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Impurity-Assisted Inelastic Tunneling: Many-Electron Theory

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The one-electron theory of impurity-assisted tunneling is extended to a many-electron system. A formal derivation of the wave function through second order in the interaction potential is given for an arbitrary barrier potential and an arbitrary interaction potential. Application to a one-dimensional square-barrier model with energy-loss mechanisms confined to the barrier region is made. The magnitude of the inelastic current resulting from the excitation of a molecular impurity is in agreement with the results of the transfer-Hamiltonian model if the appropriate current-carrying wave functions are used to calculate the transfer matrix elements. Additional second-order terms which give rise to logarithmic singularities and step-function decreases in the barrier-penetration factor are found for interaction potentials which are large near the boundaries of the tunnel barrier. Numerical calculations show that, for a molecular impurity at the boundary, the line shapes in d^2I/dV^2 versus V are fundamentally different from those for an impurity inside the barrier by more than $\sim\frac{1}{2}$ K.

I. INTRODUCTION

In a previous paper,[1] a theory of one electron interacting with a molecular impurity in a tunneling barrier was given. We here extend the theory to a many-electron system. The need for a many-electron theory arises because the tunneling experiments of Jaklevic and Lambe[2,3] reveal structure in the curves of d^2I/dV^2 versus voltage due to the energy-loss mechanisms in the barrier which explicitly involve the statistics of the many-electron system.

In Sec. II, we derive a general theory of many electrons interacting with a vibrator in first Born approximation. (As in I, the vibrator is representative of the molecular impurity, or, in general, of phonons, magnetic impurities in a magnetic field, etc.) Since it is unnecessary to restrict the formal analysis in Sec. II to one dimension or to interactions entirely within the barrier, the results of this section are quite general and may be useful for problems other than that considered in this paper. For simplicity, however, we first apply the general theory (first Born approximation) to a one-dimensional square-barrier model with the interactions confined to the barrier region in Sec. III. Since it appears that the results of first Born approximation are sufficient for the interpretation of the experiments by Jaklevic and Lambe,[2,3] and since this provides a simple picture of the physical processes involved, we calculate the current neglecting any other terms which are of the same order (second) in the interaction potential in this section for the one-dimensional model. We also discuss the results for a three-dimensional model. In Sec. IV, the general theory of Sec. II is extended to second Born approximation. In Sec. V, the general theory (second Born approximation) is applied to the one-dimensional model of Sec. III. An examination of the second-order terms omitted from the current in Sec. III is given and the implications of such terms for the interpretation of a variety of experiments are discussed. Our conclusions are stated in Sec. VI.

II. GENERAL THEORY: FIRST BORN APPROXIMATION

In this section a general theory of many electrons interacting with a single vibrator is formulated in first Born approximation. The direct Coulomb interaction between electrons is neglected except insofar as it can be represented by an effective self-consistent field which is contained in the one-particle Hamiltonian. The positions of the N electrons comprising the system are labeled by $1, 2, \ldots, N$. The internal coordinate of the vibrator is ξ. The Hamiltonian for the system is given by

$$\mathcal{H}(1, 2, \ldots, N; \xi) = \sum_i \mathcal{H}_e(i) + \mathcal{H}_v(\xi) + \sum_i \mathcal{H}_{ev}(i, \xi), \tag{2.1}$$

where $\mathcal{H}_e(i)$ is the Hamiltonian for the ith electron, $\mathcal{H}_v(\xi)$ is the Hamiltonian for the vibrator, and $\mathcal{H}_{ev}(i, \xi)$ is the interaction Hamiltonian for the ith electron interacting with the vibrator. We expand the wave function $\Psi(1, 2, \ldots, N; \xi)$ for the system

$$\Psi(1, 2, \ldots, N; \xi) = \sum_n \chi_n(1, 2, \ldots, N)\Phi_n(\xi), \tag{2.2}$$

where Ψ satisfies the Schrödinger equation

$$\mathcal{H}(1, 2, \ldots, N; \xi)\Psi(1, 2, \ldots, N; \xi) = E\Psi(1, 2, \ldots, N; \xi), \tag{2.3}$$

the vibrator eigenfunctions $\Phi_n(\xi)$ satisfy Eq. (I2.3)

(in paper I) and E is the total energy of the system. If we restrict the sum in Eq. (2.2) to the ground state and the first excited state of the vibrator, we find

$$\sum_i \mathcal{H}_e(i)\chi_0(1,2,\ldots,N)+\sum_i U(i)\chi_1(1,2,\ldots,N)$$

$$=\epsilon\chi_0(1,2,\ldots,N), \tag{2.4a}$$

$$\sum_i \mathcal{H}_e(i)\chi_1(1,2,\ldots,N)+\sum_i U(i)\chi_0(1,2,\ldots,N)$$

$$=(\epsilon-\hbar\omega)\chi_1(1,2,\ldots,N), \tag{2.4b}$$

where

$$U(i)=\int d\xi\ \Phi_1^*(\xi)\mathcal{H}_{ev}(i,\xi)\Phi_0(\xi)\ , \tag{2.5a}$$

$$\epsilon=E-E_{v0}\ , \tag{2.5b}$$

$$\hbar\omega=E_{v1}-E_{v0}\ . \tag{2.5c}$$

We assume that $U(i)$ is real and we neglect terms such as

$$\int d\xi\ \Phi_0^*(\xi)\mathcal{H}_{ev}(i,\xi)\Phi_0(\xi)\ .$$

We have not been able to find the exact solution to Eq. (2.4) even for as simple an interaction potential as Eq. (I3.1). The reason is that Eq. (2.4) is not separable which means that the exact χ_0 and χ_1 can not be taken as a simple product (or suitably antisymmetrized linear combination) of the form $\prod_i \psi_i(i)$. We can, however, use a generalization of the first Born approximation (Sec. II of I).

In lowest order,

$$\sum_i \mathcal{H}_e(i)\chi_0^{(0)}(1,2,\ldots,N)=\epsilon\chi_0^{(0)}(1,2,\ldots,N)\ . \tag{2.6}$$

We assume that the eigenvalues for the system ϵ are essentially continuous so that ϵ can be regarded as a parameter. That is, for every solution of the unperturbed problem with energy ϵ [Eq. (2.6)], there is a corresponding solution of the perturbed problem [Eq. (2.4)] with the same energy ϵ. A solution to Eq. (2.6) is

$$\chi_0^{(0)}(1,2,\ldots,N)=\psi_\alpha(1)\psi_\beta(2)\cdots\psi_\omega(N)\ , \tag{2.7}$$

where

$$\mathcal{H}_e(i)\psi_\mu(i)=\epsilon_\mu\psi_\mu(i),\quad \mu=\alpha,\beta,\ldots,\omega\ , \tag{2.8a}$$

$$\epsilon=\epsilon_\alpha+\epsilon_\beta+\cdots+\epsilon_\omega. \tag{2.8b}$$

We assume that we know the eigenfunctions $\psi_\mu(i)$ and eigenvalues ϵ_μ of $\mathcal{H}_e(i)$.

In first order,

$$\left[\sum_i \mathcal{H}_e(i)-\epsilon+\hbar\omega\right]\chi_1^{(1)}(1,2,\ldots,N)$$

$$=-\sum_i U(i)\chi_0^{(0)}(1,2,\ldots,N). \tag{2.9}$$

Equation (2.9) is inhomogeneous with the sum over i on the right-hand side representing a number of sources. Clearly, the solution $\chi_1^{(1)}$ is a superposition of solutions, one for each source. Therefore, we find

$$\chi_1^{(1)}(1,2,\ldots,N)=\psi'_\alpha(1)\psi_\beta(2)\cdots\psi_\omega(N)$$

$$+\psi_\alpha(1)\psi'_\beta(2)\cdots\psi_\omega(N)+\cdots+\psi_\alpha(1)\psi_\beta(2)\cdots\psi'_\omega(N)\ , \tag{2.10}$$

where

$$\left[\mathcal{H}_e(i)-\epsilon_\mu+\hbar\omega\right]\psi'_\mu(i)=-U(i)\psi_\mu(i)\ . \tag{2.11}$$

We can find $\psi'_\mu(i)$ in a manner similar to that used to find $\psi'(x)$ in Sec. II of I.

To take into account the statistics of the electrons correctly, we should write Eq. (2.7) not as a simple product but as a Slater determinant. It is straightforward to show that if

$$\chi_0^{(0)}(1,2,\ldots,N)$$

$$=(N!)^{-1/2}\begin{vmatrix}\psi_\alpha(1) & \psi_\beta(1) & \cdots & \psi_\omega(1)\\ \psi_\alpha(2) & \psi_\beta(2) & \cdots & \psi_\omega(2)\\ & & \cdots & \\ \psi_\alpha(N) & \psi_\beta(N) & \cdots & \psi_\omega(N)\end{vmatrix} \tag{2.12a}$$

$$\equiv D(\psi_\alpha\psi_\beta\cdots\psi_\omega) \tag{2.12b}$$

[we use the symbol D to represent the determinant in (2.12a) made up of the functions ψ_α, ψ_β, ..., and ψ_ω],
then

$$\chi_1^{(1)}(1,2,\ldots,N)=D(\psi'_\alpha\psi_\beta\cdots\psi_\omega)$$

$$+D(\psi_\alpha\psi'_\beta\cdots\psi_\omega)+\cdots+D(\psi_\alpha\psi_\beta\cdots\psi'_\omega)\ . \tag{2.13}$$

The wave functions $\psi_\mu(i)$ are to include a spin function, either spin up or spin down, in addition to a function of position. We note that $\psi'_\mu(i)$ has the same spin function as $\psi_\mu(i)$ if $U(i)$ contains no spin-flip terms. In general, $U(i)$ may contain a slip-flip term if the impurity is magnetic, in which case $\psi'_\mu(i)$ will contain a term with a spin function opposite to that of $\psi_\mu(i)$. The wave function $\psi'_\mu(i)$ is first order in U and Eq. (2.13) is called first Born approximation in this paper.

To calculate the current of the system of electrons through order U^2 (the lowest order of the effects of the vibrator on the current) we ultimately

must go to second Born approximation (to include all of the terms of order U^2). To do so, we observe the following. In the first determinant of Eq. (2.13), we can replace $\psi'_\alpha(i)$ by

$$f_\alpha(i) = \psi'_\alpha(i) - \sum'_\eta \langle \psi_\eta | \psi'_\alpha \rangle \psi_\eta(i),$$

where the sum is over all occupied states. [By "occupied" or "unoccupied," we refer to states occupied or unoccupied in $\chi_0^{(0)}$.] The prime on the summation sign indicates that only occupied states are considered. This does not change the value of the determinant, since we are adding to the first column multiples of other columns in the determinant. The term $\eta = \alpha$ can be included because the $\langle \psi_\alpha | \psi'_\alpha \rangle$ term makes a negligible contribution to the sum on η for the nearly continuous spectrum of eigenfunctions we are considering, since there is a finite energy difference $\hbar\omega$ between ψ_α and ψ'_α. In general, then, we can make the replacement

$$\psi'_\mu(i) \to f_\mu(i),$$

where

$$f_\mu(i) = \psi'_\mu(i) - \sum'_\eta \langle \psi_\eta | \psi'_\mu \rangle \psi_\eta(i). \quad (2.14)$$

(The sum on η is over occupied states.) Clearly, $f_\mu(i)$ possesses the same spin function as $\psi'_\mu(i)$ and $\psi_\mu(i)$ if $U(i)$ contains no spin-flip terms. Equation (2.13) becomes

$$\chi_1^{(1)}(1, 2, \cdots, N) = D(f_\alpha \psi_\beta \cdots \psi_\omega) + D(\psi_\alpha f_\beta \cdots \psi_\omega) + \cdots + D(\psi_\alpha \psi_\beta \cdots f_\omega). \quad (2.15)$$

In first Born approximation, then, the wave function for the system (electrons plus vibrator) is given by Eq. (2.2) with χ_0 obtained from Eq. (2.12) and χ_1 from Eq. (2.15). All other χ_n $(n = 2, 3, \ldots)$ are set equal to zero.

III. ONE-DIMENSIONAL MODEL IN FIRST BORN APPROXIMATION

A. Calculation of $\chi_0^{(0)}$

In Sec. III, we solve for the many-electron wave function for a vibrator in a square barrier in first Born approximation, such as we did for a single electron in Sec. II of I. We again restrict the analysis to one dimension and ignore the spin of the electrons for simplicity. We first obtain $\chi_0^{(0)}(1, 2, \ldots, N)$. The Hamiltonian for an electron is given by Eq. (I2.2). The eigenfunctions of the Hamiltonian in Eq. (I2.2) are of two types. The first is a current-carrying state representing an electron approaching the barrier from the left which we call a left-hand state,

$$\psi_l(k, x) = (2L)^{-1/2}[e^{ikx} + R(k)e^{-ikx}], \quad x < 0$$
$$= (2L)^{-1/2}[C(k)e^{-Kx} + D(k)e^{Kx}], \quad 0 < x < b$$
$$= (2L)^{-1/2}T(k)e^{ik(x-b)}, \quad b < x. \quad (3.1a)$$

$$\epsilon(k) = \hbar^2 k^2/2m, \quad K = \{2m[V_0 - \epsilon(k)]/\hbar^2\}^{1/2}. \quad (3.1b)$$

We normalize in the interval $-L < x < L (L \gg b)$. $R(k)$ is given by Eq. (I2.11b), $D(k)$ by (I2.11c), $T(k)$ by (I2.11d), and $C(k)$ by (I2.11e).

