Tunneling theory without the transfer-Hamiltonian formalism. II. Resonant and inelastic tunneling across a junction of finite width

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A novel theory of electronic tunneling between two semi-infinite systems separated by an insulating barrier of finite width is developed. The theory based on Keldysh's perturbation theory for nonequilibrium processes does not invoke the transfer-Hamiltonian formalism. The analysis is a reasonably straightforward extension of the theory developed in the first paper of this series, dealing with the abrupt junction (of zero width). The results for the abrupt junction are shown to correspond to those of the finite junction in the zero-thickness limit. The general formalism is applied to the study of effects of impurities, incorporated into the barrier, on the tunneling-current energy distribution. It is shown that tunneling resonances may reflect "interfacial" as well as "atomic" impurity states localized within the barrier. The general discussion is illustrated by somewhat more detailed analysis of two common models for such impurities: the Anderson model for the localized resonant (impurity) state, and the elementary δ-function pseudopotential. The entire formalism is developed so as to allow for explicitly time-dependent potentials in the barrier region. This feature of the formalism is being applied to a phenomenological analysis of inelastic tunneling associated with localized vibrational excitations in the barrier region, i.e., the vibrating-impurity problem. This work will be reported separately. The theory allows a clear separation between the normal tunneling and the so-called resonant and inelastic channels. In the normal channel the energy density of tunneling current displays the expected dependence on the product of the local densities of states in the right and left electrodes evaluated at the interfaces. The other channels have a characteristically different dependence on these quantities, and are inherently capable of producing a left-right asymmetry in the tunneling current. Besides opening the new channels the (time-dependent) impurity potential also affects the normal channel by modifying the elastic barrier transmissivity. An extension of the one-dimensional theory to three dimensions is being developed.

I. INTRODUCTION

This is the second of a series of papers concerned with the development of a many-body theory of electronic tunneling between two semi-infinite systems separated by an insulating barrier of finite width. The theory is based on a perturbation theory for nonequilibrium processes, developed by Keldysh,[1] and obviates the transfer-Hamiltonian formalism which is generally applied in current analysis of tunneling phenomena.[2-7] The motivation for our work and our general approach are discussed at length in the first paper of this series,[8] dealing with the abrupt junction (of zero width). In the present paper we extend the theory to include junctions of finite width. Furthermore, we allow the potential in the barrier region to include an explicitly time-dependent term. The time-dependent term may represent an external modulation, or the pseudopotential for a vibrating impurity. The formalism is applied in a discussion of resonant tunneling across barriers containing impurities.[9-11] Application to inelastic tunneling across a barrier containing vibrating impurities is considered in a separate publication.

The formal analysis, while somewhat lengthy, is a fairly obvious extension of the work reported in I.[8] This analysis is presented in Secs. II and III, and is essentially self-contained. However, to avoid duplication of the extensive discussion in I, verbal arguments are kept to a bare minimum.

In Sec. II, we determine the single-particle thermal-equilibrium Green's function for the entire junction, G, in terms of the thermal-equilibrium "uncoupled Green's functions" for the three uncoupled subregions of the junction g_α. The pseudo-Hamiltonian which "couples" the subregions and hence determines G in terms of g_α is also derived.

In Sec. III, the tunneling current is expressed in terms of the correlation function G^+ which has to satisfy Keldysh's matrix Dyson equation, relating it to the uncoupled Green's functions g_α. The latter (matrix) equation is used to express the tunneling current in a form which manifestly reduces to the corresponding expression for the abrupt static junction, when both the spatial width and the time-dependent component of the potential in the barrier tend to zero.

In Sec. IV the general expression for the tunneling current in a finite time-dependent junction is compared with the result derived in I. The current is shown to include two contributions. The first, or "normal," channel can be expressed in a form

similar to that deduced by means of the transfer-Hamiltonian formalism, provided that the left and right densities of states are interpreted as appropriate "local" densities of states. However, in contrast to the transfer-Hamiltonian formalism, our derivation leads to an explicit expression for the energy-dependent "matrix element." The second, "resonant and inelastic" channel exhibits a characteristic dependence on the local densities of states in the electrodes which cannot be obtained from the transfer Hamiltonian. This channel "closes" when the density of states vanishes in the static barrier. Thus, it does not contribute to the current across the static junction of zero width.

In Sec. V we apply our formal results to discuss resonant tunneling. Specifically we consider the effect of atomic impurities within the barrier on the "matrix element" and the resonant enhancement of the current in the normal channel, as well as the effect of the impurity density of states on the resonant channel. In this analysis the impurity is represented by a static pseudopotential. The "uncoupled" Green's function for the perturbed barrier is calculated within an approximation corresponding to an Anderson model for the localized impurity states, in which we neglect the Coulomb repulsion between two electrons at the impurity.[12,13]

Readers who wish to avoid the detailed, occasionally involved algebra may find the discussion in Sec. IV and subsections V A and V B adequate.

In Sec. VI we present a summary of our results.

II. EQUILIBRIUM GREEN'S FUNCTION

A. Definitions

In this section we shall compute the single-particle Green's function for a one-dimensional junction of arbitrary width in the absence of an external potential in terms of the Green's functions of the three uncoupled subregions: left electrode, barrier, right electrode; these are defined by writing the entire Hamiltonian in the form indicated below:

$$\mathcal{H}=\Theta(-(x-L))\mathcal{H}_L+\Theta(x-L)\Theta(-(x-R))\mathcal{H}_B + \Theta(x-R)\mathcal{H}_R \ . \tag{2.1}$$

The Hamiltonians $\mathcal{H}_\alpha$ $\alpha=L, B, R$, characterize the uncoupled subregions. The Green's functions for these subregions g_α will be referred to as "uncoupled" Green's functions. These are required, as in I, to satisfy general homogenous boundary conditions at the interfaces and at infinity. As in I, we shall ultimately specialize these boundary conditions, and require the normal derivatives to vanish at the interfaces, in order to obtain the preferred "transfer-Hamiltonian-like" form for the tunneling current. Thus, the uncoupled Green's functions satisfy the equations

$$[\hbar\omega-\mathcal{H}_\alpha(x)]g_\alpha(x,x';\omega)=\delta(x-x'); \quad \alpha=L,B,R \ . \tag{2.2}$$

At the interfaces, we impose general homogeneous (and self-adjoint) boundary conditions,

$$\begin{aligned}
&\left(\alpha_L+\beta_L\frac{\partial}{\partial x}\right)g_L(x,x'<L;\omega)|_{x=L}=0\\
&\quad=\left(\alpha_L+\beta_L\frac{\partial}{\partial x'}\right)g_L(x<L,x';\omega)|_{x'=L}\\
&\left(\alpha_R+\beta_R\frac{\partial}{\partial x}\right)g_R(x,x'>R;\omega)|_{x=R}=0\\
&\quad=\left(\alpha_R+\beta_R\frac{\partial}{\partial x'}\right)g_R(x>R,x';\omega)|_{x'=R}\\
&\left(\alpha_{L,R}+\beta_{L,R}\frac{\partial}{\partial x}\right)g_B(x,L<x'<R;\omega)|_{x=L,R}=0\\
&\quad=\left(\alpha_{L,R}+\beta_{L,R}\frac{\partial}{\partial x'}\right)g_B(L<x<R,x';\omega)|_{x'=L,R} \ .
\end{aligned} \tag{2.3}$$

The (homogeneous) boundary conditions imposed on $g_{L,R}$ at $\pm\infty$ are

$$\begin{aligned}
&\lim_{x\to-\infty}\left(a_-+b_-\frac{\partial}{\partial x}\right)g_L(x,x'<L;\omega)=0\\
&\quad=\lim_{x'\to-\infty}\left(a_-+b_-\frac{\partial}{\partial x'}\right)g_L(x<L,x';\omega) \ ,\\
&\lim_{x\to\infty}\left(a_++b_+\frac{\partial}{\partial x}\right)g_R(x,x'>R;\omega)=0\\
&\quad=\lim_{x'\to\infty}\left(a_++b_+\frac{\partial}{\partial x'}\right)g_R(x>R,x';\omega) \ .
\end{aligned} \tag{2.4}$$

The Green's function for the entire junction is defined by

$$[\hbar\omega-\mathcal{H}(x)]G(x,x';\omega)=\delta(x-x') \tag{2.5}$$

and satisfies at $\pm\infty$ the boundary conditions imposed respectively on $g_{R,L}$. Here it should be recalled that the "out-going-wave" boundary conditions are a particular case of the general homogeneous boundary conditions.

B. Calculation of the equilibrium Green's function

An application of Green's theorem over the appropriate domains leads to the following expression for $G(x,x';\omega)$ in terms of the "uncoupled" Green's functions g_α:

$$G(x,x';\omega)=g_L(x,x';\omega)\Theta(-x'+L)$$
$$-\frac{\hbar^2}{2m}\left(g_L(x,x_1;\omega)\frac{\partial}{\partial x_1}G(x_1,x';\omega)-\frac{\partial}{\partial x_1}[g_L(x,x_1;\omega)]\,G(x_1,x';\omega)\right)\Big|_{x_1=L^-},\quad x\le L$$

$$G(x,x';\omega)=g_B(x,x';\omega)\Theta(x'-L)\Theta(-x'+R)$$
$$-\frac{\hbar^2}{2m}\left(g_B(x,x_1;\omega)\frac{\partial}{\partial x_1}G(x_1,x';\omega)-\frac{\partial}{\partial x_1}[g_B(x,x_1;\omega)]\,G(x_1,x';\omega)\right)\Big|_{x_1=L^+}^{x_1=R^-},\quad L\le x\le R \tag{2.6}$$

$$G(x,x';\omega)=g_R(x,x';\omega)\Theta(x'-R)$$
$$+\frac{\hbar^2}{2m}\left(g_R(x,x_1;\omega)\frac{\partial}{\partial x_1}G(x_1,x';\omega)-\frac{\partial}{\partial x_1}[g_R(x,x_1;\omega)]\,G(x_1,x';\omega)\right)\Big|_{x_1=R^+},\quad x\ge R\ .$$

