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Dynamic properties of double-barrier resonant-tunneling structures

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In this paper we present an approach to the dynamic transport properties of a double-barrier resonant-tunneling system. Based on the nonequilibrium-Green's-function technique and the Feynman-path-integral theory, the essential ingredients of this microstructure will be properly treated in a self-consistent way: the quantum interference across the structure, the nonequilibrium distribution of tunneling electrons driven by the applied bias voltage, and the effect of reservoirs (electrodes). The transient behavior of the tunneling current, immediately after the switching on of a dc bias voltage, is characterized by the building-up process of tunneling electrons in the quantum well. The novel negative differential conductance demonstrates itself as a function of frequency of the small ac signal superimposed upon a dc bias. The imaginary part of admittance is shown to be related to the conductance via a Kronig-Kramers relation.

I. INTRODUCTION

For years the double-barrier resonant-tunneling system (DBRTS) has been the focus of intense experimental and theoretical investigations.[1–19] On the one hand, this is due to its technological importance. On the other hand, the DBRTS provides us with an ideal prototype system where nonequilibrium and quantum effects of a small-sized open system may become significant. Since its conception by Tsu and Esaki[1] and the first realization of significant negative differential resistance by Sollner *et al.*,[2] many aspects of this system have been intensively studied, e.g., dc characteristics,[3–7] phonon and laser-assisted tunneling,[8,9] time-dependent processes,[10–12] frequency response,[13–15] noise characteristics,[16,17] and effects of elastic scattering.[18,19] The steady-state properties of the DBRTS have been understood quite well and are mainly characterized by an I-V curve shown in Fig. 1, where a regime of pronounced negative differential resistance (NDR) appears. However, the dynamical aspects of the system, which are of particular importance both for the physical understanding and for the device applications, need to be carefully investigated on the basis of a time-dependent quantum statistical treatment. Traditionally, most theoretical analyses are based upon solving the Schrödinger equation for the scattering wave function and integrating the obtained transmission coefficient to derive the stationary tunneling current as a function of dc bias voltage. This kind of approach may not be capable of describing the dynamic processes of the system such as frequency response and noise processes because, in this prevalent scattering approach, the quantum interference is well accounted for, but the nonequilibrium statistics cannot be self-consistently derived. Actually, the nonequilibrium distribution of tunneling electrons is crucial to the novel negative differential resistance phenomenon in this kind of system, which needs to be consistently determined by bias voltage and by the coupling of the electrodes (reservoirs). Recently, we were able to employ the nonequilibrium-Green's-function approach to get a better understanding of the dynamic properties of the DBRTS. The preliminary results have been reported in Refs. 12, 15, and 17. In this paper, we shall provide the details of this method in Sec. II. Based on a time-dependent quantum statistical treatment, the following topics will be studied, respectively, in Secs. III and IV: (i) The transient behavior of the tunneling current in response to a sudden switch on of a dc bias V; (ii) the frequency-dependent response of the DBRTS to a small ac signal $u(t)\sim u_0 e^{-i\Omega t}$ superimposed upon a dc bias voltage V. The final section consists of a conclusion and a discussion.

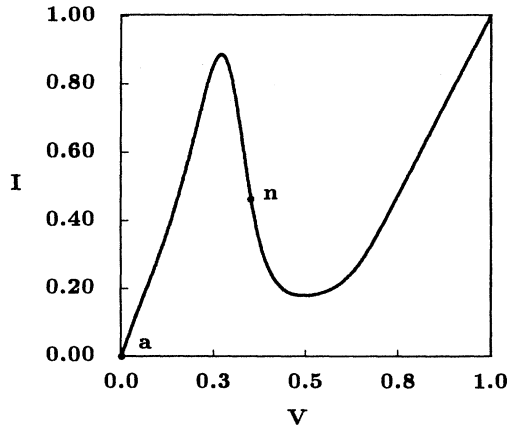

FIG. 1. A typical (qualitative) current-voltage characteristic of the DBRTS. Point a—zero biased, n—biased so that the resonance level is equal to the conduction-band bottom of the emitter electrode.