The second type of state is that corresponding right-hand state which is found by replacing x by $b - x$ in Eq. (3.1)

$$\psi_r(k, x) = (2L)^{-1/2}T(k)e^{-ikx}, \quad x < 0$$
$$= (2L)^{-1/2}[C(k)e^{-K(b-x)} + D(k)e^{K(b-x)}], \quad 0 < x < b$$
$$= (2L)^{-1/2}[e^{-ik(x-b)} + R(k)e^{ik(x-b)}], \quad b < x. \quad (3.2)$$

If we restrict k to positive-integer multiples of π/L, we find that the states (3.1) and (3.2) form an orthonormal set in the limit $L \to \infty$ which is complete for our purposes.

In the limit that $U \to 0$, $\chi \to \chi_0^{(0)}$. Therefore, the state $\chi_0^{(0)}$ is the ground state of the electrons at $T = 0$ K with a net current flowing through the barrier when there are no interactions between the electrons and the vibrator. Such a state is made up by filling all the left-hand states with energy less than the Fermi level on the left and all the right-hand states with energy less than the Fermi level on the right. One can show that such a choice for $\chi_0^{(0)}$ gives the correct independent-particle current as obtained by more conventional means. To avoid complicating the wave functions of Eqs. (3.1) and (3.2), the shift of the energy zero on one side of the barrier relative to the other due to the bias voltage will be neglected. We instead simulate the effect of the bias voltage V across the barrier by increasing the Fermi energy E_F on the side of the barrier from which electrons flow. Thus, to make up the state $\chi_0^{(0)}$, we fill all the left-hand states with $\epsilon(k) \le E_{Fl} = \hbar^2 k_{Fl}^2/2m$ and all the right-hand states with $\epsilon(k) \le E_{Fr} = \hbar^2 k_{Fr}^2/2m$. We let $E_{Fl} - E_{Fr} = eV$; at equilibrium, $E_{Fl} = E_{Fr} = E_F$ and $V = 0$. This is only a convenient simplification and is not essential, but it is reasonably accurate for the low-bias voltages of interest.

B. Calculation $\chi_1^{(1)}$

In first Born approximation, we must solve equations of the following form [see Eq. (2.11)] for left-hand states,

$$[\mathcal{H}_e(x) - \epsilon(k) + \hbar\omega]\psi'_l(k, x) = -U(x)\psi_l(k, x). \quad (3.3)$$

The solution is

$$\psi'_l(k, x) = \int_0^b dx' K(\epsilon(k) - \hbar\omega, x, x') U(x') \psi_l(k, x'), \quad (3.4)$$

where $K(\epsilon, x, x')$ is given by Eq. (I2.14). [Note that k and K appearing in Eq. (I2.14) are determined by Eqs. (I2.14h) and (I2.14i) with $\epsilon = \epsilon(k) - \hbar\omega$.] We consider $U(x)$ to be nonzero only for $0 < x < b$.

Outside the barrier region, we find from Eq. (I2.14a)

$$\psi_l'(k, x) = (2L)^{-1/2} R_l'(k) e^{-ik'x}, \quad x < 0$$
$$= (2L)^{-1/2} T_l'(k) e^{ik'(x-b)}, \quad b < x \tag{3.5a}$$

where

$$k' = \{2m[\epsilon(k) - \hbar\omega]/\hbar^2\}^{1/2}, \tag{3.5b}$$

$$R_l'(k) = (2L)^{1/2} \times \int_0^b dx' K(\epsilon(k) - \hbar\omega, 0, x') U(x') \psi_l(k, x'), \tag{3.5c}$$

$$T_l'(k) = (2L)^{1/2} \times \int_0^b dx' K(\epsilon(k) - \hbar\omega, b, x') U(x') \psi_l(k, x'). \tag{3.5d}$$

In a similar manner, we find for right-hand states

$$\psi_r'(k, x) = \int_0^b dx' K(\epsilon(k) - \hbar\omega, x, x') U(x') \psi_r(k, x') \tag{3.6a}$$

$$= (2L)^{-1/2} T_r'(k) e^{-ik'x}, \quad x < 0$$
$$= (2L)^{-1/2} R_r'(k) e^{ik'(x-b)}, \quad b < x \tag{3.6b}$$

where

$$T_r'(k) = (2L)^{1/2} \times \int_0^b dx' K(\epsilon(k) - \hbar\omega, 0, x') U(x') \psi_r(k, x'), \tag{3.6c}$$

$$R_r'(k) = (2L)^{1/2} \times \int_0^b dx' K(\epsilon(k) - \hbar\omega, b, x') U(x') \psi_r(k, x'). \tag{3.6d}$$

We note that $T_r'(k)$ is found from $T_l'(k)$ by replacing $\psi_l(k, x')$ by $\psi_r(k, x')$ and $K(\epsilon(k) - \hbar\omega, 0, x')$ by $K(\epsilon(k) - \hbar\omega, b, x')$ in the integrand of Eq. (3.5c). Similar considerations apply to $R_l'(k)$ and $R_r'(k)$.

We now wish to find the $f_\mu(i)$ functions of Eq. (2.14) corresponding to $\psi_l'(k, x)$. We must subtract out of $\psi_l'(k, x)$ its projection on the occupied states. Consider first the occupied left-hand states, letting q run over the occupied left-hand states, we find

$$\sum_{q<k_{Fl}} \langle \psi_l(q) | \psi_l'(k) \rangle \psi_l(q, x) = \sum_{q<k_{Fl}} (2iL)^{-1} [R^*(q) R_l'(k) + T^*(q) T_l'(k) \left(\frac{1 - \exp[-i(q - k')L]}{q - k'} \right)$$

$$\times (2L)^{-1/2} \begin{cases} [e^{iqx} + R(q) e^{-iqx}], & x < 0 \\ [C(q) e^{-Qx} + D(q) e^{Qx}], & 0 < x < b \\ T(q) e^{iq(x-b)}, & b < x \end{cases} \tag{3.7a}$$

where

$$Q = \{2m[V_0 - \epsilon(q)]/\hbar^2\}^{1/2}. \tag{3.7b}$$

[We neglect terms $\propto \{1 - \exp[-i(q + k')L]\}/(q + k')$ since the denominator never vanishes, and we neglect the overlap in the barrier which is $\propto b/L \to 0$.] Considering $x < 0$ and $b < x$ first, we see that only those states with $q \simeq k'$ are important, so we can evaluate the slowly varying functions $R^*(q)$ and $T^*(q)$ at $q = k'$ (slowly varying on the scale of $1/L$). We next replace $\sum_{q<k_{Fl}} \cdots$ by

$$(L/\pi) \int_0^{k_{Fl}} dq \cdots.$$

Equation (3.6) becomes

$$\sum_{q<k_{Fl}} \langle \psi_l(q) | \psi_l'(k) \rangle \psi_l(q, x) = (2\pi i)^{-1} [R^*(k') R_l'(k) + T^*(k') T_l'(k)]$$

$$\times (2L)^{-1/2} \begin{cases} [e^{ik'x} I^+(k_{Fl}, k', x) + R(k') e^{-ik'x} I^-(k_{Fl}, k', x)], & x < 0 \\ T(k') e^{ik'(x-b)} I^+(k_{Fl}, k', x - b), & b < x \end{cases} \tag{3.8}$$

where ($k > 0$)

$$I^\pm(a, k, x) = \int_{-k}^{a-k} dz\, z^{-1} e^{\pm izx} (1 - e^{-izL}) \tag{3.9a}$$

$$= \mathrm{Ci}[|(a - k)x|] - \mathrm{Ci}(k|x|) \pm i\{\mathrm{Si}[(a - k)x] + \mathrm{Si}(kx)\}$$
$$- \mathrm{Ci}[|(a - k)(L \mp x)|] + \mathrm{Ci}(k|L \mp x|)$$
$$+ i\{\mathrm{Si}[(a - k)(L \mp x)] + \mathrm{Si}[k(L \mp x)]\}. \tag{3.9b}$$

The functions $\mathrm{Ci}(x)$ and $\mathrm{Si}(x)$ are defined as[4]

$$\mathrm{Ci}(x) = \int_\infty^x \frac{\cos t}{t} dt, \quad x > 0 \tag{3.10a}$$

$$\mathrm{Si}(x) = \int_0^x \frac{\sin t}{t} dt, \tag{3.10b}$$

and their limiting forms are[4]

$$\mathrm{Ci}(x) \to 0, \quad \mathrm{Si}(x) \to \tfrac{1}{2}\pi\, \mathrm{sgn}(x), \quad x \gg 1 \tag{3.11a}$$

$$\mathrm{Ci}(x)\to\ln x,\quad \mathrm{Si}(x)\to 0,\quad x\ll 1. \tag{3.11b}$$

In the region of $x\sim 1$, $\mathrm{Ci}(x)$ and $\mathrm{Si}(x)$ oscillate about 0 and $\frac{1}{2}\pi$, respectively. We are interested in the region $0\ll|x|\ll L$ where $I^{\pm}(a, k, x)$ becomes

$$I^{\pm}(a, k, x)=2\pi i\theta(a-k)\theta(\pm x),\quad 0\ll|x|\ll L \tag{3.12}$$

and $\theta(t)$ is the unit-step function. Substituting into Eq. (3.8) gives

$$\sum_{q<k_{Fl}}\langle\psi_l(q)|\psi_l'(k)\rangle\psi_l(q, x)=[R^*(k')R_l'(k)+T^*(k')T_l'(k)]\times(2L)^{-1/2}\begin{cases}R(k')e^{-ik'x}, & -L\ll x\ll 0\\ T(k')e^{ik'(x-b)}, & b\ll x\ll L.\end{cases} \tag{3.13}$$

[The factor $\theta(k_{Fl}-k')$ is always positive, since $k'<k\le k_{Fl}$ for left-hand states.] Equation (3.13) is the projection of $\psi_l'(k, x)$ on the occupied left-hand states. The projection of $\psi_l'(k, x)$ on the occupied right-hand states is found in a similar manner. Letting q run over the occupied right-hand states, we find

$$\sum_{q<k_{Fr}}\langle\psi_r(q)|\psi_l'(k)\rangle\psi_r(q, x)=[T^*(k')R_l'(k)+R^*(k')T_l'(k)]\theta(k_{Fr}-k')\times(2L)^{-1/2}\begin{cases}T(k')e^{-ik'x}, & -L\ll x\ll 0\\ R(k')e^{ik'(x-b)}, & b\ll x\ll L.\end{cases} \tag{3.14}$$

Hence, from Eqs. (2.14), (3.5), (3.13), and (3.14), we see that

$$f_l(k,x)=O(T^2)\theta(k'-k_{Fr})e^{-ik'x},\quad -L\ll x\ll 0$$
$$=(2L)^{-1/2}\tilde{T}_l'(k)e^{ik'(x-b)},\quad b\ll x\ll L \tag{3.15a}$$

where

$$\tilde{T}_l'(k)=[T_l'(k)-T(k')R^*(k')R_l'(k)+O(T^3)]\theta(k'-k_{Fr}). \tag{3.15b}$$

These steps follow because

$$|R(k)|^2+|T(k)|^2=1$$

and

$$T^*(k)R(k)+R^*(k)T(k)=0.$$

Let us remark that $T\sim e^{-Kb}\ll 1$ and that we need to calculate quantities such as the current only through order T^2. Therefore, we keep only those terms which contribute to order T in any transmission coefficients, to order T^2 in any reflection coefficients which contains other terms of order 1, and to order T in any reflection term which contains no terms of order 1.

Now from Eq. (I2.11), (I2.14), (3.1), and (3.2), for $0<x'<b$

$$K(\epsilon(k), 0, x')=(-mi/\hbar^2k)(2L)^{1/2}\psi_l(k, x') \tag{3.16a}$$

and

$$K(\epsilon(k), b, x')=(-mi/\hbar^2k)(2L)^{1/2}\psi_r(k, x'). \tag{3.16b}$$

Thus, substituting into Eq. (3.15g), we find

$$\tilde{T}_l'(k)=(-2imL/\hbar^2k')\int_0^b dx'[\psi_r(k', x')-T(k')R^*(k')\psi_l(k', x')]U(x')\psi_l(k, x')+O(T^3),\quad k'>k_{Fr}. \tag{3.17}$$

From Eqs. (I2.11), (3.1), and (3.2), it is easy to show that

$$\psi_r(k, x)-T(k)R^*(k)\psi_l(k, x)=R(k)\psi_r^*(k, x)+O(T^2). \tag{3.18}$$

Substituting into Eq. (3.17), we find, then, that

$$\tilde{T}_l'(k)=[(-2imL/\hbar^2k')R(k')\int_0^b dx'\psi_r^*(k', x')\times U(x')\psi_l(k, x')+O(T^2)]\theta(k'-k_{Fr}). \tag{3.19}$$

We note that the matrix element appearing in Eq. (3.19) is between a left-hand state and a right-hand state with the interaction potential. This result is similar to the transfer-Hamiltonian model[5] except that Eq. (3.19) contains orthogonal current-carrying states, whereas, the transfer-Hamiltonian model uses nonorthogonal standing-wave states which are eigenfunctions of a slightly different Hamiltonian than Eq. (I2.2). (A complete discussion of this is given in Ref. 5.) The result depends upon the requirement of orthogonality of the scattered wave with the rest of the occupied states. For one electron interacting with a vibrator, the inelastic-transmission amplitude is just $T_l'(k)$, and not $\tilde{T}_l'(k)$, which is a somewhat different matrix element involving ψ_r, and not ψ_r^* [see Eqs. (3.5d), (3.16b), and (I2.15)]. It is found in the Secs. IV–VI, however, that first Born approximation is sufficiently accurate for the calculation of the current when all inelastic-reflection coefficients are negligible, and therefore, in this case the distinction between $T_l'(k)$

and $\tilde{T}_l'(k)$ is unimportant for $k' > k_{Fr}$. [For $k' < k_{Fr}$, $\tilde{T}_l'(k)$ vanishes.]