An alternative representation of $G(x,x';\omega)$ is

$$G(x,x';\omega)=g_L(x,x';\omega)\Theta(-x+L)$$
$$+\frac{\hbar^2}{2m}\left(G(x,x_1';\omega)\frac{\partial}{\partial x_1}g_L(x_1,x';\omega)-\frac{\partial}{\partial x_1}[G(x,x_1;\omega)]\,g_L(x_1,x';\omega)\right)\Big|_{x_1=L^-},\quad x'\le L$$

$$G(x,x';\omega)=g_B(x,x';\omega)\Theta(x-L)\Theta(-x+R)$$
$$+\frac{\hbar^2}{2m}\left(G(x,x_1;\omega)\frac{\partial}{\partial x_1}g_B(x_1,x';\omega)-\frac{\partial}{\partial x_1}[G(x,x_1;\omega)]\,g_B(x_1,x';\omega)\right)\Big|_{x_1=L^+}^{x_1=R^-},\quad L\le x'\le R \tag{2.7}$$

$$G(x,x';\omega)=g_R(x,x';\omega)\Theta(x-R)$$
$$-\frac{\hbar^2}{2m}\left(G(x,x_1;\omega)\frac{\partial}{\partial x_1}g_R(x_1,x';\omega)-\frac{\partial}{\partial x_1}[G(x,x_1;\omega)]\,g_R(x_1,x';\omega)\right)\Big|_{x_1=R^+};\quad x'\ge R\ .$$

At $x=x'$, all Green's functions are continuous; their first derivatives display at this point a characteristic discontinuity,

$$\frac{\partial}{\partial x}G(x,x';\omega)\Big|_{x=x'-}^{x=x'+}=\frac{2m}{\hbar^2}=\frac{\partial}{\partial x'}G(x,x';\omega)\Big|_{x'=x^-}^{x'=x^+}, \tag{2.8}$$

and their mixed second derivative is again continuous. One easily verifies that a substitution of Eqs. (2.7) into Eqs. (2.6) leads to an expression of $G(x,x';\omega)$ in terms of its "boundary values," i.e., G and its first derivative evaluated with both arguments located at the interfaces. These boundary values have to be determined self-consistently. In the present case it is simplest to impose Eqs. (2.8) at the interfaces. In particular, whenever the coefficients $\beta_{L,R}$ in Eqs. (2.3) do not vanish, the following matrix equations hold:

$$\begin{pmatrix} G(L,L;\omega) & G(L,R;\omega)\\ G(R,L;\omega) & G(R,R;\omega)\end{pmatrix}$$
$$=\begin{pmatrix} g_L(L,L;\omega) & 0\\ 0 & g_R(R,R;\omega)\end{pmatrix}\begin{pmatrix} g_L(L,L;\omega)+g_B(L,L;\omega) & g_B(L,R;\omega)\\ g_B(R,L;\omega) & g_R(R,R;\omega)+g_B(R,R;\omega)\end{pmatrix}^{-1}\begin{pmatrix} g_B(L,L;\omega) & g_B(L,R;\omega)\\ g_B(R,L;\omega) & g_B(R,R;\omega)\end{pmatrix}$$
$$=\begin{pmatrix} g_B(L,L;\omega) & g_B(L,R;\omega)\\ g_B(R,L;\omega) & g_B(R,R;\omega)\end{pmatrix}\begin{pmatrix} g_L(L,L;\omega)+g_B(L,L;\omega) & g_B(L,R;\omega)\\ g_B(R,L;\omega) & g_R(R,R;\omega)+g_B(R,R;\omega)\end{pmatrix}^{-1}\begin{pmatrix} g_L(L,L;\omega) & 0\\ 0 & g_R(R,R;\omega)\end{pmatrix}. \tag{2.9}$$

Equations (2.9) apply in particular when the coefficients $\alpha_{L,R}$ in Eqs. (2.3) vanish, i.e., when the normal derivatives of the uncoupled Green's functions g_α vanish at the interfaces. In that case the following equation applies:

$$\begin{pmatrix} \Gamma(L,L;\omega) & \Gamma(L,R;\omega) \\ \Gamma(R,L;\omega) & \Gamma(R,R;\omega) \end{pmatrix} = \frac{2m}{\hbar^2} \begin{pmatrix} g_L(L,L;\omega)+g_B(L,L;\omega) & -g_B(L,R;\omega) \\ -g_B(R,L;\omega) & g_R(R,R;\omega)+g_B(R,R;\omega) \end{pmatrix}^{-1} . \tag{2.10}$$

where

$$\Gamma(\alpha,\beta;\omega) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x\, \partial x_1} G(x,x_1;\omega)\Big|_{\substack{x=\alpha \\ x_1=\beta}} . \tag{2.11}$$

When the coefficients $\beta_{L,R}$ in Eqs. (2.3) vanish, then Eqs. (2.9) are invalid. Denoting the uncoupled Green's functions which vanish at the interfaces by $\bar{g}_\alpha$, we can now verify that

$$\begin{pmatrix} G(L,L;\omega) & G(L,R;\omega) \\ G(R,L;\omega) & G(R,R;\omega) \end{pmatrix} = \frac{2m}{\hbar^2} \begin{pmatrix} \bar{\gamma}_L(L,L;\omega)+\bar{\gamma}_B(L,L;\omega) & -\bar{\gamma}_B(L,R;\omega) \\ -\bar{\gamma}_B(R,L;\omega) & \bar{\gamma}_R(R,R;\omega)+\bar{\gamma}_B(R,R;\omega) \end{pmatrix}^{-1} , \tag{2.9'}$$

where now

$$\bar{\gamma}_\alpha(\beta,\gamma;\omega) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x \partial x_1} \bar{g}_\alpha(x,x_1;\omega)\Big|_{\substack{x=\beta \\ x_1=\gamma}} . \tag{2.12}$$

The matrix equations (2.9), (2.9′) and (2.10) are obvious generalizations of Eqs. (2.18), (2.18″), and (2.24) of I. We note that when Eq. (2.10) applies, then Eq. (2.7) implies that

$$\begin{pmatrix} \frac{\partial G}{\partial x}(x, L \geq x';\omega)\big|_{x=L^+} & \frac{\partial}{\partial x} G(x, L \leq x' \leq R;\omega)\big|_{x=L^-} & \frac{\partial}{\partial x} G(x, R \leq x';\omega)\big|_{x=L} \\ \frac{\partial G}{\partial x}(x, L \geq x';\omega)\big|_{x=R} & \frac{\partial}{\partial x} G(x, L \leq x' \leq R;\omega)\big|_{x=R^+} & \frac{\partial}{\partial x} G(x, R \leq x';\omega)\big|_{x=R^-} \end{pmatrix}$$

$$= \begin{pmatrix} \Gamma(L,L;\omega) & \Gamma(L,R;\omega) \\ \Gamma(R,L;\omega) & \Gamma(R,R;\omega) \end{pmatrix} \begin{pmatrix} g_L(L,x';\omega) & -g_B(L,x';\omega) & 0 \\ 0 & g_B(R,x';\omega) & -g_R(R,x';\omega) \end{pmatrix} . \tag{2.13}$$

Thus, when the normal derivative of the uncoupled Green's functions g_α vanishes at the interfaces, Eqs. (2.7), (2.10), and (2.13) determine the thermal-equilibrium Green's function for the entire junction in terms of the functions g_α. Similarly G can be determined in terms of the uncoupled Green's functions $\bar{g}_\alpha$ which vanish at the interfaces. In this case, Eqs. (2.7) and (2.9′), and (2.14), given below apply:

$$\begin{pmatrix} G(L,x'<L;\omega) & G(L,L<x'<R;\omega) & G(L,R<x';\omega) \\ G(R,x'<L;\omega) & G(R,L<x'<R;\omega) & G(R,R<x';\omega) \end{pmatrix}$$

$$= \frac{\hbar^2}{2m} \begin{pmatrix} G(L,L;\omega) & G(L,R;\omega) \\ G(R,L;\omega) & G(R,R;\omega) \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial x} g_L(x,x';\omega)\big|_{x=L^-} & -\frac{\partial}{\partial x} g_B(x,x';\omega)\big|_{x=L^+} & 0 \\ 0 & \frac{\partial}{\partial x} g_B(x,x';\omega)\big|_{x=R^-} & -\frac{\partial}{\partial x} g_R(x,x';\omega)\big|_{x=R^+} \end{pmatrix} . \tag{2.14}$$

In concluding this section we note that just as in I, the functions g_α can be combined into a piecewise continuous "uncoupled" Green's function g and that consequently Eqs. (2.6) can be written in a more concise fashion,

$$G(x,x';\omega) = g(x,x';\omega) + \int_{-\infty}^{\infty} g(x,x_1;\omega)\mathcal{H}'(x_1)G(x_1,x';\omega)\,dx_1$$

$$= g(x,x';\omega) + \int_{-\infty}^{\infty} G(x,x_1;\omega)\mathcal{H}'^{\dagger}(x_1)g(x_1,x';\omega)\,dx_1 , \tag{2.15}$$

where the pseudo-Hamiltonian $\mathcal{H}'(x)$ is given below,

$$\mathcal{H}'(x) = -[\mathcal{H}'(x)]^{\dagger} = \lim_{\epsilon\to 0^+} \frac{\hbar^2}{2m} \left([\delta(x-R-\epsilon) - \delta(x-R+\epsilon) + \delta(x-L-\epsilon) - \delta(x-L+\epsilon)], \frac{\partial}{\partial x} \right)_+ . \tag{2.16}$$

The relation of $\mathcal{H}'(x)$ to the transition current introduced by Bardeen in his analysis of tunneling is discussed in I.[14]

Equations (2.9) and (2.9′) represent different generalizations of the "surface Green's function" introduced by Garcia-Moliner and Rubio.[15,16] It is clear that they represent a convenient starting point for the discussion of interfacial states or resonances. This point of view will be pursued in Sec. V.

III. GENERAL EXPRESSION FOR THE TUNNELING CURRENT

A. Introduction

In this section we shall extend the formalism developed in Sec. III of I to apply to a junction of finite width with a barrier region subject to a single-particle time-dependent perturbing potential $V(x,t)$.