II. GENERAL DESCRIPTION

In order to describe the essential ingredients of a double-barrier resonant-tunneling structure, we choose the following Hamiltonian for a one-dimensional model system:

$$H_T = H + H'(t) , \tag{2.1}$$

where

$$H = \sum_k \varepsilon_k^L a_k^\dagger a_k + \varepsilon_c c^\dagger c + \sum_p \varepsilon_p^R b_p^\dagger b_p + \sum_k (T_{Lk} c^\dagger a_k + T_{Lk}^* a_k^\dagger c) + \sum_p (T_{Rp} b_p^\dagger c + T_{Rp}^* c^\dagger b_p) \tag{2.2}$$

is the Hamiltonian of a DBRTS under a dc bias voltage V and

$$H'(t) = c^\dagger c[-\alpha e u(t)] + \sum_p b_p^\dagger b_p[-e u(t)] \tag{2.3}$$

is the perturbation due to the ac signal $u(t)$, which is superimposed upon the bias V. a_k ($a_k^\dagger$), c ($c^\dagger$), and b_p ($b_p^\dagger$) are, respectively, the annihilation (creation) operators of electrons (fermions) in the left electrode, in the central quantum well, and in the right electrode. $\varepsilon_c = \varepsilon_0 - \alpha e V$ (α is structure dependent, $\alpha \simeq 0.5$ for a symmetrical structure) is the resonance level as affected by the dc bias. $\varepsilon_k^L = k^2/2m$ and $\varepsilon_p^R = p^2/2m - eV$ are the single-particle energy of the left and right electrodes. The starting point for the energy level is chosen to be the conduction-band bottom of the left electrode and αeV and eV are, respectively, the potential drops of the resonance level and the conduction-band bottom of the right electrode caused by the bias V. [Actually, the choice of the energy starting point is arbitrary. When it is chosen as the position of the resonance level, the difference thus brought is only a constant $\varepsilon_c(\sum_k a_k^\dagger a_k + c^\dagger c + \sum_p b_p^\dagger b_p)$ which does not effect any physics.] The fourth and the fifth terms of Eq. (2.2) describe the coupling between quantum-well electrons and the two reservoirs. The tunneling matrices T_{Lk} and T_{Rp} depend on the barrier profile including the effect of the bias V.

Since the electrode electrons respond to an applied field much faster than the quantum-well electrons, they are generally treated as reservoirs. Thus the density matrix for the DBRTS can be written as

$$\rho = e^{-\beta \sum_k (\varepsilon_k^L - \mu_L) a_k^\dagger a_k} \rho_c e^{-\beta \sum_p (\varepsilon_p^R - \mu_R) b_p^\dagger b_p} , \tag{2.4}$$

where $1/\beta$ is the temperature of the system. The left and right electrode subsystems are separately in their own equilibrium states with chemical potentials μ_L and μ_R, respectively ($\mu_L - \mu_R = e[V + u(t)]$). The central quantum-well electrons are in a nonequilibrium state with the density matrix ρ_c to be determined by their coupling to the two reservoirs and to the applied electric field. In the practical calculation of the present problem, the path-integral method not only enables us to treat the tunneling coupling nonperturbatively, which is essential to the resonant phenomenon, but it also allows us to work out analytically the statistical average with a nonequilibrium density matrix as shown in Eq. (2.4) in a tractable fashion. Moreover, the two density matrices for the two electrode subsystems (with different chemical potentials) can be incorporated into the effective-action functional by replacing the free propagators of the lead subsystems with their thermodynamic counterparts.