In a similar manner, we find for the right-hand states

$$f_r(k, x) = (2L)^{-1/2}\tilde{T}_r'(k)e^{-ik'x}, \quad -L \ll x < 0$$
$$= O(T^2)\theta(k' - k_{Fl}) \quad , \quad b \ll x \ll L \quad (3.20a)$$

where

$$\tilde{T}_r'(k) = [T_r'(k) - T(k')R^*(k')R_r'(k) + O(T^3)]\theta(k' - k_{Fl}). \quad (3.20b)$$

We can also show that

$$\tilde{T}_r'(k) = [(-2imL/\hbar^2 k')R(k') \int_0^b dx' \psi_l^*(k', x') \times U(x')\psi_r(k, x') + O(T^2)]\theta(k' - k_{Fl}). \quad (3.21)$$

When $|eV| < \hbar\omega$, all $f_l(k, x)$ and $f_r(k, x)$ vanish in the regions $-L \ll x \ll 0$ and $b \ll x \ll L$ because there are no occupied states where k' could exceed k_{Fl} or k_{Fr}, whichever is smaller. This means that there are no electrons which inelastically tunnel by excitation of the vibrator when $|eV| < \hbar\omega$. In the region of the barrier, however, $f_l(k, x)$ and $f_r(k, x)$ do not vanish, and can serve as sources for the second-order terms considered in Secs. IV and V.

C. Current, Conductance, and d^2J/dV^2

The current flowing in the negative x direction for a system described by a normalized wave function $\Psi(x_1, x_2, \cdots, x_N; \xi)$ is

$$J(x) = -\frac{ie\hbar}{2m} \int dx_1 \int dx_2 \cdots \int dx_N \int d\xi \sum_{i=1}^{N} [\psi^*(x_1, x_2, \cdots, x_n; \xi)\frac{\partial \Psi}{\partial x_i}(x_1, x_2, \cdots, x_N; \xi) - \Psi(x_1, x_2, \cdots, x_N; \xi)\frac{\partial \Psi^*}{\partial x_i}(x_1, x_2, \cdots, x_N; \xi)]\delta(x_i - x) \quad (3.22a)$$

$$= J_0'(x) + J_1'(x), \quad (3.22b)$$

where

$$J_j'(x) = -\frac{ie\hbar}{2m} \int dx_1 \int dx_2 \cdots \int dx_N \sum_{i=1}^{N} [\chi_j^*(x_1, x_2, \ldots, x_N)\frac{\partial \chi_j}{\partial x_i}(x_1, x_2 \ldots, x_N) - \chi_j(x_1, x_2, \ldots, x_N)\frac{\partial \chi_j^*}{\partial x_i}(x_1, x_2, \ldots, x_N)]\delta(x_i - x), \quad j = 0, 1. \quad (3.22c)$$

Since $\Psi(x_1, x_2, \ldots, x_N; \xi)$ represents a stationary state, $J(x)$ must be independent of x from the continuity equation. (In what follows, we retain only terms through order U^2.) The normalization of the wave function calculated thus far is not unity, but is

$$\text{Norm} = 1 + \sum_\eta' \langle f_\eta \mid f_\eta \rangle \ , \quad (3.23)$$

where the sum on η runs over occupied states [see Eqs. (2.2), (2.14), (2.15), (2.32), and (2.34)]. Therefore, we must divide χ_0 as given by Eq. (2.32) by $(\text{Norm})^{1/2}$ to be correct. For the wave functions we have derived in this paper to make sense physically, $\sum_\eta' \langle f_\eta \mid f_\eta \rangle$ must be small compared to unity, that is, the probability of finding the system in the excited state relative to the probability of finding the system in the ground state,

$$\frac{\int dx_1 \int dx_2 \cdots \int dx_N \mid \chi_1(x_1, x_2, \ldots, x_N)\mid^2}{\int dx_1 \int dx_2 \cdots \int dx_N \mid \chi_0(x_1, x_2, \ldots, x_N)\mid^2} \simeq \sum_\eta' \langle f_\eta \mid f_\eta \rangle \ ,$$

must be small. Now, in this paper we have solved for the wave function of the many-electron-vibrator coupled system. The physical system of interest contains many electrons, a vibrator, *and* a contact with a thermal sink which keeps the vibrator in the ground state most of the time. Our theory does not contain a contact with a thermal sink. We rely solely on boundary conditions to stimulate the thermal sink. In the one-electron theory, this presents no difficulties since we imagine an electron as a wave packet incident on the barrier with the vibrator in the ground state, the wave packet being made up of states $\chi_0(x)$ like Eq. (I3.7a). The boundary condition assures us that the vibrator is in the ground state for the incident wave packet which, physically, is what the thermal sink does. So long as the contact with the thermal sink is not so strong as to modify the nature of the vibrator states, the only effect that the thermal sink has is to deexcite the vibrator after the wave packet has been scattered off the barrier. This subsequent deexcitation can have no effect on the various scattering probabilities of the wave packet. In the many-electron system, if we imagine the occupied $\psi_\mu(x)$ as represent-

ing wave packets, the best we can do is to put the vibrator in the ground state before any wave packet impinges on the barrier. Then, we scatter *all* the wave packets in the system off the barrier. Physically, we would like to deexcite the vibrator (if excited) after each wave packet scatters off the barrier, but we can not accomplish this in the solution of the many-electron-vibrator coupled system. We must, therefore, assume that the total probability for the excitation of the vibrator by scattering of all N electrons in the system is small. Obviously in a large system, particularly a three-dimensional system, this assumption is not valid. This is an inherent difficulty in our approach, resulting from our inability to solve the many-electron-vibrator system with a thermal sink. We proceed formally by assuming the smallness of $\sum_\eta' \langle f_\eta \mid f_\eta \rangle$ (by making U as small as necessary), calculating the current through order U^2, and assuming that the answer is correct for physically reasonable values of U.

If $k_{Fl} > k_{Fr}$ $(V > 0)$, it is convenient to calculate $J(x)$ in the region $b \ll x \ll L$ and if $k_{Fl} < k_{Fr}$, it is convenient to calculate $J(x)$ in the region $-L \ll x \ll 0$. Under these circumstances, we find

$$J_0'(x) = \sum_\eta' \langle \psi_\eta \mid J \mid \psi_\eta \rangle / (1 + \sum_\eta' \langle f_\eta \mid f_\eta \rangle) , \tag{3.24a}$$

$$J_1'(x) = \sum_\eta' \langle f_\eta \mid J \mid f_\eta \rangle + (\sum_\eta' \langle \psi_\eta \mid J \mid \psi_\eta \rangle)(\sum_\eta' \langle f_\eta \mid f_\eta \rangle) , \tag{3.24b}$$

where

$$\langle \psi \mid J \mid \psi \rangle = \frac{-ie\hbar}{2m} \left(\psi^*(x) \frac{\partial \psi(x)}{\partial x} - \psi(x) \frac{\partial \psi^*(x)}{\partial x} \right) . \tag{3.24c}$$

We have taken into account Eq. (3.23). If we combine the second term of Eq. (3.24b) with Eq. (3.24a), we have

$$J(x) = J_0(x) + J_1(x) , \tag{3.25a}$$

$$J_0(x) = \sum_\eta' \langle \psi_\eta \mid J \mid \psi_\eta \rangle , \tag{3.25b}$$

$$J_1(x) = \sum_\eta' \langle f_\eta \mid J \mid f_\eta \rangle . \tag{3.25c}$$

Now, $J_0(x)$ is the elastic current and is quite clearly the same for $-L \ll x \ll 0$ and $b \ll x \ll L$; whereas, $J_1(x)$ [as given by Eq. (3.25c)] vanishes for $-L \ll x \ll 0$ if $V > 0$, and vanishes for $b \ll x \ll L$ if $V < 0$. Yet we know that $J(x)$ is independent of x. The resolution of the difficulty is that in addition to the term $\langle f_\eta \mid J \mid f_\eta \rangle$, terms of the form

$$-\mathrm{Re} \sum_\mu' \langle f_\eta \mid f_\mu \rangle \langle \psi_\mu \mid J \mid \psi_\eta \rangle$$

should appear in Eq. (3.25c). These latter terms arise from the nonorthogonality of f_η with f_μ $(\mu \neq \eta)$. It can be shown that these terms contribute to the current in the region $-L \ll x \ll b$ when $V > 0$ (or in the region $b \ll x \ll L$ when $V < 0$) the proper amount to ensure current conservation across the barrier. It can also be shown that these do not give a contribution of $O(T^2)$ to the current in the region $b \ll x \ll L$ when $V > 0$ (or in the region $-L \ll x \ll 0$ when $V < 0$). So, Eq. (3.25c) is correct if $J_1(x)$ is evaluated in the region $b \ll x \ll L$ for $V > 0$ and in the region $-L \ll x \ll 0$ for $V < 0$. This means that we do have current conservation across the barrier in the inelastic channel.

Consider $V > 0$ so that $k_{Fl} > k_{Fr}$. We calculate $J_0(x)$ and $J_1(x)$ in the region $b \ll x \ll L$. We note that only those states $\psi_l(k, x)$, $k_{Fr} < k < k_{Fl}$, can contribute to $J_0(x)$, since for every left-hand state with $k < k_{Fr}$, there exists a right-hand state with equal and opposite current. Hence,

$$J_0(x) = \sum_{k_{Fr} < k < k_{Fl}} \langle \psi_l(k) \mid J \mid \psi_l(k) \rangle , \; k_{Fr} < k_{Fl} \quad (0 < V). \tag{3.26}$$

We recall that $f_l(k, x)$ and $f_r(k, x)$ vanish for $k' = (k^2 - 2m\omega/\hbar)^{1/2} < k_{Fr}$ in the region $b \ll x \ll L$. This means that only the $f_l(k, x)$ for which $k' > k_{Fr}$ can contribute to $J_1(x)$ (for $V > 0$), which requires $eV > \hbar\omega$ for there to be any inelastic current when $V > 0$. Hence,

$$J_1(x) = \sum_{k_{Fr}'' < k < k_{Fl}} \langle f_l(k) \mid J \mid f_l(k) \rangle , \tag{3.27a}$$

$$k_{Fr}'' = (k_{Fr}^2 + 2m\omega/\hbar)^{1/2} < k_F \quad (\hbar\omega < eV)$$

$$= 0 , \qquad 0 < eV < \hbar\omega . \tag{3.27b}$$

From Eqs. (3.1a), (3.15b), and (3.24c), we find

$$J_0(x) = \sum_{k_{Fr} < k < k_{Fl}} \frac{e\hbar k}{2mL} \mid T(k) \mid^2 , \quad V > 0 \tag{3.28a}$$

$$J_1(x) = \sum_{k_{Fr}'' < k < k_{Fl}} \frac{e\hbar k'}{2mL} \mid \tilde{T}_l'(k) \mid^2 , \; \hbar\omega < eV$$

$$= 0 , \quad 0 < eV < \hbar\omega . \tag{3.28b}$$

In a similar manner, we can show that

$$J_0(x) = -\sum_{k_{Fl} < k < k_{Fr}} \left(\frac{e\hbar k}{2mL} \right) \mid T(k) \mid^2 , \quad V < 0 \tag{3.29a}$$

$$J_1(x) = -\sum_{k_{Fl}'' < k < k_{Fr}} \left(\frac{e\hbar k'}{2mL} \right) \mid \tilde{T}_r'(k) \mid^2 , \quad eV < -\hbar\omega$$

$$= 0, \quad -\hbar\omega < eV < 0 . \tag{3.29b}$$

We recall that $E_{Fl} - E_{Fr} = eV$; and for $V > 0$, $E_{Fr} = E_F$, $k_{Fr} = k_F$, and for $V < 0$, $E_{Fl} = E_F$, $k_{Fl} = k_F$,

where E_F and k_F are the equilibrium Fermi energy and momentum. We can rewrite Eqs. (3.28) and (3.29) as

$$J_0(V) = \mathrm{sgn}(V)\frac{e}{h}\int_0^{|eV|} d\epsilon\ D_0(\epsilon)\ , \qquad (3.30a)$$

$$J_1(V) = \mathrm{sgn}(V)\frac{e}{h}\int_0^{|eV|} d\epsilon\ D_1(\epsilon, V)\ , \qquad (3.30b)$$

where

$$D_0(\epsilon) = |T(k)|^2 \qquad (3.30c)$$

$$D_1(\epsilon, V) = (k'/k)|\tilde{T}_l'(k)|^2, \quad 0 < V$$
$$= (k'/k)|\tilde{T}_r'(k)|^2, \quad V < 0 \qquad (3.30d)$$

$$k = \left(\frac{2m(\epsilon + E_F)}{\hbar^2}\right)^{1/2},$$

$$k' = \left(\frac{2m(\epsilon + E_F - \hbar\omega)}{\hbar^2}\right)^{1/2}, \qquad (3.30e)$$

where T, $\tilde{T}_l'$, and $\tilde{T}_r'$ are given by Eqs. (2.11d), (3.19), and (3.21), respectively. (We drop the x variable, since current is independent of x, and indicate the dependence on bias voltage V.)