It is easy to see that the Green's functions for such a system are no longer invariant under time translation. The ensemble-averaged current can always be expressed in terms of the Green's function

$$G^+(x,t;x',t') = i\langle \psi^+(x',t')\psi(xt)\rangle \ , \tag{3.1}$$

namely

$$\langle J(x,t)\rangle = -\frac{e\hbar}{2m}\lim_{x',t'\to x,t}\left(\frac{\partial}{\partial x}-\frac{\partial}{\partial x'}\right)G^+(x,t;x',t') \ . \tag{3.2}$$

The time Fourier transform of $\langle J(x,t)\rangle$ is

$$-\frac{2m}{e\hbar}\langle J(x;\bar{\omega})\rangle = \lim_{x'\to x}\left(\frac{\partial}{\partial x}-\frac{\partial}{\partial x'}\right)\times\int_{-\infty}^{\infty} G^+(x,x';\omega,\omega-\bar{\omega})\frac{d\omega}{2\pi} \ . \tag{3.3}$$

We note here that when the spectrum of $V(x,t)$ includes a set of discrete frequencies, $\bar{\omega}=0,\Omega,\ldots$, then the generalized transform of the current is

$$\langle J(x;\bar{\omega})\rangle = \langle J(L)\rangle\delta(\bar{\omega}) + \sum_n \langle J(x,\Omega_n)\rangle\delta(\bar{\omega}-\Omega_n) + \langle J_c(x;\bar{\omega})\rangle \ . \tag{3.4}$$

The one-dimensional version of the conservation of current implies that the time independent term of the current, which is proportional to $\delta(\bar{\omega})$, is also position independent.[17] We therefore singled out that term in Eq. (3.4). The choice to evaluate $\langle J(x)\rangle$ at $x=L$ is arbitrary; $x=R$ could also have been chosen. However, one or the other has to be chosen if a clumsy formulation of the theory is to be avoided. J_c represents the analytic component of the Fourier transform of $\langle J(x;t)\rangle$, i.e., the contribution of the continuous spectrum to $\langle J(x;\bar{\omega})\rangle$.

In the following we shall be interested only in the zero-frequency component of $\langle J(x;\bar{\omega})\rangle$, or rather in the time-independent component of the tunneling current. Nevertheless we shall continue, for a while, to keep the analysis general.

B. Determination of the nonequilibrium Green's functions

Following the procedure outlined in Sec. III B of I, we can use Keldysh's matrix Dyson equations to determine G^+, on the right side of Eq. (3.3), in terms of the "uncoupled" or "unperturbed" Green's functions g_α and the "perturbation." In the present paper we consider only perturbations consisting of nonretarded single-particle interactions having a generalized time Fourier transform $\mathcal{H}_1(x;\omega)$. In particular we shall consider

$$\mathcal{H}_1(x;\omega) = \mathcal{H}'(x)\delta(\omega) + V_1(x;\omega) \ , \tag{3.5}$$

where $\mathcal{H}'(x)$ is the pseudo-Hamiltonian defined by Eq. (2.16), and $V_1(x;\omega)$ is the time Fourier transform of an arbitrary time-dependent perturbing potential. It is shown in Appendix A that for any perturbation $\mathcal{H}_1(x;\omega)$, Keldysh's equations assume the form

$$G^\pm(x,x';\omega,\omega') - g^\pm(x,x'\omega)2\pi\delta(\omega-\omega') = \int_{-\infty}^{\infty}dx_1\int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}g^r(x,x_1;\omega)\mathcal{H}_1(x_1;\omega_1)G^\pm(x_1,x';\omega-\omega_1,\omega') + \int_{-\infty}^{\infty}dx_1\int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}g^\pm(x,x_1;\omega)\mathcal{H}_1(x_1;\omega_1)G^a(x_1,x',\omega-\omega_1,\omega') \ , \tag{3.6}$$

and

$$G^{r,a}(x,x';\omega,\omega') - g^{r,a}(x,x';\omega)2\pi\delta(\omega-\omega') = \int_{-\infty}^{\infty}dx_1\int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}g^{r,a}(x,x_1;\omega)\mathcal{H}_1(x_1;\omega_1)G^{r,a}(x_1,x';\omega-\omega_1,\omega') \ . \tag{3.7}$$

Whenever the homogenous equations

$$G^{r,a}_{\rm res}(x,x';\omega,\omega') = \int_{-\infty}^{\infty} g^{r,a}(x,x_1,\omega)\mathcal{H}_1(x_1;\omega_1)G^{r,a}_{\rm res}(x_1,x';\omega-\omega_1,\omega')\,dx_1\frac{d\omega_1}{2\pi}$$

$$= \int_{-\infty}^{\infty} G^{r,a}_{\rm res}(x,x';\omega,\omega'-\omega_1)\mathcal{H}_1^{\dagger}(x_1;\omega_1)g^{r,a}(x,x_1;\omega')\,dx_1\frac{d\omega_1}{2\pi}\ , \tag{3.8}$$

have no nontrivial solutions, Eq. (3.6) can be inverted with the help of Eq. (3.7) to yield a unique explicit expression for $G^{\pm}$,

$$G^{\pm}(x,x';\omega;\omega') - g^{\pm}(x,x';\omega)2\pi\delta(\omega-\omega')$$

$$= \delta g^{\pm}(x,x';\omega,\omega') = \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}G^{r}(x,x_1;\omega,\omega'-\omega_1)\mathcal{H}_1^{\dagger}(x_1,\omega_1)g^{\pm}(x_1,x';\omega')$$

$$+\int_{-\infty}^{\infty} dx_1 \int \frac{d\omega_1}{2\pi}\, g^{\pm}(x,x_1;\omega)\mathcal{H}_1(x_1,\omega_1)G^{a}(x_1,x';\omega-\omega_1,\omega')$$

$$+\int_{-\infty}^{\infty} dx_1\,dx_2\prod_{i=1}^{3}\frac{d\omega_i}{2\pi}G^{r}(x,x_1;\omega,\omega_2-\omega_1)\mathcal{H}_1^{\dagger}(x_1,\omega_1)g^{\pm}(x_1,x_2;\omega_2)\mathcal{H}_1(x_2,\omega_3)G^{a}(x_2,x';\omega_2-\omega_3,\omega')\ . \tag{3.9}$$

Whenever Eqs. (3.8) have non-trivial solutions, we shall assume that the standard conditions for the existence of a solution of Eq. (3.6) is satisfied, i.e., that the inhomogenous terms in Eq. (3.6) are orthogonal to the solutions of the adjoint (or associated) homogenous equation, Eq. (3.8).[18] In this case we have to modify the left side of Eq. (3.9) and write

$$\delta g^{\pm}(x,x';\omega,\omega') = G^{\pm}(x,x';\omega,\omega') - G^{\pm}_{\rm res}(x,x';\omega,\omega') - g^{\pm}(x,x';\omega)2\pi\delta(\omega-\omega')\ . \tag{3.10}$$

Alternatively, the difficulty may be eliminated by redefining the "unperturbed" functions g^{ν}, and the perturbation $\mathcal{H}_1$, by including an appropriate part of $\mathcal{H}_1$ in the unperturbed Hamiltonian. This way one can make sure that the modified version of Eq. (3.8) has no nontrivial solution. Equations (3.6)–(3.9) simplify considerably for static perturbing potentials, i.e., when

$$V_1(x,\omega) = V_1(x)2\pi\delta(\omega)\ . \tag{3.11}$$

In this case the time translational invariance is restored to the problem, and the time Fourier transforms of the Green's functions depend only on a single frequency. Formally this implies that

$$G^{\nu}(x,x';\omega,\omega') = G^{\nu}(x,x';\omega)2\pi\delta(\omega-\omega')\ . \tag{3.12}$$

The several Green's functions entering Eqs. (3.6)–(3.9) are defined below in terms of the field operators ψ and $\psi^{\dagger}$:

$$g^{+}(x,t;x',t') = i\langle\psi^{\dagger}(x',t')\psi(x,t)\rangle_0$$

$$g^{-}(x,t;x',t') = -i\langle\psi(x,t)\psi^{\dagger}(x',t')\rangle_0$$

$$g^{r,a}(x,t;x',t') = \mp i\langle[\psi(x,t),\psi^{\dagger}(x',t')]_{+}\rangle_0 \times\Theta(\pm(t-t'))\ . \tag{3.13}$$

The subscript 0 denotes that the averaging is to be performed with respect to the unperturbed (equilibrium) density-matrix operator. The full Green's functions G are defined in the same way, except that the averaging is with respect to the full (nonequilibrium) density-matrix operator. The time Fourier transforms of the equilibrium or "uncoupled" Green's functions g satisfy the following relations:

$$g^{\pm}(x,x';\omega) = -2i\begin{Bmatrix} f(\omega) \\ f(\omega)-1 \end{Bmatrix}[-\tfrac{1}{2}\rho(x,x';\omega)]\ , \tag{3.14}$$

$$g^{r}(x,x';\omega) = P\int_{-\infty}^{\infty}\frac{\rho(x,x';\omega_1)}{\omega-\omega_1}\frac{d\omega_1}{2\pi} - i\rho(x,x';\omega) = [g^{a}(x,x';\omega)]^{\dagger}\ , \tag{3.15}$$

where

$$f(\omega) = \{1+\exp[(\hbar\omega-\mu)(k_B T)^{-1}]\}^{-1}\ . \tag{3.16}$$

P denotes the principal part of the integral. The complex spectral density function $\rho(x,x';\omega)$ vanishes over energy intervals in which the local density of states,

$$\rho(x,\omega) = \frac{1}{2\pi}\rho(x,x;\omega)\ , \tag{3.17}$$

vanishes.[19–22]

