle_R\frac{\partial}{\partial z}\langle m|\psi^\dagger(\mathbf{r})|0\rangle_L\Big]. \quad (3.9)$$

A number of points must now be made concerning the role interactions in the barrier play in the above derivation. We have assumed that both the left- and right-hand states have been diagonalized with respect to interactions in the barrier. Because of our use of product wave function this may lead to an overcounting of the degrees of freedom in the barrier. In practice, this overcounting does not appear to be a problem. As an example, consider a single ion (localized phonon mode) in the barrier region at $\mathbf{R}_0$. First let $\mathbf{R}_0$ be near metal L so that its interaction wi th the electrons in this electrode need not be negligible. It is then natural not to consider the dynamic interaction with this ion for the metal R states since these effects should lead to corrections of order the coupling constant squared times something like $|T|^2$. In the above derivation of the expression for the matrix element the only requirement was that the right and left wave functions be eigenfunctions of H up to the surface at which the expectation value of

the current is taken. If we take the surface z_0 to the right-hand side of $\mathbf{R}_0$ the above expression is correct. If z_0 were chosen to be to the left-hand side of $\mathbf{R}_0$ then in expression (3.5) it would be necessary to omit the term describing the interaction between the electrons and this localized mode. The electron ion interaction does not drop out of (3.6) and

$$M_{mn}=J_{mn}+\int \Psi^{mn*}H_{ep}\Psi_0 d\tau. \tag{3.10}$$

The extra term when analyzed is the expression usually given for assisted tunneling. As must be the case a detailed calculation shows that these two expressions for M_{mn} are identical. The usual assisted tunneling is contained in the expression for the current whenever the surface is to the right-hand side of $\mathbf{R}_0$. Both expressions are capable of including corrections due to the fact that $\mathbf{R}_0$ is near metal L. If these corrections are not important one need not diagonalize either side with respect to this interaction and M_{mn} has the form (3.10) independent of the location of z_0. The independence of the assisted term on the method of calculation enhances our confidence in the procedure's ability to handle barrier excitations. Returning now to Eq. (3.9) and assuming that the interactions are confined to the electrodes, we first need to analyze the behavior of the spectral amplitude $\langle m|\psi^\dagger(\mathbf{r})|0\rangle_L$ in the barrier region. To do this we introduce the left-hand Green's function

$$G^L(\mathbf{r},\mathbf{r}';E)=\sum_m \frac{\langle 0|\psi(\mathbf{r})|m\rangle_L\langle m|\psi^\dagger(\mathbf{r}')|0\rangle_L}{E-E_{m0}} + \sum_{m'} \frac{\langle 0|\psi^\dagger(\mathbf{r}')|m'\rangle_L\langle m'|\psi(\mathbf{r})|0\rangle_L}{E-E_{m'0}}. \tag{3.11}$$

The equation satisfied by $G^L(r,r';E)$ is

$$\int\left\{\left[E-\left(-\frac{\nabla_r^2}{2m}+V(\mathbf{r})\right)\right]\delta(\mathbf{r}-\mathbf{r}'')-\Sigma(\mathbf{r},\mathbf{r}'';E)\right\} \times G^L(\mathbf{r}'',\mathbf{r}';E)d^3r''=\delta(\mathbf{r}-\mathbf{r}'), \tag{3.12}$$

where $\Sigma(\mathbf{r},\mathbf{r}'',E)$ is the usual self-energy operator, and $V(\mathbf{r})$ includes the static barrier potential. For finite volume, the sums on m are discrete sums so consistency of (3.12) for E near E_{m0} requires that

$$\int d^3r\left\{\left[E_{m0}-\left(-\frac{\nabla_r^2}{2m}+V(\mathbf{r})\right)\right]\delta(\mathbf{r}-\mathbf{r}')-\Sigma(\mathbf{r},\mathbf{r}';E_{m0})\right\} \times\langle m|\psi^\dagger(\mathbf{r}')|0\rangle_L=0. \tag{3.13}$$

For $\mathbf{r}$ in the barrier $\Sigma(\mathbf{r},\mathbf{r}';E)=0$ and

$$\langle m|\psi^\dagger(\mathbf{r})|0\rangle_L =C\exp\{-[2m(V-E_{m0}+\epsilon_{k||})]^{1/2}z\}\, e^{i\mathbf{k}_{||}\cdot\mathbf{r}}, \tag{3.14}$$

where we have assumed a plane wave solution parallel to the junction interface with wave vector $k_{||}$ which has energy $\epsilon_{k||}$.