Let us now calculate the conductance in first Born approximation

$$G(V) = \frac{dJ}{dV} \qquad (3.31a)$$

$$= G_0(V) + G_1(V)\ , \qquad (3.31b)$$

where the background conductance is [Eq. (I2.11d)]

$$G_0(V) = (e^2/\hbar)D_0(|eV|) \qquad (3.32a)$$

$$= \frac{16e^2k^2K^2}{h(k^2+K^2)^2}\ e^{-2Kb}\ , \qquad (3.32b)$$

and now

$$k = [2m(|eV| + E_F)/\hbar^2]^{1/2}\ , \qquad (3.32c)$$

$$K = [2m(V_0 - |eV| + E_F)/\hbar^2]^{1/2}\ . \qquad (3.32d)$$

In the calculation of $G_1(V)$ when first Born approximation is valid for the calculation of the current, we can replace $\tilde{T}_l'(k)$ by $T_l'(k)$ for $k' > k_{Fr}$ and $V > 0$, and $\tilde{T}_r'(k)$ by $T_r'(k)$ for $k' > k_{Fl}$ and $V < 0$. Hence,

$$G_1(V) = (e/h)(k'/k)[\,|T_l'(k)|^2\,\theta(eV - \hbar\omega)$$
$$+ |T_r'(k)|^2\,\theta(-eV - \hbar\omega)]\ , \qquad (3.33a)$$

where

$$k' = [2m(|eV| + E_F - \hbar\omega)/\hbar^2]^{1/2} \qquad (3.33b)$$

and $T_l'(k)$ is given by Eq. (3.5d) and $T_r'(k)$ by Eq. (3.6c).

Since we have considered a symmetric barrier potential $V(x)$, the background conductance $G_0(V)$ is symmetric about zero bias. The background is assumed to be slowly varying for the bias voltages of interest. (We can also allow V_0 to be a function of V and to fit the background, if necessary.)

The inelastic conductance associated with the excitation of the vibrator $G_1(V)$ vanishes for $|eV| < \hbar\omega$ (see Fig. 1), where conservation of energy forbids the excitation of the vibrator (at $T = 0$ K). At $eV = \hbar\omega$, a step increase in the conductance occurs which is proportional to the probability for inelastic transmission $|T_l'(k)|^2$. Likewise, at $eV = -\hbar\omega$, a step increase occurs which is proportional to $|T_r'(k)|^2$. Since $T_l'(k)$ is the same as T' in I, we see that inelastic current is relatively insensitive to the position of the vibrator, and hence, the step increases in the conductance at $eV = \pm\hbar\omega$ are approximately the same size, being slightly larger for $eV = \hbar\omega$ if the vibrator is located near the right-hand edge of the barrier, etc., which is in agreement with experiment.[2,3]

Experimentally, $d^2J/dV^2 = dG/dV$ is often measured. The inelastic current contributes a positive peak for $eV = \hbar\omega$ and a negative peak for $eV = -\hbar\omega$. The heights of the peaks are, of course, proportional to the step increases in the conductance. The width of the peaks depend upon temperature and the distribution of vibrator frequencies. We emphasize again, that the above remarks are strictly valid only when inelastic reflection is negligible.

D. Further Results

Let us quote the results in first Born approximation for the model which is a generalization of one-dimensional model of Secs. I and II to three dimen-

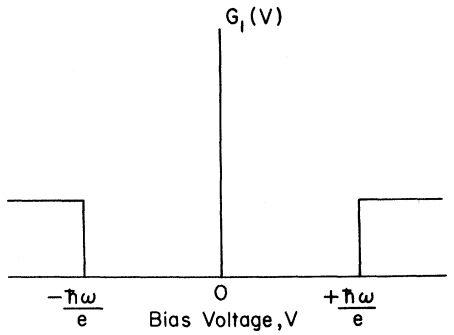

FIG. 1. Inelastic conductance $G_1(V)$ versus bias voltage V. No inelastic current flows for $|eV| < \hbar\omega$ by conservation of energy. Step increases in the conductance occur at $eV = \pm\hbar\omega$ owing to the onset of inelastic tunneling associated with the excitation of the vibrator.

sions. We find by techniques similar to those used for one dimension that for $b \ll x \ll L$

$$f_l(\vec{k},\vec{r}) = \sum_{\vec{p}} (2LA)^{-1/2} \tilde{T}_l'(\vec{k},\vec{p}) \times \exp[ip_x(x-b) + i\vec{p}_t \cdot \vec{\rho}\,]\,\theta(\epsilon(\vec{k}) - \hbar\omega - E_{Fr}) , \tag{3.34}$$

where the sum on $\vec{p}$ is over all $\vec{p}$ with $\hbar^2 p^2/2m = (\hbar^2 k^2/2m) - \hbar\omega$. In the plane of the barrier, the projections of $\vec{p}$ and $\vec{r}$ are $\vec{p}_t$ and $\vec{\rho}$. The area of the barrier, equal to the area of the tunnel junction, is A. (As before, the barrier extends from 0 to b.) The amplitude for inelastic transmission from $\vec{k}$ on the left to $\vec{p}$ on the right is

$$\tilde{T}_l'(\vec{k},\vec{p}) = \frac{-2imL}{\hbar^2 p_x} \int d^3r\ \psi_r^*(\vec{p},\vec{r}) U(\vec{r}) \psi_l(\vec{k},\vec{r}). \tag{3.35}$$

The left- and right-hand states $\psi_r(\vec{p},\vec{r})$ and $\psi_l(\vec{k},\vec{r})$ are obtained from Eqs. (3.1) and (3.2) by multiplying by the appropriate plane-wave factors $A^{-1/2} \times \exp(i\vec{p}_t \cdot \vec{\rho}\,)$ and $A^{-1/2} \exp i\vec{k}_t \cdot \vec{\rho}$. We assume the three-dimensional interaction potential $U(\vec{r}\,)$ vanishes outside the barrier. Similar results hold for $f_r(\vec{k},\vec{r}\,)$.

The matrix element $\tilde{T}_l'(\vec{k},\vec{p}\,)$ is similar to that which appears in the transfer-Hamiltonian model,[5] except that orthogonal current-carrying states occur in Eq. (3.35), whereas, nonorthogonal standing-wave states occur in the matrix elements of the transfer-Hamiltonian model. The difference in most cases is, however, unimportant.

We conclude the calculations in first Born approximation by remarking that for interaction potentials which do not give rise to significant inelastic reflection, we can calculate the inelastic current from the one-electron theory of I (or its appropriate three-dimensional generalization) by the following prescription. We calculate the amplitude T' for inelastic transmission of a single electron by the methods of I. We then calculate the inelastic current for that electron. Now, the total inelastic current for the many-electron system is the sum of all the inelastic contributions from the single electrons consistent with the initial state being occupied and the final state being unoccupied. In one-dimension, the result is Eq. (3.30b). In three dimensions, the result for the inelastic current due to a single vibrator for $V > 0$ is (including spin)

$$\frac{2e\hbar}{m} \sum_{\vec{k}} \sum_{\vec{p}} p_x \left| \tilde{T}_l'(\vec{k},\vec{p}) \right|^2 . \tag{3.36}$$

The sum on $\vec{k},\vec{p}$ is over all states such that $\hbar^2 k^2/2m < E_{Fl}$ and $\hbar^2 p^2/2m = (\hbar^2 k^2/2m) - \hbar\omega > E_{Fr}$, where $E_{Fl} = E_F + eV$ and $E_{Fr} = E_F$ for $V > 0$. Similar results hold for $V < 0$. The amplitude $\tilde{T}_l'(\vec{k},\vec{p}\,)$ is given by Eq. (3.35).

Finally, we make connection with the results of Scalapino and Marcus[6] for molecular excitations. Instead of evaluating the amplitude $\tilde{T}_l'(\vec{k},\vec{p}\,)$ in Eq. (3.35), we obtain the inelastic current from the three-dimensional generalization of I. The one-electron elastic and inelastic wave functions obey the coupled equations

$$[H_e(\vec{r}) - \epsilon]\,\chi_0(\vec{r}) + U(\vec{r})\,\chi_1(\vec{r}) = 0 , \tag{3.37a}$$

$$[H_e(\vec{r}) - \epsilon + \hbar\omega]\,\chi_1(\vec{r}) + U(\vec{r})\,\chi_0(\vec{r}) = 0, \tag{3.37b}$$

where $U(\vec{r}\,)$ is the dipole (plus image) potential,[6]

$$U(\vec{\rho}\,,x) = 2eP_x x/(x^2+\rho^2)^{3/2} \tag{3.38}$$

(in our notation) and P_x is the dipole moment in the x direction of a molecule near $x = 0$.

We write $\chi_0(\vec{r}\,)$ as

$$e^{i\vec{k}_t \cdot \vec{\rho}}\,\psi(x) , \tag{3.39}$$

where $\vec{k}_t$ is the transverse momentum and $\chi_0(x)$ is an incoming wave on the left [see Eq. (I2.11)]. We take the electron energy to be $\epsilon = \hbar^2(k_x^2 + k_t^2)/2m$. It is straightforward to show that in first Born approximation

$$\chi_1(\vec{r}\,) = \int \frac{d^2p_t}{(2\pi)^2}\ e^{i\vec{\rho}_t \cdot \vec{\rho}} \int d^2\rho'\ e^{i(\vec{k}_t - \vec{p}_t)\cdot\vec{\rho}\,'} \times \int dx'\ K(\epsilon - \hbar\omega - \hbar^2 p_t^2/2m, x, x')\, U(\vec{\rho}\,', x')\psi(x') , \tag{3.40}$$

where the Green's function $K(\epsilon, x, x')$ is given by Eq. (I2.14). Now, *if* $U(\vec{\rho}\,', x')$ is slowly varying in $\vec{\rho}\,'$, only $\vec{p}_t \simeq \vec{k}_t$ will contribute to Eq. (3.40), so we replace p_t by k_t in $K(\epsilon - \hbar\omega - \hbar^2 p_t^2/2m, x, x')$. Hence we find for $x > b$

$$\chi_1(\vec{r}\,) = T' e^{i\vec{k}_t \cdot \vec{\rho}} e^{ik_x'(x-b)} ,$$

where

$$T' = \int_0^b dx'\ t(\epsilon - \hbar\omega - \hbar^2 k_t^2/2m, x')\, U(\vec{\rho}\,, x')\, \psi(x')$$

and

$$k_x' = \left(\frac{2m(\epsilon - \hbar\omega - \hbar^2 k_t^2/2m)}{\hbar^2} \right)^{1/2}$$

in analogy with Eq. (I2.15). We note that T' depends upon $\vec{\rho}$, so that the inelastic current due to a single electron incident from the left with energy ϵ and transverse momentum $\vec{k}_t$ and one molecule is

$$\int d^2\rho\ (\hbar k_x'/m) \left| T' \right|^2 .$$

Similar results hold for electrons incident from

the right. If we add up the inelastic current from all electrons that can make inelastic transitions, our results are equivalent to those of Scalapino and Marcus.[6]

IV. GENERAL THEORY: SECOND BORN APPROXIMATION

We now extend the analysis of Sec. II to second Born approximation. In second order,

$$[\sum_i H_e(i) - \epsilon]\chi_0^{(2)}(1, 2, \ldots, N)$$

$$= -\sum_i U(i)\,\chi_1^{(1)}(1, 2, \ldots, N), \tag{4.1}$$

where $\chi_1^{(1)}$ is given by Eq. (2.15). As before, the right-hand side is a sum of sources, each of which gives a contribution to $\chi_0^{(2)}$. There are two types of terms on the right-hand side of Eq. (4.1), one of which we call direct and the other indirect. As an example of a direct term, consider a term of the form

$$-U(1)f_\alpha(1)\,\psi_\beta(2)\cdots\psi_\omega(N)\ .$$

Such a term gives a contribution to $\chi_0^{(2)}$ which is

$$\psi''_\alpha(1)\,\psi_\beta(2)\cdots\psi_\omega(N)\quad ,$$

where

$$[H_e(1) - \epsilon_\alpha]\psi''_\alpha(1) = -U(1)f_\alpha(1)\ .$$

We can solve for $\psi''_\alpha(1)$ in a manner similar to that used to find $\psi'(x)$ in Sec. II of I. Clearly, $\psi''_\alpha(1)$ possesses the same spin as $f_\alpha(1)$ and $\psi_\alpha(1)$ [if $U(i)$ contains no spin-flip terms]. Similar considerations hold for $\beta, \ldots, \omega$. It is straightforward to show that the total contribution of the direct terms to $\chi_0^{(2)}$ is

$$\chi_0^{(2)}(1, 2, \ldots, N)_{\text{direct}} = D(\psi''_\alpha\psi_\beta\cdots\psi_\omega)$$

$$+D(\psi_\alpha\psi''_\beta\cdots\psi_\omega)+\cdots+D(\psi_\alpha\psi_\beta\cdots\psi''_\omega)\quad , \tag{4.2}$$

where

$$[H_e(i) - \epsilon_\mu]\psi''_\mu(i) = -U(i)f_\mu(i)\ . \tag{4.3}$$

In addition, there are source terms of the following form which are called indirect,

$$-U(2)f_\alpha(1)\,\psi_\beta(2)\,\psi_\gamma(3)\cdots\psi_\omega(N)\quad .$$

The contribution of this source term to $\chi_0^{(2)}$ is of the form

$$F(1, 2)\,\psi_\gamma(3)\cdots\psi_\omega(N)\quad , \tag{4.4}$$

where

$$[H_e(1) + H_e(2) - \epsilon_\alpha - \epsilon_\beta]F(1, 2) = -U(2)f_\alpha(1)\,\psi_\beta(2)\ . \tag{4.5}$$

Unfortunately, Eq. (4.5) is not separable and cannot be solved as simply as Eq. (4.3). Therefore, we expand $f_\alpha(1)$ as

$$f_\alpha(1) = \sum_\eta \langle\psi_\eta|f_\alpha\rangle\,\psi_\eta(1)\ . \tag{4.6}$$

(The sum is formally over all states.) Since f_α is already orthogonal to all occupied states ψ_α, only unoccupied states need to be included in the sum.