C. Calculation of the current

In the following we shall explicitly restrict $V_1(x,t)$ to the barrier[23]:

$$V_1(x,t) = V(x,t)\Theta(x-L)\Theta(x+R) \ . \tag{3.18}$$

Furthermore, we specialize the general homogenous boundary conditions imposed on the Green's functions g_α at the interfaces, and require that their normal derivatives vanish at the interfaces, i.e.,

$$\begin{aligned}
&\frac{\partial}{\partial x} g_L(x, x'<L;\omega)|_{x=L} = 0 \\
&\quad = \frac{\partial}{\partial x'} g_L(x<L, x';\omega)|_{x'=L} \ , \\
&\frac{\partial}{\partial x} g_B(x, L<x'<R;\omega)|_{x=L,R} = 0 \\
&\quad = \frac{\partial}{\partial x'} g_B(L<x<R, x';\omega)|_{x'=L,R} \ , \\
&\frac{\partial}{\partial x} g_R(x, x'>R;\omega)|_{x=R} = 0 \\
&\quad = \frac{\partial}{\partial x'} g_R(x>R, x';\omega)|_{x'=R} \ .
\end{aligned} \tag{3.19}$$

In order to calculate the Fourier transform of the current we substitute Eq. (3.6) into Eq. (3.3) and impose on the resultant expression Eqs. (3.18). Thus in the case where x tends to L from the left,[24]

$$\begin{aligned}
\frac{2m}{e\hbar}\langle J(L,\bar\omega)\rangle = &-\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}[g_L^r(L,L;\omega) - g_L^a(L,L;\omega)] \\
&\times \Gamma^+(L,L;\omega,\omega-\bar\omega) \\
&-\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}[g_L^+(L,L,\omega)\Gamma^a(L,L;\omega,\omega-\bar\omega) \\
&- g_L^+(L,L;\omega-\bar\omega)\Gamma^r(L,L;\omega,\omega-\bar\omega)].
\end{aligned} \tag{3.20}$$

Here,

$$\Gamma^\nu(\alpha,\beta;\omega,\omega') = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x\,\partial x'} G^\nu(x,x';\omega,\omega')|_{\substack{x=\alpha\\x'=\beta}}, \quad \nu = +,-,r,a \ . \tag{3.21}$$

The cumbersome expression for $\langle J(L,\bar\omega)\rangle$ simplifies considerably in the case of primary interest to us, when $\bar\omega = 0$. Using the identity[25]

$$G^a - G^r = G^+ - G^- \ , \tag{3.22}$$

Eq. (3.20) reduces now to,

$$\begin{aligned}
&\frac{2m}{e\hbar}\langle J(L;\bar\omega=0)\rangle \\
&\quad = -\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}[g_L^+(L,L;\omega)\Gamma^-(L,L;\omega,\omega) \\
&\qquad - g_L^-(L,L;\omega)\Gamma^+(L,L;\omega,\omega)] \ .
\end{aligned} \tag{3.23}$$

An analogous expression can be derived for the current at $x=R$:

$$\begin{aligned}
&\frac{2m}{e\hbar}\langle J(R;\bar\omega=0)\rangle \\
&\quad = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}[g_R^+(R,R;\omega)\Gamma^-(R,R;\omega,\omega) \\
&\qquad - g_R^-(R,R;\omega)\Gamma^+(R,R;\omega,\omega)] \ .
\end{aligned} \tag{3.24}$$

The position independence of the zero-frequency component of the current implies that the right sides of Eqs. (3.23) and (3.24) are identical.[26] Equations (3.23) and (3.24) are the generalizations of Eqs. (3.20) and (3.21) of I. Both pairs of equations do not separate the effects of the barrier from those of the two metals. To achieve such a separation, we follow the procedure of Sec. III of I; Eqs. (3.9), (3.18), and (3.19) are used to evaluate $\Gamma^\pm(\alpha,\beta;\omega,\omega)$. The resultant expression reduces after some algebra, relegated to Appendix B, to a two-dimensional matrix integral equation,

$$\begin{aligned}
&\frac{2m}{\hbar^2}\underline{\Gamma}^\pm(\omega,\omega) \\
&\quad = -\int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}\frac{d\omega_2}{2\pi}\underline{\Gamma}^r(\omega,\omega_1)\{[\underline{g}^\pm(\omega_1) + \delta\underline{g}_B^\pm(\omega_1)] \\
&\qquad \times 2\pi\delta(\omega_1-\omega_2) + \delta\underline{g}_B^\pm(\omega_1,\omega_2)\}\underline{\Gamma}^a(\omega_2\omega) \ .
\end{aligned} \tag{3.25}$$

The two-dimensional matrices entering Eq. (3.25) are defined below:

$$\underline{\Gamma}^\nu(\omega,\omega') = \begin{pmatrix} \Gamma^\nu(L,L;\omega,\omega') & \Gamma^\nu(L,R;\omega,\omega') \\ \Gamma^\nu(R,L;\omega,\omega') & \Gamma^\nu(R,R;\omega,\omega') \end{pmatrix}, \tag{3.26}$$

$$\underline{g}^\nu(\omega) = \begin{pmatrix} g_L^\nu(L,L;\omega) + g_B^\nu(L,L;\omega) & -g_B^\nu(L,R;\omega) \\ -g_B^\nu(R,L;\omega) & g_R^\nu(R,R;\omega) + g_B^\nu(R,R;\omega) \end{pmatrix}, \tag{3.27}$$

$$\underline{g}_B^\nu(\omega)+\delta\underline{g}_B^\nu(\omega)=\underline{G}_{B_0}^{\ \nu}(\omega)=\begin{pmatrix} G_{B_0}^\nu(L,L;\omega) & -G_{B_0}^\nu(L,R;\omega)\\ -G_{B_0}^\nu(R,L;\omega) & G_{B_0}^\nu(R,R;\omega)\end{pmatrix}, \tag{3.28}$$

and

$$\underline{G}_{B_0}^\nu(\omega)2\pi\delta(\omega-\omega')+\delta\underline{g}_B^\nu(\omega,\omega')=\underline{G}_B^\nu(\omega,\omega')=\begin{pmatrix} G_B^\nu(L,L;\omega,\omega') & -G_B^\nu(L,R;\omega,\omega')\\ -G_B^\nu(R,L;\omega,\omega') & G_B^\nu(R,R;\omega,\omega')\end{pmatrix},\quad \nu=\pm,r,a\ . \tag{3.29}$$

The "intermediate"-barrier Green's functions $G_{B_0}^\nu$, G_B^ν are exact-barrier Green's functions in the presence of the perturbing potentials $V(x)$, $V(x,t)$, but they satisfy at the interfaces the homogenous boundary conditions imposed on the uncoupled Green's functions g_B^ν; thus in analogy to Eq. (3.7), we have

$$\delta g_B^{r,a}(x,x',\omega)=G_{B_0}^{r,a}(x,x';\omega)-g_B^{r,a}(x,x';\omega)=\int_L^R G_{B_0}^{r,a}(x,x_1;\omega)V(x_1)g_B^{r,a}(x_1,x';\omega')\,dx_1$$

$$=\int_L^R g_B^{r,a}(x,x_1;\omega)V(x_1)G_{B_0}^{r,a}(x_1,x';\omega)\,dx_1\ , \tag{3.30}$$

and

$$\delta g_B^{r,a}(x,x';\omega,\omega')=G_B^{r,a}(x,x';\omega,\omega')-G_{B_0}^{r,a}(x,x';\omega)2\pi\delta(\omega-\omega')$$
$$=\int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}\int_L^R dx_1 G_B^{r,a}(x,x_1;\omega,\omega_1)V^*(x_1,\omega'-\omega_1)G_{B_0}^{r,a}(x_1,x';\omega')$$
$$=\int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}\int_L^R dx_1 G_{B_0}^{r,a}(x,x_1;\omega)V(x_1,\omega-\omega_1)G_B^{r,a}(x_1,x';\omega,\omega')\ . \tag{3.31}$$

Similarly, we have in analogy to Eq. (3.9),

$$\delta g_B^{\pm}(x,x';\omega)=G_{B_0}^{\pm}(x,x';\omega)-g_B^{\pm}(x,x';\omega)$$
$$=\int_L^R dx_1 g_B^{\pm}(x,x_1;\omega)V(x_1)G_{B_0}^{a}(x_1,x';\omega)+\int_L^R dx_1 G_{B_0}^{r}(x,x_1;\omega)V(x_1)g_B^{\pm}(x_1,x';\omega)$$
$$+\int_L^R dx_1\,dx_2 G_{B_0}^{r}(x,x_1;\omega)V(x_1)g^{\pm}(x_1,x_2;\omega)V(x_2)G_{B_0}^{a}(x_2,x';\omega)\ , \tag{3.32}$$

and

$$\delta g_B^{\pm}(x,x';\omega,\omega')=G_B^{\pm}(x,x';\omega,\omega')-G_{B_0}^{\pm}(x,x';\omega)2\pi\delta(\omega-\omega')$$
$$=\int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}\int_L^R dx_1 G_{B_0}^{\pm}(x,x_1;\omega)V(x_1,\omega-\omega_1)G_{B_0}^{a}(x_1,x';\omega_1,\omega')$$
$$+\int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}\int_L^R dx_1 G_B^{r}(x,x_1;\omega,\omega_1)V^*(x_1,\omega'-\omega_1)G_{B_0}^{\pm}(x_1,x';\omega')$$
$$+\int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}\frac{d\omega_2}{2\pi}\frac{d\omega_3}{2\pi}\int_L^R dx_1\,dx_2 G_B^{r}(x,x_1,\omega,\omega_1)V^*(x_1,\omega_2-\omega_1)G_{B_0}^{\pm}(x_1,x_2;\omega_2)$$
$$\times V(x_2,\omega_2-\omega_3)G_B^{a}(x_2,x';\omega_3,\omega')\ . \tag{3.33}$$

In the preceding discussion we separated the static component $V(x)$ from the explicitly time dependent potential $V(x,t)$. The former is defined by the relation

$$\lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{T}|V(x,t)-V(x)|\,dt=0\ . \tag{3.34}$$