The value of C depends on the over-alln ormalization of $\langle m|\psi^\dagger(\mathbf{r})|0\rangle_L$ determined in the bulk as well as the detailed matching of this solution on to that in the bulk. The normalization of $\langle m|\psi^\dagger(\mathbf{r})|0\rangle_L$ can be obtained by looking for the residue at $E=E_{0m}$ of the integral

$$\int d^3r\, G(\mathbf{r},\mathbf{r};E). \tag{3.15}$$

This integral is determined by the value of G in the bulk of the electrode. In the bulk $G(\mathbf{r},\mathbf{r};E)$ is independentof $\mathbf{r}$:

$$G(\mathbf{r},\mathbf{r};E)=\frac{1}{V}\sum_{\mathbf{k}}\frac{1}{[E-\epsilon_{\mathbf{k}}-\Sigma_{\mathbf{k}}(E)]}. \tag{3.16}$$

Since the $\langle m|\Psi^\dagger(\mathbf{r})|0\rangle$ must be characterized by a $\mathbf{k}$ vector in the bulk E_{0m} must be one of the zeros of $[E-\epsilon_{\mathbf{k}}-\Sigma_{\mathbf{k}}(E)]=0$ say $E_{\mathbf{k}_n}$. The residue is then $(1-\partial\Sigma_{\mathbf{k}}{}^{(E)}/\partial E|_{E_{\mathbf{k}n}})^{-1}$. From this we see that the functions $\langle m|\psi^\dagger(\mathbf{r})|0\rangle$ are exactly identical to the $\varphi_{\mathbf{k}n}(\mathbf{r})$ used in Sec. II and the expression for the current is exactly that obtained there. This expression is therefore independent of the form of the interactions considered within the validity of the WKB approximation.

Instead of relating the current to the bulk spectral functions as we have done one can go on from the expression (3.9) for M_{mn} to write an expression for the current in terms of the Green's functions of the two metals *evaluated in the barrier.* Defining

$$\mathrm{Im}G(\mathbf{r},\mathbf{r}',\omega)=\frac{1}{2i}[G(\mathbf{r},\mathbf{r}',\omega+i\delta)-G(\mathbf{r},\mathbf{r}',\omega-i\delta)]$$

one finds without difficulty

$$I=-2\pi e\int\frac{d\omega}{\pi}\theta(\omega)\int\frac{d\omega'}{\pi}[1-\theta(\omega')]\delta(\omega-\omega'+eV)\int d^3r d^3r'\,\delta(z-z_0)\delta(z'-z_0)\frac{1}{(2m)^2} \times\left\{\mathrm{Im}G^R(\mathbf{r}',\mathbf{r},\omega)\frac{\partial^2}{\partial z\partial z'}\mathrm{Im}G^L(\mathbf{r},\mathbf{r}',\omega')+\frac{\partial^2}{\partial z\partial z'}\mathrm{Im}G^R(\mathbf{r}',\mathbf{r},\omega)\,\mathrm{Im}G^L(\mathbf{r},\mathbf{r}',\omega')\right. -\frac{\partial}{\partial z}\mathrm{Im}G^R(\mathbf{r}',\mathbf{r};\omega)\frac{\partial}{\partial z'}\mathrm{Im}G^L(\mathbf{r},\mathbf{r}',\omega')-\frac{\partial}{\partial z'}\mathrm{Im}G^R(\mathbf{r}',\mathbf{r};\omega)\frac{\partial}{\partial z}\mathrm{Im}G^L(\mathbf{r},\mathbf{r}',\omega')\Big\}. \tag{3.17}$$

An expression like (3.17) was derived previously by Zawadowski[9] by a different method. However, Zawadowski then assumed that the Green's function of the metal in the presence of the barrier could be written in a diagonal form by a suitable choice of one-electron wave functions. This incorrect assumption introduces all the difficulties associated with the tunneling Hamiltonian.

In concluding this section we want to consider further the effect of the local variation of the self-energy near the barrier. Up until now we have treated these effects within the WKB approximation which is valid provided their spatial variation is characterized by a wavelength long compared with the Fermi wavelength and the self-energy is zero inside the barrier. This approximation leads to a small decrease in the conductance proportional to the imaginary part of the self-energy. This decrease is due to dissipation caused by back scattering in the electrode. For normal metal tunneling the use of the WKB approximation may not be correct. For example, the self-energy may exhibit Friedel-like oscillations due to the presence of the barrier. One must then go beyond the WKB approximation and the conductance will depend on both the real and imaginary parts of the self-energy. The magnitude and even the sign of these contributions depend on the behavior of the self-energy near the barrier. Such effects although small may have been seen in a number of cases[4,10] and are currently under further investigation.

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Spin Correlations in the Electron Liquid*

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An expression for the frequency- and wave-vector–dependent paramagnetic susceptibility of the electron gas at metallic densities is derived, using a previously given generalization of the random-phase approximation which takes short-range correlations between the electrons into account. The enhancement factor for the susceptibility is given as a functional of the difference between the correlation functions for pairs of electrons with parallel and antiparallel spins, which are determined in a self-consistent manner by means of the fluctuation-dissipation theorem. Explicit numerical calculations of these correlation functions are presented and compared with the results of previous theories. The present expression of the dynamic susceptibility for the paramagnetic case is a generalization of the expression given earlier by Izuyama, Kim, and Kubo, where the internal field is now a function of the wave vector.

I. INTRODUCTION

In an earlier paper,[1] hereafter referred to as I, a generalization of the random-phase approximation[2] (RPA) for the electron gas on a uniform positive background was given, which takes the short-range correlations between the electrons into account. In this formulation, the dielectric function is a functional of the pair correlation function, and the latter is evaluated in a self-consistent manner using the fluctuation-dissipation theorem. The calculated pair correlation function was found to satisfy the requirement of positive-definiteness for all values of $r_s \lesssim 4$, and to

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