Substituting Eq. (4.6) into Eq. (4.5) gives

$$F(1, 2) = \sum_\eta \langle\psi_\eta|f_\alpha\rangle\,\psi_\eta(1)\,h_\beta(\epsilon_\alpha + \epsilon_\beta - \epsilon_\eta,\ 2)\ , \tag{4.7}$$

where for any ϵ

$$[H_e(2) - \epsilon]h_\beta(\epsilon,\ 2) = -U(2)\,\psi_\beta(2). \tag{4.8}$$

The contribution of such terms to $\chi_0^{(2)}$ is of the form

$$\sum_\eta \langle\psi_\eta|f_\alpha\rangle\,D(\psi_\eta h_\beta(\epsilon_\alpha + \epsilon_\beta - \epsilon_\eta)\,\psi_\gamma\cdots\psi_\omega)\ . \tag{4.9}$$

The above terms involve only replacements in the (α, β) pair among the states $\psi_\alpha\psi_\beta\cdots\psi_\omega$. The total contribution of indirect terms will involve all other pairs formed from the occupied states of $\chi_0^{(0)}$, such as (γ, β), (α, γ), etc.

Now the principal contribution to the sum in Eq. (4.9) corresponds to the states ψ_η with energies $\epsilon_\eta \simeq \epsilon_\alpha - \hbar\omega$. This means that for the ψ_η of importance

$$\langle\psi_\beta|\,h_\beta(\epsilon_\alpha + \epsilon_\beta - \epsilon_\eta)\rangle \simeq \langle\psi_\beta|\,h_\beta(\epsilon_\beta + \hbar\omega)\rangle\ . \tag{4.10}$$

Such a term can be neglected in any sum over states since there is a finite energy difference $\hbar\omega$ between ψ_β and $h_\beta(\epsilon_\beta + \hbar\omega)$.

Hence, in Eq. (4.9) we can make the replacement

$$h_\beta(\epsilon_\alpha + \epsilon_\beta - \epsilon_\eta, i) \to l_\beta(\epsilon_\alpha + \epsilon_\beta - \epsilon_\eta, i)$$

$$+\langle\psi_\alpha|\,h_\beta(\epsilon_\alpha + \epsilon_\beta - \epsilon_\eta)\rangle\,\psi_\alpha(i), \tag{4.11}$$

where

$$l_\beta(\epsilon_\alpha + \epsilon_\beta - \epsilon_\eta, i) = h_\beta(\epsilon_\alpha + \epsilon_\beta - \epsilon_\eta, i)$$

$$-\sum'_\nu \langle\psi_\nu|\,(h_\beta(\epsilon_\alpha + \epsilon_\beta - \epsilon_\eta)\rangle\,\psi_\nu(i)\ , \tag{4.12}$$

the sum being over all occupied states. Substituting Eq. (4.11) into Eq. (4.9), we obtain two terms

$$\sum_\eta \langle\psi_\eta|f_\alpha\rangle\,D(\psi_\eta\,l_\beta(\epsilon_\alpha + \epsilon_\beta - \epsilon_\eta)\,\psi_\gamma\cdots\psi_\omega)$$

$$-\sum_\eta \langle\psi_\eta\,|f_\alpha\rangle\langle\psi_\alpha|\,h_\beta(\epsilon_\alpha + \epsilon_\beta - \epsilon_\eta)\rangle\,D(\psi_\alpha\,\psi_\eta\,\psi_\gamma\cdots\psi_\omega)\ . \tag{4.13}$$

The sum on η is over unoccupied states since, according to Eq. (2.14), the projection of f_α on the occupied states has been subtracted out. The first term in Eq. (4.13) is doubly orthogonal to $\chi_0^{(0)}$,

i.e., both ψ_η and $l_\beta(\epsilon_\alpha+\epsilon_\beta-\epsilon_\eta)$ are each orthogonal to ψ_α and ψ_β. In the calculation of the current, or of a matrix element of any single-particle operator, any term which is doubly orthogonal to $\chi_0^{(0)}$ cannot give a contribution of order U^2 by interfering with $\chi_0^{(0)}$. Therefore, we can drop such a term because it will give only a term of order U^4 in the current. The second term in Eq. (4.13) is only singly orthogonal to $\chi_0^{(0)}$ and must be kept.

Consider now all pairs involving β such as (α,β), (γ,β), etc. We can combine these indirect terms [such as the second term in Eq. (2.28)] to obtain

$$D(\psi_\alpha\,\varphi_\beta\,\psi_\gamma\cdots\psi_\omega)\ ,$$

where

$$\varphi_\beta(i)=-\sum{}'_\nu\sum_\eta\langle\psi_\eta|f_\nu\rangle\,\langle\psi_\nu|h_\beta(\epsilon_\nu+\epsilon_\beta-\epsilon_\eta)\rangle\,\psi_\eta(i)\ .$$

The sum on ν is over all occupied states and the sum on η need be over unoccupied states only. [The term $\nu=\beta$ can be included in the sum since it is negligibly small.] Now, h_β has the same spin as ψ_β, so φ_β will also have the same spin as ψ_β [if $U(i)$ contains no spin-flip terms]. The remaining terms can be treated in a similar manner which allows us to write $\chi^{(2)}_{0,\text{indirect}}$ (with doubly orthogonal terms omitted) as

$$\chi_0^{(2)}(1,2,\ldots,N)_{\text{indirect}}=D(\varphi_\alpha\,\psi_\beta\circ\circ\psi_\omega)+D(\psi_\alpha\varphi_\beta\circ\circ\psi_\omega)+\circ\circ\circ+D(\psi_\alpha\,\psi_\beta\circ\circ\varphi_\omega)\ , \tag{4.14}$$

where

$$\varphi_\mu(i)=-\sum{}'_\nu\sum_\eta\langle\psi_\eta|f_\nu\rangle\,\langle\psi_\nu|h_\mu(\epsilon_\nu+\epsilon_\mu-\epsilon_\eta)\rangle\,\psi_\eta(i)\ . \tag{4.15}$$

Both ψ_μ'' and φ_μ are second order in U^2.

In Eq. (4.2), we can make the replacement

$$\psi_\mu''(i)\to g_\mu(i)\ ,$$

where

$$g_\mu(i)=\psi_\mu''(i)-\sum{}'_\eta\langle\psi_\eta|\psi_\mu''\rangle\,\psi_\eta(i)\ . \tag{4.16}$$

The sum on η is over all occupied states. [The $\eta=\mu$ term in $g_\mu(i)$ can be included since we can always add a constant times the homogeneous solution of Eq. (4.3) to the inhomogeneous solution.]

Through order U^2, we can combine Eqs. (2.12), (4.3), and (4.14) to obtain

$$\chi_0(1,2,\ldots,N)=\chi_0^{(0)}(1,2,\ldots,N)+\chi_0^{(2)}(1,2,\circ\circ\circ,N) \tag{4.17a}$$

$$=D(\tilde\psi_\alpha\,\tilde\psi_\beta\cdots\tilde\psi_\omega)\ , \tag{4.17b}$$

where

$$\tilde\psi_\mu(i)=\psi_\mu(i)+g_\mu(i)+\varphi_\mu(i)\ . \tag{4.18}$$

From Eqs. (4.15) and (4.16), through order U^2 for any occupied states μ and ν,

$$\langle\tilde\psi_\mu|\tilde\psi_\nu\rangle=\delta_{\mu\nu}\ , \tag{4.19}$$

since g_μ and φ_μ are orthogonal to ψ_μ. (We assume the ψ_μ form a complete orthonormal set.)

Through order U^2, χ_1 is given by $\chi_1^{(1)}$ [see Eq. (2.15)], the next order term being order U^3. This completes the formal derivation of the many-electron wave function with a single vibrator through second order in the interaction potential.

V. ONE-DIMENSIONAL MODEL: SECOND BORN APPROXIMATION

A. Calculation of $\chi_0^{(2)}$

We now calculate $\chi_0^{(2)}$ for the one-dimensional model of Sec. III. We must first evaluate Eq. (3.7a) in the region $0<x<b$. This we do by evaluating $C(q)$, $D(q)$, and Q at $q=k'$, but we must apply a cutoff to the $q\ll k'$ since $\psi_l(q,x)$ decreases exponentially as q decreases (except at $x=0$). We find

$$\sum_{q<k_{Fl}}\langle\psi_l(q)|\psi_l'(k)\rangle\,\psi_l(q,x)=(2\pi i)^{-1}[R^*(k')R_l'(k)+T^*(k')T_l(k)]\,\psi_l(k',x)\times\left(\ln\left|\frac{k_{Fl}-k'}{k_c}\right|+i\pi\theta(k_{Fl}-k')\right),\ 0<x<b \tag{5.1}$$

where k_c is a cutoff. In a similar manner, we find

$$\sum_{q<k_{Fr}}\langle\psi_r(q)|\psi_l'(k)\rangle\,\psi_r(q,x)=(2\pi i)^{-1}[T^*(k')R_l'(k)+R^*(k')T_l'(k)]\,\psi_r(k',x)\times\left(\ln\left|\frac{k_{Fr}-k'}{k_c}\right|+i\pi\theta(k_{Fr}-k')\right),\ 0<x<b\ . \tag{5.2}$$

In Eq. (5.1), k' is always less than k_{Fl} for left-hand states. Hence, we never encounter the singularity at $k'=k_{Fl}$ in the ln term or the step in the θ term. Since we are concerned only with the second-order terms which show structure (we cannot distinguish slowly varying terms from the background), we can neglect the slowly varying contribution Eq. (5.1) to $f_l(k,x)$ in the region $0<x<b$ when we calculate $\psi_l''(k,x)$ using a source involving $f_l(k,x)$. As for Eq. (5.2), we cannot, in general, neglect this contribution to $f_l(k,x)$ since, for $eV>\hbar\omega$, there exist left-hand states for which k'

$= k_{Fr}$. This term will, therefore, give structure to the second-order reflection and transmission amplitudes. For convenience, we define

$$\varphi_l(k,x,k_{Fr}) = -(2\pi i)^{-1}[T^*(k')R_l'(k) + R^*(k')T_l'(k)] \times \psi_r(k',x)[\ln|(k_{Fr}-k')/k_c| - i\pi\theta(k'-k_{Fr})], \quad 0<x<b \ . \quad (5.3)$$

The function $\varphi_l(k,x,k_{Fr})$ differs from the right-hand side of Eq. (5.2) only in sign and in the neglect of a slowly varying term associated with rewriting the θ term. Hence, in computing $\psi_l''(k,x)$ from a source involving $f_l(k,x)$, we keep only $\varphi_l(k,x,k_{Fr})$. Likewise, we find for right-hand states the most important contribution to $f_r(k,x)$ for $0<x<b$ is

$$\varphi_r(k,x,k_{Fl}) = -(2\pi i)^{-1}[T^*(k')R_r'(k) + R^*(k')T_r'(k)] \times \psi_l(k',x)[\ln|(k_{Fl}-k')/k_c| - i\pi\theta(k'-k_{Fl})], \quad 0<x<b \ . \quad (5.4)$$

From Eq. (4.3), we see that the second-order terms arise from equations of the form

$$[H_e(x)-\epsilon(k)]\psi_l''(k,x) = -U(x)f_l(k,x) \ . \quad (5.5)$$

Neglecting all terms in $f_l(k,x)$ except Eq. (5.3), we find

$$\psi_l''(k,x) = (2L)^{-1/2}R_l''(k)e^{-ikx}, \quad x<0$$
$$= (2L)^{-1/2}T_l''(k)e^{ik(x-b)}, \quad b<x \quad (5.6a)$$

where

$$R_l''(k) = (2L)^{1/2} \times \int_0^b dx' K(\epsilon(k),\ 0,\ x')U(x')\varphi_l(k,x',k_{Fr}) \ , \quad (5.6b)$$

$$T_l''(k) = (2L)^{1/2} \times \int_0^b dx' K(\epsilon(k), b, x')U(x')\varphi_l(k,x',k_{Fr}) \ . \quad (5.6c)$$