Three relatively obvious but important consequences of Eqs. (3.30)–(3.34) should be noted. First, if $V(x,t)=V(x)$, then the generalized Fourier transform $V(x,\omega)$ of $V(x,t)-V(x)$ vanishes. Consequently, it follows that $\delta g^\nu(\omega,\omega')\equiv 0$. Second, $G_{B_0}^\nu(x,x';\omega)$, in contrast to $G_B^\nu(x,x';\omega,\omega')$, are thermal-equilibrium Green's functions. That is,

they satisfy Eqs. (3.14)–(3.17) with an appropriately modified spectral density. Third, it follows from Eq. (3.32) that in general $G_B^{\pm}(x, x'; \omega)$ vanish over the same forbidden energy gaps as $g_B^{\pm}(x, x'; \omega)$. The exception to this result occurs when the perturbation $V(x)$ gives rise to a localized density of states in the "original" gaps. The mathematical manifestation of this physically important phenomenon is the occurrence of nontrivial solutions of the homogenous version of Eq. (3.30). The exigency has already been noted in our discussion of Eq. (3.9). In the following we shall assume that the "intermediate" barrier Green's functions include, where necessary, a "resonant" term, which in the specific instance being considered satisfies the equation

$$G_{B_0}^{\pm}(x, x'; \omega) = \int_L^R dx_1 g_B(x, x_1; \omega) V(x_1) G_{B_0}^{\pm}(x_1, x'; \omega) = \int_L^R dx_1 G_{B_0}^{\pm}(x, x_1; \omega) V(x_1) g_B(x_1, x'; \omega) , \tag{3.35}$$

where, since

$$g_B^{\pm}(x, x'; \omega) = 0 , \tag{3.36}$$

we denoted

$$g_B^r(x, x'; \omega) = g_B(x, x'; \omega) = g_B^a(x, x'; \omega) . \tag{3.37}$$

If we now substitute Eq. (3.25) into Eq. (3.23) we obtain the following expression for the tunneling current:

$$\frac{\hbar}{e}\langle J(L; \bar{\omega} = 0)\rangle = \frac{\hbar}{e}\langle J_1(\bar{\omega} = 0)\rangle + \langle J_2(\bar{\omega} = 0)\rangle , \tag{3.38}$$

where

$$\frac{\hbar}{e}\langle J_1\rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\frac{d\omega_1}{2\pi}[g_L^+(L, L; \omega) g_R^-(R, R; \omega_1) - g_L^-(L, L; \omega) g_R^+(R, R; \omega_1)] \times \left|\frac{\hbar^2}{2m}\Gamma^r(L, R; \omega, \omega_1)\right|^2 , \tag{3.39}$$

and

$$\frac{\hbar}{e}\langle J_2\rangle = \sum_{\alpha,\beta}\int \frac{d\omega}{2\pi}\frac{d\omega_1}{2\pi}\frac{d\omega_2}{2\pi}[g_L^+(L, L; \omega) G_B^-(\alpha, \beta; \omega_1, \omega_2) - g_L^-(L, L; \omega) G_B^+(\alpha, \beta; \omega_1 \omega_2)] \left(\frac{\hbar^2}{2m}\right)^2 \Gamma^r(L; \alpha, \omega, \omega_1)\, \Gamma^a(\beta, L; \omega_2, \omega) . \tag{3.40}$$

Equations (3.38)–(3.40) represent the most important result derived in this section. These equations will be applied in the next sections in a discussion of resonant tunneling. The application of Eqs. (3.33)–(3.40) to a phenomenological analysis of the inelastic tunneling across a barrier containing a vibrating impurity is considered in another publication.

IV. COMPARISON WITH THE ABRUPT JUNCTION

Before we proceed to apply Eqs. (3.38)–(3.40) we shall briefly compare present results with those derived in I for the abrupt static junction.

When we use Eqs. (3.14)–(3.16) to eliminate the "uncoupled" Green's functions from Eqs. (3.39) and (3.40), the first term on the right side of Eq. (3.38) reduces to a "transfer-Hamiltonian-like" expression:

$$\frac{\hbar}{e}\langle J_1(\bar{\omega} = 0)\rangle = \int_{\infty}^{\infty} d\omega d\omega_1 [f_L(\omega) - f_R(\omega_1)] \times \rho_L(L, \omega)\rho_R(R, \omega_1)\, |\Lambda^r(\omega, \omega_1)|^2 . \tag{4.1}$$

Here, $f_{L,R}$ are the Fermi distribution functions characterizing the left and right subregions. The chemical potentials of these two regions are displaced with respect to one another by the external potential U. The effective matrix element in Eq. (4.1) is defined below:

$$\Lambda^r(\omega, \omega_1) = -\left(\frac{\hbar^2}{2m}\right)^2 \frac{\partial^2}{\partial x\, \partial x_1} G^r(x, x_1; \omega, \omega_1)\Big|_{\substack{x=L \\ x_1=R}} . \tag{4.2}$$

For the static-barrier potential Eq. (3.12) applies, and thus the expression for the matrix element simplifies to

$$\Lambda^r(\omega, \omega_1) = \Lambda^r(\omega) 2\pi\delta(\omega - \omega_1) \tag{4.3}$$

and

$$\Lambda^r(\omega) = -\frac{\hbar^2}{2m}\frac{\partial}{\partial x} G^r(x, x_1; \omega)\Big|_{\substack{x=L \\ x_1=R}} . \tag{4.4}$$

Substituting Eqs. (4.3) and (4.4) into Eq. (4.1) we obtain

$$\langle J_1(\bar{\omega} = 0)\rangle = \delta(0)\langle J_1\rangle , \tag{4.5}$$

where

$$\langle J_1\rangle = \frac{e}{\hbar}\int_{-\infty}^{\infty}(2\pi)^2\, d\omega[f_L(\omega)-f_R(\omega)] \times\rho_L(L;\omega)\rho_R(R;\omega)\,|\Lambda^r(\omega)|^2 . \tag{4.6}$$

The singular factor $\delta(0)$ in Eq. (4.5) is easily interpreted: It occurs in Eq. (3.4) and in Eq. (4.5) because in both cases we took a formal time Fourier transformation of a time-independent function. If the Fourier transforms are interpreted as distributions, then this is a perfectly acceptable procedure which allows us to treat simultaneously barrier potentials with a time dependence exhibiting a discrete frequency spectrum and those with a continuous spectrum. The abrupt junction can be viewed as the limit of the finite junction as $L\to 0^-$ and $R\to 0^+$. Evidently, the continuity of the mixed second derivative of G assures that

$$\lim_{\substack{R\to 0^+\\ L\to 0^-}}\Lambda^r(\omega) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x\,\partial x_1}G(x,x_1;\omega)\big|_{x=0=x_1} . \tag{4.7}$$

This expression agrees with the form of the effective matrix element derived in I, as can be checked by substituting Eq. (2.24) of I into Eq. (3.25) of I. Thus we conclude that the expression (4.4) of I derived directly for the (static) abrupt junction is indeed the limit of $\langle J_1\rangle$ as the width of the barrier vanishes.

Turning to the second term in Eq. (3.38), we note that this term is essentially different from the first one, for it does not involve products of the form $g_L^+(L,L;\omega)g_R^-(R,R;\omega)$. That is, it cannot be cast into a "transfer-Hamiltonian-like" form. For a static barrier, we have

$$\langle J_2(\bar\omega=0)\rangle = \delta(0)\langle J_2\rangle \tag{4.8}$$

and

$$\langle J_2\rangle = \frac{e}{\hbar}\sum_{\alpha,\beta}\int_{-\infty}^{\infty}d\omega[g_L^+(L,L;\omega)G_{B_0}^-(\alpha,\beta;\omega) - g_L^-(L,L;\omega)G_{B_0}^+(\alpha,\beta;\omega)]\left(\frac{\hbar^2}{2m}\right)^2\Gamma^r(L,\alpha;\omega) \times\Gamma^a(\beta,L;\omega) . \tag{4.9}$$

The functions $G_{B_0}^{\pm}$ were defined by Eq. (3.32). It was already noted that unless the perturbing potential gives rise to a "resonant" localized density of states in the barrier, these "intermediate" Green's functions vanish over the same energy intervals as the "uncoupled" Green's functions $g_B^{\pm}$. Hence the only nonvanishing contribution to $\langle J_2\rangle$ arises from energies at which either the barrier is transparent (i.e., $g_B^{\pm}\neq 0$) or the perturbation gives rise to a density of states in what previously was an energy gap. Thus, the tunneling-current energy distribution for a static barrier naturally separates into two terms: The "normal" term (or nonresonant channel) is given by the integrand of Eq. (4.6). The "resonant" term is given by the integrand of Eq. (4.9), provided that $G_{B_0}^{\pm}$ satisfies Eq. (3.35). In the Sec. V we shall examine resonant tunneling more closely. We shall see that the introduction of a density of states into a forbidden energy gap of the unperturbed ("uncoupled") barrier clearly manifests itself also in the energy dependence of the normal-tunneling-current energy distribution. Nevertheless there exists a meaningful distinction between the two terms based on their manifestly different form. The normal term $\langle J_1(\bar\omega=0)\rangle$ has the manifest symmetry with respect to the right and left subregions which characterizes the transfer-Hamiltonian formulations of elastic tunneling. The second term represents the strictly resonant and/or inelastic channel. As defined in Eq. (3.40) this term seems to single out the left interface L. This is not the case, and a symmetrized expression follows from the position independence of $\langle J(\bar\omega=0)\rangle$, i.e.,

$$\langle J(L;\bar\omega=0)\rangle = \langle J(R;\bar\omega=0)\rangle = \tfrac{1}{2}[\langle J(L;\bar\omega=0)\rangle + \langle J(R;\bar\omega=0)\rangle] . \tag{4.10}$$

However, regardless of the symmetrization, $\langle J_2(\bar\omega=0)\rangle$ clearly exhibits a different, more complicated dependence on the density of states than that of the normal (nonresonant) elastic channel $\langle J_1(\bar\omega=0)\rangle$.