Similarly,

$$\psi_r''(k,x) = (2L)^{-1/2}T_r''(k)e^{-ikx}, \quad x<0 \quad (5.7a)$$
$$= (2L)^{-1/2}R_r''(k)e^{ik(x-b)}, \quad b<x \quad (5.7b)$$

where

$$T_r''(k) = (2L)^{1/2} \times \int_0^b dx' K(\epsilon(k),\ 0,\ x')U(x')\varphi_r(k,x',k_{Fl}) \ , \quad (5.7c)$$

$$R_r''(k) = (2L)^{1/2} \times \int_0^b dx' K(\epsilon(k),\ b,\ x')U(x')\varphi_r(k,x',k_{Fl}). \quad (5.7d)$$

According to Eq. (4.16), we must find the functions $g_\mu(i)$ which correspond to subtracting out of $\psi_l''(k,x)$ and $\psi_r''(k,x)$ their projections on the occupied states. First, for left-hand states, we find by methods similar to those used to find $f_l(k,x)$

$$g_l(k,x) = (2L)^{-1/2}G_{l1}e^{-ikx}, \quad -L \ll x \ll 0$$
$$= (2L)^{-1/2}G_{l2}e^{ik(x-b)}, \quad b \ll x \ll L \quad (5.8a)$$

where

$$G_{l1} = -T^*(k)G_{l2}/R^*(k) \quad (5.8b)$$

and

$$G_{l2} = T_l''(k) - T(k)R^*(k)R_l''(k) + \theta(T^3), \quad k>k_{Fr}$$
$$= 0, \quad k<k_{Fr} \ . \quad (5.8c)$$

We can rewrite G_{l2} as

$$G_{l2} = (-2imL/\hbar^2 k)R(k) \times \int_0^b dx' \psi_r^*(k,x')U(x')\varphi_l(k,x',k_{Fr}) + O(T^2), \quad k>k_{Fr} \quad (5.9)$$

where we have made use of Eqs. (3.16), (3.18), and (5.6). Substituting Eq. (5.3) into Eq. (5.9), we find

$$G_{l2} = \frac{-2i}{\pi kk'}\left(\frac{mL}{\hbar^2}\right)^2 R(k)\int_0^b dx' \psi_r^*(k,x')U(x')\psi_r(k',x') \times \int_0^b dx' \psi_r^*(k',x')U(x')\psi_l(k,x') \times [\ln|(k_{Fr}-k')/k_c| - i\pi\theta(k'-k_{Fr})] + O(T^2), \quad k>k_{Fr}$$
$$= 0, \quad k<k_{Fr} \ . \quad (5.10)$$

In deriving Eq. (5.10), we have made use of the results leading to Eq. (3.19). In a similar manner, we find for right-hand states

$$g_r(k,x) = (2L)^{-1/2}G_{r2}e^{-ikx}, \quad -L \ll x \ll 0$$
$$= (2L)^{-1/2}G_{r1}e^{ik(x-b)}, \quad b \ll x \ll L \quad (5.11a)$$

where

$$G_{r2} = \frac{-2i}{\pi kk'}\left(\frac{mL}{\hbar^2}\right)^2 R(k)\int_0^b dx' \psi_l^*(k,x')U(x')\psi_l(k',x') \times \int_0^b dx' \psi_l^*(k',x')U(x')\psi_r(k,x')$$

$$\times[\ln|(k_{Fl}-k')/k_c| - i\pi\theta(k'-k_{Fl})] + O(T^2),\quad k>k_{Fl}$$

$$=0,\quad k<k_{Fl} \tag{5.11b}$$

and

$$G_{r1} = -T^*(k)\,G_{r2}/R^*(k)\ . \tag{5.11c}$$

From Eq. (5.10) we note that G_{l2} contributes structure to the transmission amplitude (coefficient of $e^{ik(x-b)}$ terms for $x \gg b$) for left-hand states, which is second order in U and has a logarithmic singularity for $k'=k_{Fr}$. Likewise, G_{r2} contributes similar structure to the right-hand states when $k'=k_{Fl}$. It has been shown previously[6-8] that whenever one has interactions with a boson of energy $\hbar\omega$ (e.g., optical phonon) in the electrode region (say $b<x<L$), it is possible to have logarithmic singularities (suitably rounded off) in the spectral weight function which is reflected in the conductance of the tunnel junction in essentially the same manner as the logarithmic singularities in the transmission amplitudes above [Eqs. (5.10) and (5.11)] are. (We explicitly calculate the conductance below.) This result indicates that the presence of a logarithmic singularity in the conductance of a tunnel junction can arise from structure in the barrier-penetration factor as well as in the spectral weight function. We note that no such singularity appears in the one-electron theory[1] since the singularity results from the statistics of the many-electron system.

In addition to the Eqs. (5.10) and (5.11), the $\varphi_\mu(i)$ terms of Eq. (4.15) also contribute structure to the transmission amplitudes in the form of logarithmic singularities. In the Appendix, we show that for left-hand states

$$\varphi_l(k,x) = (2L)^{-1/2}\,F_{l1}e^{-ikx},\quad -L\ll x<0$$
$$= (2L)^{-1/2}F_{l2}e^{ik(x-b)},\quad b\ll x\ll L \tag{5.12a}$$

where

$$F_{l1} = -T^*(k)\,F_{l2}/R^*(k) \tag{5.12b}$$

and

$$F_{l2} = \frac{2i}{\pi k k''}\left(\frac{mL}{\hbar^2}\right)^2 R(k)\int_0^b dx'\,\psi_l^*(k,x')\,U(x')\,\psi_l(k'',x')$$
$$\times\int_0^b dx'\,\psi_r^*(k'',x')\,U(x')\,\psi_l(k,x')$$
$$\times\left(\ln\left|\frac{k-k'_{Fl}}{k_c}\right| - i\pi\theta(k'_{Fl}-k)\right) + O(T^2),\quad k>k_{Fr}$$

$$=0,\quad k<k_{Fr} \tag{5.12c}$$

$$k'' = (k^2+2m\omega/\hbar)^{1/2}\ , \tag{5.12d}$$

$$k'_{Fl} = (k_{Fl}^2 - 2m\omega/\hbar)^{1/2}\ . \tag{5.12e}$$

For right-hand states,

$$\varphi_r(k,x) = (2L)^{-1/2}F_{r2}e^{-ikx},\quad -L\ll x\ll 0$$
$$= (2L)^{-1/2}F_{r1}e^{ik(x-b)},\quad b\ll x\ll L \tag{5.13a}$$

where

$$F_{r2} = \frac{2i}{\pi k k''}\left(\frac{mL}{\hbar^2}\right)^2 R(k)\int_0^b dx'\,\psi_r^*(k,x')\,U(x')\,\psi_r(k'',x')$$
$$\times\int_0^b dx'\,\psi_l^*(k'',x')\,U(x')\,\psi_r(k,x')$$
$$\times\left(\ln\left|\frac{k-k'_{Fr}}{k_c}\right| - i\pi\theta(k'_{Fr}-k)\right) + O(T^2),\quad k>k_{Fl}$$

$$=0,\quad k<k_{Fl} \tag{5.13b}$$

and

$$F_{r1} = -T^*(k)\,F_{r2}/R^*(k)\ . \tag{5.13c}$$

We note that all of these terms [Eqs. (5.10), (5.11b), (5.12c), and (5.13b)] involve essentially reflection matrix elements of the type $\int dx\ \psi_r^* U\psi_r$ or $\int dx\ \psi_l^* U\psi_l$. Although these terms are present in the transfer-Hamiltonian approach, they are usually not considered[5] except in the magnetic-impurity scattering.[9,10]

We are now in a position to evaluate the $\tilde{\psi}_\mu(i)$ of Eq. (4.18). Combining Eqs. (3.1a), (5.8a), and (5.12a), we find

$$\tilde{\psi}_l(k,x) = (2L)^{-1/2}\tilde{R}_l(k)\,e^{-ikx},\quad -L\ll x\ll 0$$
$$= (2L)^{-1/2}\,\tilde{T}_l(k)\,e^{ik(x-b)},\quad b\ll x\ll L \tag{5.14a}$$

where

$$\tilde{R}_l(k) = R(k) - T^*(k)\,(G_{l2}+F_{l2})/R^*(k) \tag{5.14b}$$

and

$$\tilde{T}_l(k) = T(k) + G_{l2} + F_{l2}\ . \tag{5.14c}$$

If we substitute Eqs. (5.10) and (5.12c) into Eq. (5.14), we find through order U^2

$$|\tilde{T}_l(k)|^2 = |T(k)|^2 + \mathrm{Re}\left\{\left(\frac{-im^2}{\pi\hbar^4k^2}\,T^*(k)R(k)\right)\left[\frac{k}{k'}\,M_{rr}(k,k')\,M_{rl}(k',k)\left(\ln\left|\frac{k_{Fr}-k'}{k_c}\right| - i\pi\theta(k'-k_{Fr})\right)\right.\right.$$

$$-\frac{k}{k''}M_{ll}(k'',k)M_{rl}(k,k'')\left(\ln\left|\frac{k-k'_{Fl}}{k_c}\right|-i\pi\theta(k'_{Fl}-k)\right)\Bigg]+O(T^3)\Bigg\}\ \theta(k-k_{Fr})\ , \tag{5.15a}$$

where

$$M_{ij}(k,q)=2L\int_0^b dx\,\psi_i^*(k,x)\,U(x)\,\psi_j(q,x),\quad i,j=r,l\ . \tag{5.15b}$$

For $k<k_{Fr}$, we can see that $\tilde{\psi}_l(k,x)=\psi_l(k,x)$ for the regions $-L\ll x\ll 0$ and $b\ll x\ll L$. In addition, from Eq. (5.14b) we see that $|\tilde{R}_l(k)|$ can be determined from the condition of current conservation across the barrier in the elastic channel

$$|\tilde{R}_l(k)|^2+|\tilde{T}_l(k)|^2=1\ . \tag{5.16}$$

Also, Eq. (5.16) can be derived from the requirement of orthogonality of $\tilde{\psi}_l(k,x)$ to states $\tilde{\psi}_l(q,x)$, q nearly equal to k. For right-hand states,

$$\tilde{\psi}_r(k,x)=(2L)^{-1/2}\tilde{T}_r(k)\,e^{-ikx}=(2L)^{-1/2}\tilde{R}_r(k)\,e^{ik(x-b)}\ , \tag{5.17a}$$

where

$$\tilde{T}_r(k)=T(k)+G_{r2}+F_{r2}\ , \tag{5.17b}$$

$$\tilde{R}_r(k)=R(k)-T^*(k)(G_{r2}+F_{r2})/R^*(k)\ . \tag{5.17c}$$

From Eqs. (5.11b) and (5.13b), we find

$$|\tilde{T}_r(k)|^2=|T(k)|^2+\mathrm{Re}\Bigg\{\left(\frac{-im^2}{\pi\hbar^4k^2}\,T^*(k)R(k)\right)\left[\frac{k}{k'}M_{ll}(k,k')M_{lr}(k',k)\left(\ln\left|\frac{k_{Fl}-k'}{k_c}\right|-i\pi\theta(k'-k_{Fl})\right)\right.$$
$$\left.-\frac{k}{k''}M_{rr}(k'',k)M_{lr}(k,k'')\left(\ln\left|\frac{k-k'_{Fr}}{k_c}\right|-i\pi\theta(k'_{Fr}-k)\right)\right]+O(T^3)\Bigg\}\ \theta(k-k_{Fl})\ . \tag{5.18}$$

Also, we can see that $\tilde{\psi}_r(k,x)=\psi_r(k,x)$ for $k<k_{Fl}$, $-L\ll x\ll 0$ or $b\ll x\ll -L$, and that an expression analogous to Eq. (5.16) holds for the reflection coefficient.