V. RESONANT TUNNELING

A. Generalities, calculation of the "transfer matrix"

In the present section we shall concern ourselves with some effects of atomic impurities in the barrier on the tunneling-current energy distribution. Specifically, we assume that the impurities can be represented by a static potential $V_1(x)$, satisfying Eq. (3.18). It follows that the tunneling-current density is given by

$$\langle J(\omega)\rangle = \langle J_1(\omega)\rangle + \langle J_2(\omega)\rangle , \tag{5.1}$$

where $\langle J_1(\omega)\rangle$ is the integrand of Eq. (4.6) and $\langle J_2(\omega)\rangle$ is the integrand of Eq. (4.9). Clearly the effect of $V_1(x)$ is to modify the barrier Green's function and hence also the "transfer matrix" $\Gamma^r(\alpha,\beta;\omega)$. We shall assume that over the energy range of interest, the local density of states in the unperturbed barrier vanishes, i.e.,

$$g_B^+(x,x';\omega) = 0 = g_B^-(x,x';\omega) . \tag{5.2}$$

However, the impurities may give rise to some nonvanishing localized density of states, i.e., for

some energies in the gap,

$$G^{\pm}_{B_0}(x, x'; \omega) \neq 0 . \tag{5.3}$$

The continuity conditions imposed on the Green's functions $G^{r,a}$ are identical to those imposed on the equilibrium Green's function, Eq. (2.8). Using these and the boundary conditions imposed on "uncoupled" functions $g^{r,a}$ [Eqs. (3.19)], it is easily checked that the "transfer matrix" satisfies the following generalization of the equilibrium relation, Eq. (2.10):

$$\frac{\hbar^2}{2m}\,\underline{\Gamma}^{r,a}(\omega) = [\underline{g}^{r,a}(\omega) + \delta\underline{g}^{r,a}_{B}(\omega)]^{-1} . \tag{5.4}$$

The matrices in Eq. (5.4) were defined by Eqs. (3.26)–(3.28). Equation (5.4) indicates that in general one should expect peaks in the energy distribution of the tunneling current to correspond to the (possibly complex) zeroes of the determinant

$$\Delta^r(\omega) + \delta\Delta^r(\omega) = \det[g^r(\alpha, \beta; \omega) + \delta g^r_B(\alpha, \beta; \omega)] . \tag{5.5}$$

These zeros can be classed into four types, depending on their relation to singularities of the uncoupled Green's functions: "Electrode resonances" occur in the neightborhood of singularities of either $g^r_L(L, L; \omega)$ or $g^r_R(R, R; \omega)$. "Impurity resonances" occur in the neighborhood of singularities of $g^r_B(\alpha, \beta; \omega)$. "Interfacial resonances" occur in the neighborhood of zeros of $\Delta^r(\omega)$ which are unrelated to singularities of the uncoupled Green's functions. These resonances represent a characteristic of the coupled system. "Impurity-induced interfacial resonances" are zeros of the $\Delta^r(\omega) + \delta\Delta^r(\omega)$ which are neither shifted interfacial resonances [i.e., shifted zeros of $\Delta^r(\omega)$] nor related to the singularities of the "uncoupled" Green's functions.[27]

In the remainder of this section we shall consider in somewhat more detail the impurity-induced resonances. We shall be guided by the heuristic, physical argument that when an impurity is embedded in the barrier its bound states are broadened and shifted. The impurity-induced tunneling resonances are manifestations of these broadened and shifted impurity states within an energy band in which the unperturbed barrier exhibited no density of states. Thus we shall have to examine the effect of an impurity on $\delta\underline{g}^r_B(\omega)$. We shall not attempt to consider this problem in its full generality. Instead, we shall consider a reasonably familiar nontrivial model.

B. Barrier Green's functions

We represent the Green's functions in the barrier by means of the bilinear formula

$$g_B(x, x'; \omega) = \sum_i g_{B;i}(\omega)\,\phi_i(x)\phi^*_i(x')$$

$$= \sum_i (\hbar\omega - \epsilon_i)^{-1}\phi_i(x)\phi^*_i(x') , \tag{5.6}$$

and

$$G^{r,a}_{B_0}(x, x'; \omega) = \sum_{ij} G^{r,a}_{B_0;ij}(\omega)\phi_i(x)\phi^*_j(x') . \tag{5.7}$$

Here,

$$G^{r,a}_{B_0;ij}(\omega) = g_{B;i}(\omega)\left[\delta_{ij} + \sum_m V_{im}G^{r,a}_{B_0;mj}(\omega)\right]$$

$$= \left[\delta_{ij} + \sum_m G^{r,a}_{B_0;im}(\omega)V_{mj}\right]g_{B;j}(\omega) , \tag{5.8}$$

and

$$V_{ij} = \int_L^R \phi^*_i(\omega)V(x)\phi_j(x)\,dx = V^*_{ji} . \tag{5.9}$$

In view of our convention concerning the boundary conditions imposed on the "uncoupled" Green's functions at the interfaces, we require the complete orthonormal basis set $\{\phi_i(x)\}$, which is to be used in the bilinear formula, to be those eigenfunctions of the Hamiltonian for the barrier whose normal derivative vanishes at the interfaces. Thus

$$(\epsilon_i - \mathcal{H}_B)\phi_i(x) = 0 , \tag{5.10}$$

and

$$\left.\frac{\partial\phi_i}{\partial x}\right|_{x=L} = 0 = \left.\frac{\partial\phi_i}{\partial x}\right|_{x=R} . \tag{5.11}$$

We are concerned with the case where the perturbing potential $V(x)$ admits of a set of σ bound states $\{\Phi_s(x); s = 1, \ldots, \sigma\}$ such that

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(x) - e_s\right]\Phi_s(x) = 0 . \tag{5.12}$$

We expect that in this case, the homogenous term of Eqs. (5.8),

$$\sum_m [\delta_{im} - g_{B;i}(\omega)V_{im}]G^{r,a}_{B_0;mj}(\omega) = 0 , \tag{5.13}$$

has σ nontrivial solutions,

$$\hbar\omega_s = e_s + \delta e_s , \quad s = 1, \ldots, \sigma . \tag{5.14}$$

These parameters characterize the shifted states e_s once V is embedded into the barrier.

We wish to examine the energy dependence of $G^{r,a}_{B_0;ij}(\omega)$, and in particular its form in the neighborhood of these "resonances." For this purpose

it is convenient to augment the basis set $\{\phi_i(x)\}$ by the set $\{\Phi_s(x)\}$. This augumented set is evidently overcomplete. Recently several workers have discussed the proper formulation of the single-particle Green's functions in terms of overcomplete basis sets.[12,28,29] Adapting the formalism of Bagchi and Cohen[29] we write

$$G^{r}_{B_0;}{}^{a}(x, x'; \omega) = \sum_{\kappa j} G'^{r}_{B_0;\kappa j}{}^{a}(\omega)\psi_\kappa(x)\phi_j^*(x'), \quad (5.15)$$

where the overcomplete basis set is designated $\{\psi_\kappa\}$, and consequently its elements can be expressed in terms of the original complete orthonormal set:

$$\psi_\kappa(x) = \sum_i \phi_i(x) S_{i\kappa}. \quad (5.16)$$

Clearly,

$$G^{r}_{B_0;}{}^{a}_{ij}(\omega) = G'^{r}_{B_0;}{}^{a}_{ij}(\omega) + \sum_{s=1}^{\sigma} S_{is} G'^{r}_{sj}{}^{a}(\omega). \quad (5.17)$$

At this point we shall simplify the problem by setting $\sigma = 1$ and considering an Anderson model of the impurity.[12,13] That is, we assume that all matrix elements V_{ij} are small enough to be treatable by an appropriate perturbation theory. Concentrating on the interaction between the impurity state Φ_s and the set $\{\phi_i\}$, we obtain the following equations derived by Bagchi and Cohen[29]:

$$(\hbar\omega - \epsilon_i) G'^{r}_{B_0;}{}^{a}_{sj}(\omega) + \mathfrak{v}_{is} G'^{r}_{B_0;}{}^{a}_{sj}(\omega) = \delta_{ij},$$

and

$$(\hbar\omega - e_s) G'^{r}_{B_0;}{}^{a}_{sj}(\omega) + \sum_i \mathfrak{v}_{si} G'^{r}_{B_0;}{}^{a}_{ij}(\omega) = S_{sj}. \quad (5.18)$$

The "matrix elements" of the effective potential are

$$\begin{aligned} \mathfrak{v}_{si} &= S_{si}(\hbar\omega - \epsilon_i) - V_{si}, \\ \mathfrak{v}_{is} &= (\hbar\omega - \epsilon_i) S_{is} - V_{is}. \end{aligned} \quad (5.19)$$

Equations (5.18) can be solved for the "pseudo" Green's function $G'_{\kappa j}(\omega)$. Upon using Eqs. (5.17) and (5.19), we find

$$\begin{aligned} G^{r}_{B_0;}{}^{a}_{ij}(\omega) = {} & g^{r}_{B;}{}^{a}_{i}(\omega)\delta_{ij} + g^{r}_{B;}{}^{a}_{i}(\omega) V_{is} \\ & \times \left[\hbar\omega - e_s - \sum_{j_1} \mathfrak{v}_{sj_1}(\omega) g^{r}_{B;}{}^{a}_{j_1}(\omega)\mathfrak{v}_{j_1 s}(\omega)\right]^{-1} \\ & \times V_{sj} g^{r}_{B;}{}^{a}_{j}(\omega). \end{aligned} \quad (5.20)$$

It is clear that when e_s falls into an energy interval excluding the singularities ϵ_i of $g_B(x, x'; \omega)$, then the "intermediate"-barrier Green's function G_{B_0} will exhibit a pole at the isolated root $\hbar\omega = e_s + \delta e_s$ of the expression

$$\begin{aligned} \hbar\omega - e_s - \sum_i \mathfrak{v}_{si}(\omega) g_{B,i}(\omega)\mathfrak{v}_{is}(\omega) \\ = \hbar\omega - \Sigma_{B,s}(\omega) - e_s = 0. \end{aligned} \quad (5.21)$$

Returning to the coordinate representation, we conclude that

$$\begin{aligned} g^{r}_{B}{}^{a}(x, x'; \omega) = \sum_{ij} & [G^{r}_{B_0;}{}^{a}_{ij}(\omega) - g^{r}_{B;}{}^{a}_{i}(\omega)\delta_{ij}] \\ & \times \phi_i(x)\phi_j^*(x') \end{aligned} \quad (5.22)$$

does indeed have a pole at the shifted energy $e_s + \delta e_s$.

The bilinearity of the determinant $\Delta^r(\omega) + \delta\Delta^r(\omega)$ in the matrix elements $G^r_{B_0}(\alpha, \beta; \omega)$ might suggest that the matrix $\underline{\Gamma}^r(\omega)$ defined by Eq. (5.4) will generally vanish at the isolated poles of $G^r_{B_0}(\alpha, \beta; \omega)$. However, it is easily verified that this is not the case whenever $\delta g_B(\alpha, \beta; \omega)$ is given by a bilinear expression such as Eq. (5.22). In fact, $\underline{\Gamma}^r(\omega)$ has neither a zero nor a pole at the root of Eq. (5.21), $e_s + \delta e_s$. On the other hand, Rouché's theorem[30] implies the $\underline{\Gamma}(\omega)$ has a complex pole at $\hbar\omega = E_s$, in the neighborhood of $e_s + \delta e_s$. At this point it is interesting to consider the rather trivial case of a δ-function impurity (pseudo) potential,

$$V(x) = V\delta(x); \quad (5.23)$$

in this case, a direct solution of Eq. (3.30) gives

$$\delta g_B(\alpha, \beta; \omega) = \frac{V}{1 - V g^r_B(0, 0; \omega)} g^r_B(\alpha, 0; \omega) g^r_B(0, \beta; \omega). \quad (5.24)$$

Evidently, also in this case, $\underline{\Gamma}^r(\omega)$ has neither a zero nor a pole at the pole of $\delta g_B(\alpha, \beta; \omega)$. Here again, if the pole of $\delta g^r_B(\alpha, \beta; \omega)$ lies isolated from the singularities of $g^r_B(\alpha, \beta; \omega)$, then a corresponding pole of $\underline{\Gamma}^r(\omega)$ is defined by one of the roots of

$$1 = V[g^r_B(0, 0; \omega) + h^r(\omega)] = 0, \quad (5.25)$$

where

$$h^r(\omega) = \frac{\partial}{\partial V} \frac{\delta\Delta^r(\omega)}{\Delta^r(\omega)}\bigg|_{V=0}. \quad (5.26)$$

C. Resonant enhancement factor

We are now ready to examine the general features of resonant tunneling predicted by our theory. This we shall do in terms of the fractional change in the energy density of the tunneling current, or the resonant enhancement factor

$$\frac{\delta\langle J(\omega)\rangle}{\langle J_{1,0}(\omega)\rangle} = \frac{\delta|\Gamma^r(L, R; \omega)|^2}{|\Gamma^r_0(L, R; \omega)|^2} + \frac{\langle J_2(\omega)\rangle}{\langle J_{1,0}(\omega)\rangle}, \quad (5.27)$$

where $\langle J_{1,0}(\omega)\rangle$ is the integrand of Eq. (4.6) in the absence of the impurity, and $\langle J_2(\omega)\rangle$ is the inte-

grand of Eq. (4.9) in the presence of the impurity. The latter quantity can be written with the help of Eqs. (3.14)–(3.17) as

$$\langle J_2(\omega)\rangle = \frac{e}{\hbar}(2\pi)^2[f_L(\omega) - f_B(\omega)]_L \rho(L;\omega) \times \sum_{\alpha,\beta}\left[\left(\frac{\hbar^2}{2m}\right)^2 \Gamma^r(L,\alpha;\omega) \times \rho_{B_0}(\alpha,\beta;\omega)\Gamma^a(\beta,L;\omega)\right], \quad (5.28)$$

where the impurity-induced spectral density in the barrier is defined by

$$\rho_{B_0}(x,x';\omega) = i[G^r_{B_0}(x,x';\omega) - G^a_{B_0}(x,x';\omega)]. \quad (5.29)$$

The first term in Eq. (5.7) represents the effect of the impurity on the normal tunneling and corresponds to a possibly pronounced peak in the energy dependence of the transmissivity of the barrier. This effect can be included in tunneling theories based on the transfer-Hamiltonian formalism by imposing on the matrix element an appropriate energy dependence. The second term in Eq. (5.27) represents the contribution of the resonant channel. Unlike the first term, this strictly resonant term displays an explicit temperature dependence and a dependence on the total energy densities of states in the two electrodes, all in addition to an explicit dependence on the impurity spectral density in the (energy gap in the) barrier. Furthermore, this term exhibits a left-right asymmetry absent from the first term in Eq. (5.27). That is, the resonant enhancement factor may depend on the direction of the tunneling. The several types of tunneling resonances have different "signatures," which we shall now examine.

The energy dependence of the matrix $\underline{\Gamma}^r(\omega)$, discussed in the preceding subsection, indicates that an impurity resonance, i.e., an isolated complex root E_s, of Eq. (5.5) manifests itself in a peak in the first term of Eq. (5.27) at the energy $\hbar\omega = \mathrm{Re}E_s$.[31] In the preceding we excluded impurity (allowed energy) bands in the energy gap of the barrier, and considered only sharp impurity states. Thus,

$$\rho_{B_0}(x,x';\omega) \propto \delta(\hbar\omega - (e_s + \delta e_s)), \quad (5.30)$$

and the resonant energy channel can only open at the energy $e_s + \delta e_s$ of the localized impurity state in the energy gap of the barrier.[31,32] That the channel is indeed open follows from the fact that $\underline{\Gamma}^r(e_s + \delta e_s) \neq 0$.[33]

$\mathrm{Re}E_s$ has a simple physical significance;

$$\mathrm{Re}E_s - e_s = \Delta e_s$$

is the shift of the "atomic" level due to the embedding of the impurity in the junction.

The quantity δe_s has a more model-dependent significance and represents the shift of the level due to the embedding in the "uncoupled" barrier.

An impurity-induced shift of an interfacial resonance manifests itself in a peak of the first term of the enhancement factor, and an associated dip at the energy of the unshifted interfacial resonance [i.e., zero of $\Delta^r(\omega)$].

A strictly impurity-induced surface resonance [i.e., a zero of $\Delta^r(\omega) + \delta\Delta^r(\omega)$] unrelated to any pole of the "uncoupled" Green's functions or any zero of $\Delta^r(\omega)$, manifests itself in a peak of the first term of the enhancement factor.

VI. DISCUSSION AND SUMMARY OF RESULTS

In the second paper of this series on tunneling, we have demonstrated that the basic approach developed in the first paper on tunneling across a junction of zero width is readily adaptable to more realistic problems. Thus we obtained in Eqs. (3.38)–(3.40) a general expression for the current across an insulating barrier of finite width, subject to an arbitrary time-independent bias and an additional possibly time-dependent single-particle potential energy of interaction. This time dependence may represent a modulated bias or a vibrating impurity potential. The theory, though not based on the transfer-Hamiltonian formalism, can be formulated so as to lead to a "transfer-Hamiltonian-like" expression for the ordinary tunneling channel [Eq. (3.39)]. However, in contrast with the transfer-Hamiltonian formulations, our theory inherently identified the additional channels for resonant and inelastic tunneling [Eq. (3.40)]. In contrast with linear-response theories of inelastic tunneling, our theory is inherently nonperturbative (or an infinite-order perturbation scheme). It also has the advantage that it preserves, at least for the noninteracting system considered in this paper, the intuitively appealing separation between the left (right) electrodes and the barrier effects. We have shown in Sec. IV that the expression for the tunneling current in a junction of zero width, calculated directly in I, represents the proper limit of our general expression when the time-dependent component of the barrier potential and the width of the junction both tend to zero. Finally we have discussed the energy density of the tunneling current when an atomic impurity is incorporated in the barrier. In Sec. V A we were able to point out several different resonant phenomena which could contribute to the resonant enhancement of the tunneling current. In Sec. V C we indicated an operational procedure for distinguishing between the several resonances in terms of their "signatures" on the

energy density of tunneling current.

Application of our formalism to the discussion of inelastic tunneling due to a vibrating impurity will be reported separately.

The results obtained clearly indicate the versatility and potential usefulness of our theory. In this initial development we have restricted ourselves to tunneling in noninteracting systems. The great attraction of the formalism is, however, in its capability of treating interacting systems. Work is presently in progress in applying our theory in this way. Work on an extension to a truly three-dimensional theory is also in progress.

APPENDIX A: DERIVATION OF THE DYSON EQUATION FOR G^+, EQS. (3.6), AND (3.9)

Keldysh's matrix Dyson equation in the time domain is

$$\underline{G}(\vec{r}, t; \vec{r}', t') = \underline{g}(\vec{r}, t; \vec{r}', t') + \int \underline{g}(\vec{r}, t; \vec{r}_1, t_1) \times \underline{\Sigma}(\vec{r}_1, t_1; \vec{r}_2 t_2) \underline{G}(\vec{r}_2, t_2; \vec{r}', t') \times d\vec{r}_1\, d\vec{r}_2\, dt_1\, dt_2 .$$

In the presence of a single-particle interaction $\mathcal{H}_1(\vec{r}, t)$ one can show directly following the original derivation of (A1) by Keldysh's or Mill's analysis that

$$\underline{G}(\vec{r}, t; \vec{r}', t') = \underline{g}(\vec{r}, t; \vec{r}', t') + \int \underline{g}(\vec{r}, t; \vec{r}_1, t_1) \times \underline{\Sigma}(r_1, t_1) \underline{G}(r_1, t_1; \vec{r}', t')\, d\vec{r}_1\, dt_1, \tag{A2}$$

where, in both Eqs. (A1) and (A2),

$$\underline{G} = \begin{pmatrix} 0 & G^a \\ G^r & 2G^{\pm} \mp (G^r - G^a) \end{pmatrix}, \tag{A3}$$

$$\underline{g} = \begin{pmatrix} 0 & g^a \\ g^r & 2g^{\pm} \mp (g^r - g^a) \end{pmatrix}, \tag{A4}$$

and in Eq. (A4)

$$\underline{\Sigma} = \begin{pmatrix} 0 & \mathcal{H}_1 \\ \mathcal{H}_1 & 0 \end{pmatrix}. \tag{A5}$$

The elements of the matrix Green's functions $\underline{G}$, $\underline{g}$ were defined by Eqs. (3.13).