B. Current and Conductance Due to $\chi_0^{(2)}$

By reasoning similar to that of Sec. III C, it is straightforward to show that the additional current due to $\chi_0^{(2)}$ is

$$J_2(V)=\mathrm{sgn}(V)\,\frac{e}{h}\int_0^{|eV|}d\epsilon\,D_2(\epsilon,V)\ , \tag{5.19}$$

where

$$D_2(\epsilon,V)=\frac{-4m^2Ke^{-Kb}}{\pi\hbar^4k(k^2+K^2)}\,\mathrm{Re}\left(\frac{k}{k'}M_{rr}(k,k')M_{rl}(k',k)\right)\left(\ln\left|\frac{k_F-k'}{k_c}\right|-i\pi\theta(k'-k_F)\right)-\frac{k}{k''}M_{ll}(k'',k)M_{rl}(k,k'')$$
$$\times\left\{\ln\left|\frac{k-[k_F^2-2m(\hbar\omega-eV)/\hbar^2]^{1/2}}{k_c}\right|-i\pi\theta\left[\left(k_F^2-\frac{2m(\hbar\omega-eV)}{\hbar^2}\right)^{1/2}-k\right]\right\}\ ,\quad V>0$$
$$=\frac{-4m^2Ke^{-Kb}}{\pi\hbar^4k(k^2+K^2)}\,\mathrm{Re}\left[\frac{k}{k'}M_{ll}(k,k')M_{lr}(k',k)\left(\ln\left|\frac{k_F-k'}{k_c}\right|-i\pi\theta(k'-k_F)\right)-\frac{k}{k''}M_{rr}(k'',k)M_{lr}(k,k'')\right.$$
$$\left.\times\left(\ln\left|\frac{k-[k_F^2-2m(\hbar\omega+eV)/\hbar^2]^{1/2}}{k_c}\right|-i\pi\theta\{[k_F^2-2m(\hbar\omega+eV)/\hbar^2]^{1/2}-k\}\right)\right]\ ,\quad V<0 \tag{5.20a}$$

and

$$k'=[2m(\epsilon+E_F-\hbar\omega)/\hbar^2]^{1/2}\ , \tag{5.20b}$$

$$k''=[2m(\epsilon+E_F+\hbar\omega)/\hbar^2]^{1/2}\ , \tag{5.20c}$$

$$K=[2m(V_0-\epsilon-E_F)/\hbar^2]^{1/2}\,. \tag{5.20d}$$

We also find that we can rewrite Eq. (3.30) as

$$D_1(\epsilon,V)=\frac{m^2}{\hbar^4kk'}\,|M_{rl}(k',k)|^2\theta(k'-k_F),\quad V>0$$
$$=\frac{m^2}{\hbar^4kk'}\,|M_{lr}(k',k)|^2\theta(k'-k_F),\quad V<0\,. \tag{5.21}$$

To a good approximation, we can make the following replacements

$$\ln|(k_F-k')/k_c|\to\ln|(\epsilon-\hbar\omega)/E_0|\,,\qquad \ln\left|\frac{k-[k_F^2-2m(\hbar\omega\mp eV)/\hbar^2]^{1/2}}{k_c}\right|\to\ln\left|\frac{\epsilon+\hbar\omega\mp eV}{E_0}\right|\,,$$

$E_0=\hbar^2k_Fk_c/m=$ energy cutoff.

Also, we note that

$$\theta(k'-k_F)=\theta(\epsilon-\hbar\omega)\,,\qquad \theta\{[k_F^2-2m(\hbar\omega\mp eV)/\hbar^2]^{1/2}-k\}=\theta(\pm eV-\epsilon-\hbar\omega)\,.$$

Hence,

$$D_2(\epsilon,V)=\frac{-4m^2Ke^{-Kb}}{\pi\hbar^4k(k^2+K^2)}\,\mathrm{Re}\left[\frac{k}{k'}M_{rr}(k,k')M_{rl}(k',k)\left(\ln\left|\frac{\epsilon-\hbar\omega}{E_0}\right|-i\pi\theta(\epsilon-\hbar\omega)\right)\right.$$
$$\left.-\frac{k}{k''}M_{ll}(k'',k)M_{rl}(k,k'')\left(\ln\left|\frac{\epsilon+\hbar\omega-eV}{E_0}\right|-i\pi\theta(eV-\epsilon-\hbar\omega)\right)\right],\quad V>0$$
$$=\frac{-4m^2Ke^{-Kb}}{\pi\hbar^4k(k^2+K^2)}\,\mathrm{Re}\left[\frac{k}{k'}M_{ll}(k,k')M_{lr}(k',k)\left(\ln\left|\frac{\epsilon-\hbar\omega}{E_0}\right|-i\pi\theta(\epsilon-\hbar\omega)\right)\right.$$
$$\left.-\frac{k}{k''}M_{rr}(k'',k)M_{lr}(k,k'')\left(\ln\left|\frac{\epsilon+\hbar\omega+eV}{E_0}\right|-i\pi\theta(-eV-\epsilon-\hbar\omega)\right)\right],\quad V<0 \tag{5.22}$$

$$D_1(\epsilon,V)=\frac{m^2}{\hbar^4kk'}\,|M_{rl}(k',k)|^2\theta(\epsilon-\hbar\omega),\quad V>0$$
$$=\frac{m^2}{\hbar^4kk'}\,|M_{lr}(k',k)|^2\theta(\epsilon-\hbar\omega),\quad V<0. \tag{5.23}$$

The inelastic conductance associated with the excitation of the vibrator is

$$G_1(V)=\frac{e^2m^2}{2\pi\hbar^5kk'}\{|M_{rl}(k',k)|^2\theta(eV-\hbar\omega)$$
$$+|M_{lr}(k',k)|^2\theta(-eV-\hbar\omega)\}, \tag{5.24a}$$

where

$$k=[2m(|eV|+E_F)/\hbar^2]^{1/2} \tag{5.24b}$$

and

$$k'=[2m(|eV|-\hbar\omega+E_F)/\hbar^2]^{1/2}. \tag{5.24c}$$

The terms in the conductance of order U^2 in the elastic channel are given by

$$G_2(V)=C_1\ln\left|\frac{eV-\hbar\omega}{E_0}\right|+C_2\theta(eV-\hbar\omega)\quad,\quad V>0$$
$$=C_3\ln\left|\frac{eV+\hbar\omega}{E_0}\right|+C_4\theta(-eV-\hbar\omega),\quad V<0 \tag{5.25a}$$

where

$$C_1=-F(eV)\,\mathrm{Re}\left(\frac{k}{k'}M_{rr}(k,k')M_{rl}(k',k)\right)_{\epsilon=eV}$$
$$+F(0)\,\mathrm{Re}\left(\frac{k}{k''}M_{ll}(k'',k)M_{rl}(k,k'')\right)_{\epsilon=0}, \tag{5.25b}$$

$$C_2=-\pi F(eV)\,\mathrm{Im}\left(\frac{k}{k'}M_{rr}(k,k')M_{rl}(k',k)\right)_{\epsilon=eV}$$
$$+\pi F(0)\,\mathrm{Im}\left(\frac{k}{k''}M_{ll}(k'',k)M_{rl}(k,k'')\right)_{\epsilon=0}, \tag{5.25c}$$

$$C_3=-F(-eV)\,\mathrm{Re}\left(\frac{k}{k'}M_{ll}(k,k')M_{lr}(k',k)\right)_{\epsilon=-eV}$$
$$+F(0)\,\mathrm{Re}\left(\frac{k}{k''}M_{rr}(k'',k)M_{lr}(k,k'')\right)_{\epsilon=0}\,, \tag{5.25d}$$

$$C_4=-\pi F(-eV)\,\mathrm{Im}\left(\frac{k}{k'}M_{ll}(k,k')M_{lr}(k',k)\right)_{\epsilon=-eV}$$

$$+\pi F(0)\,\mathrm{Im}\left(\frac{k}{k''}M_{rr}(k'', k)M_{lr}(k, k'')\right)_{\epsilon=0}, \tag{5.25e}$$

$$F(\epsilon)=2e^2m^2ke^{-Kb}/\pi^2\hbar^5k(k^2+K^2), \tag{5.25f}$$

and in Eq. (5.25)

$$k=[2m(\epsilon+E_F)/\hbar^2]^{1/2}, \tag{5.25g}$$

$$k'=[2m(\epsilon-\hbar\omega+E_F)/\hbar^2]^{1/2}, \tag{5.25h}$$

$$k''=[2m(\epsilon+\hbar\omega+E_F)/\hbar^2]^{1/2}, \tag{5.25i}$$

$$K=[2m(V_0-\epsilon-E_F)/\hbar^2]^{1/2}. \tag{5.25j}$$

Equation (5.25) represents only those terms which show some structure. Additional slowly varying terms occur which have been omitted since they cannot be distinguished from the background. We note that *if* the reflection matrix elements $M_{rr}(k, q)$ and $M_{ll}(k, q)$ (k and q arbitrary) are negligible, then there are no second-order terms in the elastic channel which give rise to structure in the conductance. Furthermore, the inelastic conductance equation (5.24) reduces to Eq. (3.33) if the reflection matrix elements (and hence, inelastic-reflection coefficients, such as R') can be neglected. Hence, the results of first Born approximation are valid when the reflection matrix elements (or inelastic-reflection coefficients) are negligible. These matrix elements are large only when the interaction potential $U(x)$ is sizeable near an edge(s) of the barrier.

The conductance $G_2(V)$ is due to an interference between the direct elastic-tunneling process, represented by $T(k)$, and a two-step process involving the virtual excitation and deexcitation of the vibrator. Such terms give rise to logarithmic singularities in the conductance and step-function changes in the conductance at $eV=\pm\hbar\omega$. The sign of these effects depends upon the relative sizes of the various matrix elements in Eq. (5.25).

To illustrate these effects, we consider an interaction potential

$$U(x)=U_0a\,\delta(x), \tag{5.26}$$

where U_0a is a constant (units of energy-distance). We find that logarithmic terms appear as in Fig. 2(a) and the step-function terms as in Fig. 2(b). The ratio of the magnitude of the step decrease in $G_2(V)$ to the magnitude of the step increase in $G_1(V)$ is approximately $2E_F/V_0$, which is greater than unity for typical metal-insulator-metal junctions. (We neglect small changes in the magnitude of the conductance between $V>0$ and $V<0$.) Hence, there is a net decrease in the conductance above threshold ($|eV|>\hbar\omega$) in addition to the logarithmically singular terms for the interaction potential (5.26).

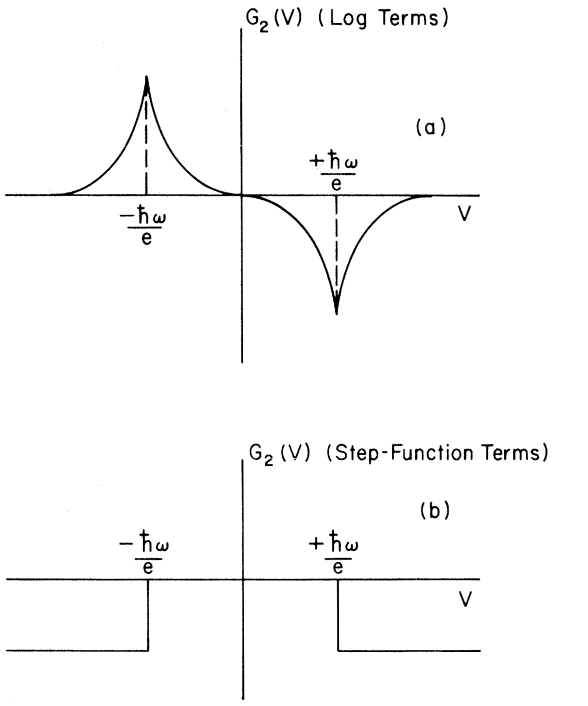

FIG. 2. (a) Logarithmically singular terms in $G_2(V)$ for the case where $U(x)\propto\delta(x)$. Singularities at $eV=\pm\hbar\omega$ arise from the interference of the direct elastic process and a two-step process involving the virtual excitation and deexcitation of the vibrator. (b) Step-function decreases at $eV=\pm\hbar\omega$ are larger than the increases of $G_1(V)$ at $eV=\pm\hbar\omega$ (Fig. 1) for typical metal-insulator-metal junctions. Positive bias voltage corresponds to current flowing in the $-x$ direction.

The coefficients of the logarithmic terms are given approximately by

$$C_3=-C_1 \tag{5.27a}$$

$$=[(V_0-E_F)/E_F]^{1/2}\pi^{-1}C_2, \tag{5.27b}$$

where

$$C_2=-\frac{64e^2m^2(U_0a)^2k''k^3K^2}{\pi\hbar^5(k^2+K^2)^4}e^{-2Kb}, \tag{5.27c}$$

where k, k'', and K are given by Eqs. (5.25g), (5.25h), and (5.25i) for $\epsilon=0$. The coefficient C_4 is approximately equal to C_2. We have taken $E_0=\hbar\omega$ to ensure the continuity of $G_2(V)$ at $V=0$ because we find that if all the terms to order U^2 are retained (including the omitted slowly varying terms), the conductance must be continuous at $V=0$.

If the interaction potential is changed from a δ function near $x=0$ [as in Eq. (5.26)], to a δ function near $x=b$, the sign of the logarithmic terms is changed, but the step-function terms remain the same. Hence, we can obtain a term in the conduc-

tance from inelastic interactions near the edge of the barrier resembling a self-energy effect but with the sign depending upon which edge gives rise to the interaction. If the junction is symmetric with identical interactions at each edge, then we expect no sizeable logarithmic terms due to cancellation. [It is possible to have a small symmetric (about $V=0$) contribution from the logarithmic terms in this case if we make no approximations in the evaluation of C_1 and C_3.]

In the molecular excitation experiments of Jaklevic and Lambe,[2,3] clear evidence of only $G_1(V)$ has been reported. This is not too surprising since the reflection-type matrix elements M_{ll} and M_{rr} pick out only a small portion of the interaction potential near the left and right boundaries, respectively, of the barrier. For molecular excitations, the interaction potential is the dipole (plus image) potential[3,6] [Eq. (3.38)]. Hence, the overlap of $U(x)$ with $\psi_l(k,x)\psi_l^*(k,x)$ or $\psi_r(k,x)\psi_r^*(k,x)$ is small. (Numerical calculations based upon this potential show extremely small effects which would be difficult to detect experimentally. Similar results hold for the induced-dipole potential.) If these matrix elements were large enough for $G_2(V)$ to be detected, the logarithmic singularities in $G_2(V)$ would resemble the self-energy effects described by Davis and Duke[6] for optical-phonon interactions in degenerate semi-conductor electrodes.