The thermal-equilibrium Green's functions are invariant under time translations; i.e., the formal Fourier transform of $\underline{g}$ with respect to both time variables (t and t') is proportional to a delta function in $\omega - \omega'$:

$$\underline{g}(\vec{r}, \vec{r}'; \omega, \omega') = \int\int_{-\infty}^{\infty} \underline{g}(\vec{r}, \vec{r}'; t - t') \times e^{i(\omega t - \omega' t')}\, dt\, dt' = \underline{g}(\vec{r}, \vec{r}'; \omega) 2\pi\delta(\omega - \omega') . \tag{A6}$$

Thus, the formal Fourier transformation of Eq. (A2) with respect to t and t' can be expressed with the help of the convolution theorem as

$$\int\int_{-\infty}^{\infty} \underline{G}(\vec{r}, \vec{r}'; t, t') e^{i(\omega t - \omega' t')}\, dt\, dt' = \underline{G}(\vec{r}, \vec{r}'; \omega, \omega') = \underline{g}(\vec{r}, \vec{r}'; \omega) 2\pi\delta(\omega - \omega') + \int_{-\infty}^{\infty} \times \left[\int \underline{g}(\vec{r}, \vec{r}_1; \omega) \underline{\Sigma}(r_1; \omega_1) \underline{G}(r_1, \vec{r}'; \omega - \omega_1)\, dr_1 \right] \frac{d\omega_1}{2\pi} . \tag{A7}$$

The integral with respect to ω_1 is evidently invariant under the transformation $\omega_1 \rightleftharpoons \omega - \omega_1$. Substituting Eqs. (A3) and (A4) into Eq. (A7) one obtains Eqs. (3.7), and using the latter to simplify Eq. (A7) one obtains Eqs. (3.6). The derivation of Eq. (3.9), i.e., the inversion of Eq. (3.6), is most conveniently obtained in terms of a symbolic (operator) notation. That is, we write Eqs. (3.6) and (3.7) as

$$G^{\pm} = g^{\pm} + g^{\pm}\mathcal{H}_1 G^a + g^r \mathcal{H}_1 G^{\pm} = (1 - g^r\mathcal{H}_1) g^{\pm} (1 + \mathcal{H}_1 G^a), \tag{A8}$$

and

$$G^{r,a} = g^{r,a} + g^{r,a}\mathcal{H}_1 G^{r,a} . \tag{A9}$$

It follows from Eq. (A9) that

$$(1 - g^r\mathcal{H}_1)^{-1} = G^r (g^r)^{-1}, \tag{A10}$$

and from the adjoint of Eq. (A9) we obtain

$$G^r (g^r)^{-1} = 1 + G^r \mathcal{H}_1^{\dagger} \tag{A11}$$

Thus, substituting Eqs. (A10) and (A11) into Eq. (A8),

$$G^{\pm} = g^{\pm} + g^{\pm}\mathcal{H}_1 G^a + g^r \mathcal{H}_1^{\dagger} g^{\pm} + G^r \mathcal{H}_1^{\dagger} g^{\pm} \mathcal{H}_1 G^a . \tag{A12}$$

Equation (A12) is the symbolic (operator) representation of Eq. (3.9). The derivation of Eq. (A12) clearly indicates that this explicit solution for $G^{\pm}$ is only valid if the operator

$$(1 - g^r\mathcal{H}_1)^{-1} = G^r (g^r)^{-1} \tag{A13}$$

exists. This in turn amounts to the requirement that the homogenous form of Eq. (A9) have no nontrivial solution.

APPENDIX B: DERIVATION OF EQ. (3.25) FOR $\Gamma^{\pm}(\omega,\omega)$

In deriving Eq. (3.25) we shall resort to the symbolic notation used in Appendix A to derive Eq. (3.9). From Eq. (3.21) we have

$$\Gamma^{\pm}(x,\beta;\omega,\omega) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x\,\partial x'}G^{\pm}(x,x';\omega,\omega)\Big|_{\substack{x=\alpha\\x'=\beta}}. \tag{B1}$$

Hence, using the boundary condition imposed on the "uncoupled" Green's functions at the interfaces [Eqs. (3.19)], we obtain from Eq. (A12) [i.e., the symbolic version of Eq. (3.9)]

$$\Gamma^{\pm}(\alpha,\beta;\omega,\omega) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x\,\partial x'}(G^r\mathcal{H}_1^{\dagger}g^{\pm}\mathcal{H}_1G^a)\Big|_{\substack{x=\alpha\\x'=\beta}}. \tag{B2}$$

where, from Eq. (3.18) we have,

$$\mathcal{H}_1(x,\omega) = \mathcal{H}'(x)\delta(\omega) + V(x,\omega)\Theta(x-L)\Theta(-x+R). \tag{B3}$$

If now $V(x,\omega)=0$, then the boundary conditions [Eqs. (3.19)], the definition of the pseudo-Hamiltonian $\mathcal{H}'$, and the continuity of the mixed second derivative of G at $x=x'$ imply

$$-\frac{2m}{\hbar^2}\Gamma^{\pm}(\alpha,\beta;\omega,\omega) = \int_{-\infty}^{\infty}\{\Gamma^r(\alpha,L;\omega,\omega_1)[g_L^{\pm}(L,L;\omega_1)+g_B^{\pm}(L,L;\omega_1)]\Gamma^a(L,\beta;\omega_1\omega)$$
$$-\Gamma^r(\alpha,L;\omega,\omega_1)g_B^{\pm}(L,R;\omega_1)\Gamma^a(R,\beta;\omega_1,\omega)-\Gamma^r(\alpha,R;\omega,\omega_1)g_B^{\pm}(R,L;\omega_1)\Gamma^a(L,\beta;\omega_1,\omega)$$
$$+\Gamma^r(\alpha,R;\omega,\omega_1)[g_R^{\pm}(R,R;\omega_1)+g_B^{\pm}(R,R;\omega_1)]\Gamma^a(R,\beta;\omega_1,\omega)\}\frac{d\omega_1}{2\pi}. \tag{B4}$$

Equation (B4) is the expanded version of Eq. (3.25) for

$$\delta g_B(\omega)\equiv 0\equiv \delta g_B(\omega,\omega'). \tag{B5}$$

Equation (B4) reduces to the corresponding Eq. (3.25) of I when we account for the time translational invariance of this simplified problem, where

$$\Gamma^{\nu}(\alpha,\beta;\omega,\omega_1)\to\Gamma^{\nu}(\alpha,\beta;\omega_1)2\pi\delta(\omega-\omega_1). \tag{B6}$$

To complete the derivation of Eq. (3.25) we now define the "perturbed" barrier problem:

$$\{\hbar\omega-[\mathcal{H}_B+V(x;\omega)]\}G_B(x,x';\omega,\omega') = \delta(x-x')\delta(\omega-\omega') \tag{B7}$$

where the "intermediate" Green's function G_B is subject to the same boundary conditions [Eq. (3.19)] as g_B. Evidently Eq. (B4) applies in this case if $g_B^{\pm}(x,x';\omega_1)$ is replaced by $G_B^{\pm}(x,x';\omega_1,\omega_2)$ and we integrate also with respect to ω_2. It is a simple matter to verify that

$$G_B^{\nu}(x,x';\omega,\omega') = [g_B^{\nu}(x,x';\omega)+\delta g_B^{\nu}(x,x';\omega)]\times 2\pi\delta(\omega-\omega')+\delta g_B^{\nu}(x,x';\omega,\omega') \tag{B8}$$

and that the several "intermediate" Green's functions can be determined by Keldysh's matrix equations in terms of the interaction

$$\mathcal{H}_1(x,\omega) = V(x;\omega)\Theta(x-L)\Theta(-x+R).$$

This, however, is the significance of Eqs. (3.28)–(3.34).

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[17]The generalized Fourier transform of a constant is proportional to a δ function $\delta(\bar{\omega})$. The coefficient of the δ function, i.e., the time-independent component of the function $f(x,t)$, is defined by the condition

$$\lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{T}|f(x,t)-f(x)|dt=0.$$

[18]This is the "Fredholm alternative"; see W. V. Lovitt, *Linear Integral Equations* (Dover, New York, 1950), p. 66.

[19]Note that for the noninteracting system as well as within the Hartree-Fock approximations for interacting systems, this assertion is self-evident: In these cases the bilinear formula for the Green's function implies

$$\rho(x,x';\omega)\,d\omega=2\pi\sum_{n}\phi_n(x)\phi_n^{*}(x'),\quad \hbar\omega<\epsilon_n<\hbar(\omega+d\omega),$$

where $\{\phi_n\}$ are the eigenfunctions of the single-particle (effective) Hamiltonian, whose eigenvalues are ϵ_n. See Refs. 20 and 21.

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[22]The sense in which $(1/2\pi)\rho(x,x;\omega)$ is a local energy density of states is discussed in Sec. IV of I.

[23]This is a convenient and nonessential restriction. If $V_1(x,t)$ extends beyond the barrier, then one can account for this by modifying $\mathcal{H}_L$ and $\mathcal{H}_R$.

[24]$\langle J(x;\bar{\omega})\rangle$ is continuous at L. However, the first derivatives of the Green's functions g_α are discontinuous at $x=L$, and $\partial G/\partial x$ is discontinuous at $x=x'$. Hence the limit $x\to L$ has to be taken with care if ambiguities are to be avoided.

[25]This identity follows directly from the definition of these functions, Eq. (3.13).

[26]See comment following Eq. (3.4).

[27]It should be noted that whereas we seem to identify resonances with singularities of the mixed second derivative of the barrier Green's (matrix) function rather than with singularities of the $G^{r,a}(\alpha,\beta;\omega)$ itself, this is in fact not the case. For the two matrices have the same spectrum of singularities. This result follows from a comparison of Eqs. (2.9) and (2.10).

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[31]Hence it is understood that the impurities are so dilute that they do not interact and the broadening of E_s is due to the interaction with the continua in the electrodes and not a manifestation of an "impurity band."

[32]We could, in principle, allow the density of states $\rho_{B_0}(x,x;\omega)$ to extend over an energy interval, i.e., an impurity band; however, the additional analysis did not seem warranted at this point. In practice $\rho_{B_0}(x,x';\omega)$ is clearly always smeared over a positive though small energy interval.

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