We now make an explicit comparison of the line shapes in d^2I/dV^2 versus V for a vibrator inside the barrier far enough for the $G_2(V)$ terms to be negligible (i.e., more than $\sim\frac{1}{2}$K) and a vibrator at the $x=b$ boundary (using δ-function interaction potentials). The conductance is given approximately by (omitting the background conductance)

$$G(V)=\pi^{-1}\Delta G_1(\hbar\omega)\left[1-\left(\frac{\eta 2E_F}{V_0}\right)\pi\theta(|eV|-\hbar\omega)-\eta\frac{2E_F}{V_0}\left(\frac{V_0-E_F}{V_0}\right)^{1/2}\ln\left|\frac{eV-\hbar\omega}{eV+\hbar\omega}\right|\right], \quad (5.28)$$

where $\Delta G_1(\hbar\omega)$ is the size of the step increase in $\Delta G_1(V)$ at $V=\hbar\omega$ (see Fig. 1), $\eta=0$ corresponds to the vibrator inside the barrier, and $\eta=1$ corresponds to the vibrator at the $x=b$ boundary. $\Delta G_1(\hbar\omega)$ may be thought to depend upon η, also, since the potential of a vibrator at a boundary can be influenced by screening, etc. To account for the finite width of the spectral line (of the vibrator) we make the replacements

$$\pi\theta(x)\to\tfrac{1}{2}\pi+\tfrac{1}{2}\tan^{-1}(x/\Gamma) \quad , \quad (5.29a)$$

$$\ln|x|\to\tfrac{1}{2}\ln(x^2+\Gamma^2) \quad . \quad (5.29b)$$

The results of a numerical calculation for typical parameters are shown in Fig. 3. We note that the line shape is essentially reversed for the vibrator at $x=b$ compared to the vibrator inside the barrier.

The occurrence of $G_2(V)$ terms associated with the virtual excitation and deexcitation of phonons in p-n junctions involving indirect semiconductors is not allowed due to the lack of the parallel direct process connecting the same initial and final states. Only the inelastic current involving the emission of phonons required by momentum conservation is observed.[11] The same considerations apply to the phonon structure seen in metal-Ge (n-type) contacts.[12] However, in p-n junctions made from direct semiconductors and metal-semiconductor contacts involving either direct or p-type semiconductors, such effects could be important in addition to the self-energy effects discussed in Ref. 6. The experimental data[13] reported for highly doped metal-semiconductor junctions are interpreted satisfactorily by the self-energy mechanism. However, at lower doping, the changes in line shape with semiconductor carrier concentration may be due to the effects discussed in this paper.[14]

IV. CONCLUSIONS

In this paper we have formulated a many-electron theory of inelastic tunneling based upon stationary

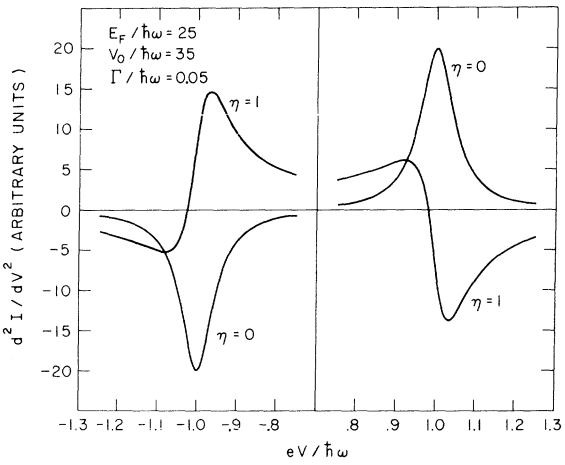

FIG. 3. Curves of d^2I/dV^2 versus V are shown for a typical parameter of a metal-insulator-metal junction. (The background conductance is omitted.) $\eta=0$ corresponds to a vibrator far enough inside the tunnel barrier (i.e., more than $\sim\frac{1}{2}$ K) for only the inelastic conductance $G_1(V)$ to be important. $\eta=1$ corresponds to a vibrator whose interaction potential is confined to a region near the $x=b$ boundary of the barrier. Γ is a parameter representing the finite width of the spectral line of the vibrator. The relative size of the $\eta=1$ compared to $\eta=0$ line shape depends upon screening and other details of the potential and no attempt has been made to estimate these effects.

current-carrying states. The theory was formally derived for an arbitrary tunneling barrier with an arbitrary interaction potential between the electrons and a vibrator, which represents a molecular impurity, a phonon, a magnetic impurity, etc. An example of the theory was given for a square-barrier potential with an interaction potential confined to the barrier. Most of the results were for a one-dimensional system for simplicity, but these results can be generalized to three-dimensions in a straightforward manner as done, for example, for the dipole potential of Scalapino and Marcus[6] in Sec. III D.

Our results for the inelastic current indicate agreement with the transfer-Hamiltonian method[5] if the appropriate matrix elements of the interaction potential are taken between orthogonal current-carrying states instead of the nonorthogonal standing-wave states used in the transfer-Hamiltonian method when the interaction potential is confined to the barrier region. (Other cases were considered only formally in Sec. II and IV.) The results of Scalapino and Marcus[6] are in approximate agreement with the transfer-Hamiltonian method and the results of the present work.

By keeping all terms of second order in the interaction potential, logarithmic singularities in the elastic-transmission coefficient were found. These singularities result from an interference between the direct elastic process (ordinary single-particle tunneling) and a two-step process involving the virtual excitation and deexcitation of the vibrator (molecular impurity, phonon, etc.). Such terms also occur in the transfer-Hamiltonian approach but have never been considered except for magnetic-impurity scattering.[9,10] In addition to the logarithmic singularities, step-function terms also occur in the elastic-transmission coefficient as well as in the inelastic-transmission coefficient.

The processes leading to the logarithmic singularities and step-function terms in the elastic-transmission coefficient are probably not important in the molecular excitation experiments[2,3] because the relevant matrix elements are not expected to be large unless the impurities are sufficiently close to the boundaries of the barrier. In this latter case, the line shapes in d^2I/dV^2 versus V are fundamentally different. In some metal-semiconductor experiments involving the optical phonons of low-doped semiconductors such processes might be important.[14]

APPENDIX

Let us repeat Eq. (4.15) as (ν and η interchanged)

$$\varphi_\mu(x) = -\sum_\eta{}' \sum_\nu \langle\psi_\nu|f_\eta\rangle\langle\psi_\eta|h_\mu(\epsilon_\eta+\epsilon_\mu-\epsilon_\nu)\rangle\psi_\nu(x) \quad , \tag{A1}$$

where the sum on η is over all occupied states and the sum on ν is over only unoccupied states. We note that $\langle\psi_\nu|f_\eta\rangle = \langle\psi_\nu|\psi'_\eta\rangle$ for ν unoccupied and η occupied. Consider first the case where $k_{Fl} > k_{Fr}$. For $\psi_\eta(x)$ equal to a right-hand state $\psi_r(p, x)$, there exist no unoccupied states $\psi_\nu(x) = \psi_l(u, x)$ or $\psi_r(u, x)$ which overlap appreciably with $\psi'_r(p, x)$, since $p' = (p^2 - 2m\omega/\hbar)^{1/2} < k_{Fr}$ and all the unoccupied states have $u > k_{Fr}$. Hence, the sum over η in Eq. (A1) is a sum over left-hand $\psi_\eta(x) = \psi_l(p, x)$, $p < k_{Fl}$, only. In the sum over ν, only the unoccupied right-hand states $\psi_\nu(x) = \psi_r(u, x)$ can have appreciable overlap with $\psi'_l(p, x)$, since the unoccupied left-hand states have $u > k_{Fl} > p'$. So,

$$\varphi_\mu(x) = -\sum_{p<k_{Fl}} \sum_{k_{Fr}<u} \langle\psi_r(u)|\psi'_l(p)\rangle \times\langle\psi_l(p)|h_\mu(\epsilon(p)+\epsilon_\mu-\epsilon(u))\rangle\psi_r(u, x), \quad k_{Fl} > k_{Fr} \quad . \tag{A2}$$

We need to consider only μ equal to a left-hand state $\psi_l(k, x)$ since μ equal to a right-hand state would give $\langle\psi_l(p)|h_\mu\rangle \sim T$ and since $\langle\psi_r(u)|\psi'_l(p)\rangle \sim T$, this would give $\varphi_\mu \sim T^2$ which we can neglect.

From Eq. (A2), we then find for left-hand states

$$h_l(k, \epsilon, x) = (2L)^{-1/2} H_{l1} e^{-iqx}, \quad x < 0$$
$$= (2L)^{-1/2} H_{l2} e^{iq(x-b)}, \quad b < x \tag{A3a}$$

$$H_{l1} = (2L)^{-1/2} \int_0^b dx' K(\epsilon, 0, x') U(x') \psi_l(k, x'), \tag{A3b}$$

$$H_{l2} = (2L)^{-1/2} \int_0^b dx' K(\epsilon, b, x') U(x') \psi_l(k, x'), \tag{A3c}$$

$$q = (2m\epsilon/\hbar^2)^{1/2} \quad .$$

Equation (A2) becomes

$$\varphi_l(k, x) = (4\pi^2)^{-1} \int_{k_{Fr}}^\infty du \int_0^{k_{Fl}} dp [R^*(p) H_{l1} + T^*(p) H_{l2}][T^*(u) R'_l(p) + R^*(u) T'_l(p)] \times \left[\frac{1 - e^{-i(p-q)L}}{p-q}\right]\left[\frac{1 - e^{-i(u-p')L}}{u-p'}\right]\psi_r(u, x) \quad , \tag{A4a}$$

$$q = [p^2 + k^2 - u^2]^{1/2} \quad , \tag{A4b}$$

$$p' = (p^2 - 2m\omega/\hbar)^{1/2} \quad . \tag{A4c}$$

The quantities H_{l1} and H_{l2} are evaluated for $\epsilon = \hbar^2 q^2/2m$ in Eqs. (A2b) and (A3c). (We limit the range of integration so that $q^2 > 0$.) Now those states for which $u \simeq p'$ and for which $p \simeq q$ contribute the most to the integral. This is equivalent to $q \simeq (k^2 + 2m\omega/\hbar)^{1/2} \simeq p$, $u \simeq k$. We evaluate the slowly varying functions $R(p)$, H_{l1}, etc., accordingly, so that

$$\varphi_l(k,\ x)=[R^*((k^2+2m\omega/\hbar)^{1/2})H_{l1}+T^*((k^2+2m\omega/\hbar)^{1/2})H_{l2}][T^*(k)R_l'((k^2+2m\omega/\hbar)^{1/2})+R^*(k)\,T_l'((k^2+2m\omega/\hbar)^{1/2})]$$

$$\times(2L)^{-1/2}\begin{cases}T(k)e^{-ikx}I(-x) & ,\quad x<0\\ [e^{-ik(x-b)}I(b-x)+R(k)e^{ik(x-b)}I(x-b)], & x>b\end{cases}\tag{A5a}$$

where

$$I(y)=(4\pi^2)^{-1}\int_{k_{Fr}}^{\infty}du\int_0^{k_{Fl}}dp\left[\frac{1-e^{-i(p-q)L}}{p-q}\right]\left[\frac{1-e^{-i(u-p')L}}{u-p'}\right]e^{i(u-k)y}.\tag{A5b}$$

We evaluate H_{l1} and H_{l2} for $\epsilon=\epsilon(k)+\hbar\omega$ in Eqs. (A3b) and (A3c) and we limit the range of integration so that $q^2>0$. We define new variables of integration

$$t=u-k,\quad s=u-p'.\tag{A6}$$

Clearly, only those states where $t\simeq 0$ and $s\simeq 0$ are important. To a good approximation,

$$p-q=kt\Big/\left(k^2+\frac{2m\omega}{\hbar}\right)^{1/2}.\tag{A7}$$

Substituting into Eq. (A5b), we obtain

$$I(y)=(4\pi^2)^{-1}\int_{k_1}^{\infty}dt\int_{k_2}^{k_c}ds\,e^{ity}\left[\frac{1-e^{-itL'}}{t}\right]\left[\frac{1-e^{-isL}}{s}\right],\tag{A8a}$$

$$k_1=k_{Fr}-k,\tag{A8b}$$

$$k_2=k-(k_{Fl}^2-2m\omega/\hbar)^{1/2},\tag{A8c}$$

$$L'=kL\Big/\left(k^2+\frac{2m\omega}{\hbar}\right)^{1/2}.\tag{A8d}$$

We also apply a cutoff k_c since we have retained nothing in the integrand to limit the contribution from large s. For $0\ll|y|\ll L$, we find

$$I(y)=\frac{i}{2\pi}\,\theta(y)\theta(k-k_{Fr})\left(-\ln\left|\frac{k-(k_{Fl}^2-2m\omega/\hbar)^{1/2}}{k_c}\right|\right.$$

$$\left.+\,i\pi\theta((k_{Fl}^2-2m\omega/\hbar)^{1/2}-k)\right).\tag{A9}$$

Substituting into Eq. (A5), and making use of Eqs. (3.16), (3.18), and (3.19), we find the result quoted in Eq. (5.12) of the text. $\varphi_r(k,\ x)$ vanishes for $k_{Fl}>k_{Fr}$ (except near the barrier) as discussed previously. Similar results hold for $k_{Fr}>k_{Fl}$.

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