To describe the nonequilibrium state of electrons in the center quantum well, the retarded, advanced, and distribution Green's functions are introduced as follows:

$$iG_r(t_1,t_2) = \theta(t_1 - t_2)\langle \{c(t_1), c^\dagger(t_2)\} \rangle , \tag{2.5}$$

$$iG_a(t_1,t_2) = -\theta(t_2 - t_1)\langle \{c(t_1), c^\dagger(t_2)\} \rangle , \tag{2.6}$$

$$iG^<(t_1,t_2) = -\langle c^\dagger(t_2) c(t_1) \rangle , \tag{2.7}$$

where $\langle \cdots \rangle$ represents the nonequilibrium statistical average $\mathrm{Tr}(\cdots)\rho$. A more symmetrical form of the nonequilibrium closed-time-path Green's functions (CTPGF) (Ref. 20) would be much easier to treat. They are defined along a closed time path that runs from $-\infty$ to $+\infty$ along the positive "+" branch and then returns from $+\infty$ back to $-\infty$ along the minus "−" branch:

$$iG_{\alpha\beta}(t_1,t_2) = \langle T_p c_\alpha(t_1) c_\beta^\dagger(t_2) \rangle , \tag{2.8}$$

where $\alpha(\beta) = +$ or $-$ means t_1 (t_2) is located on the "+" or "−" branch, respectively. T_p is the generalized chronological operator ordering physical operators along the closed time path:

$$iG_{++}(t_1,t_2) = \langle T c(t_1) c^\dagger(t_2) \rangle , \tag{2.9}$$

$$iG_{+-}(t_1,t_2) = -\langle c^\dagger(t_2) c(t_1) \rangle , \tag{2.10}$$

$$iG_{-+}(t_1,t_2) = \langle c(t_1) c^\dagger(t_2) \rangle , \tag{2.11}$$

$$iG_{--}(t_1,t_2) = \langle \tilde{T} c(t_1) c^\dagger(t_2) \rangle , \tag{2.12}$$

with T and $\tilde{T}$ being, respectively, the chronological and the antichronological ordering operators. The four components of $G_{\alpha\beta}$ are related to the physical G_r, G_a, and $G^<$ as

$$G_r = \tfrac{1}{2}\xi_\alpha \eta_\beta G_{\alpha\beta} , \tag{2.13}$$

$$G_a = \tfrac{1}{2}\eta_\alpha \xi_\beta G_{\alpha\beta} , \tag{2.14}$$

$$G^< = G_{+-} , \tag{2.15}$$

$$0 = \tfrac{1}{2}\eta_\alpha \eta_\beta G_{\alpha\beta} , \tag{2.16}$$

which can be easily proven by using the definitions of them. Here, $\xi_+ = \xi_- = \eta_+ = -\eta_- = 1$ and the repeated indices are summed over the "+" and "−" branches.

For electrons in the left electrode, the Green's functions

$$A_{\alpha\beta}(k, t_1 - t_2) \equiv \langle T_p a_{k\alpha}(t_1) a_{k\beta}^\dagger(t_2) \rangle$$

have the equilibrium form[20]

$$A_{r(a)}(k,w) = \frac{1}{\omega - \varepsilon_k^L + (-) i\eta} ,$$
$$A^<(k,\omega) = -f_L(\omega)[A_r(k,\omega) - A_a(k,\omega)] , \tag{2.17}$$

while for right electrode electrons the Green's functions

$$B_{\alpha\beta}(p,t_1-t_2)\equiv\langle T_p b_{p\alpha}(t_1)b^{\dagger}_{p\beta}(t_2)\rangle$$

are given by[20]

$$B_{r(a)}(k,\omega)=\frac{1}{\omega-\varepsilon^R_k+(-)i\eta}\ ,$$
$$B^{<}(k,\omega)=-f_R(\omega)[B_r(k,\omega)-B_a(k,\omega)]\ . \tag{2.18}$$

In Eqs. (2.17) and (2.18), $f_L(\omega)$ and $f_R(\omega)$ are, respectively, the Fermi-Dirac distribution functions with their chemical potentials as μ_L and μ_R. η is a positive infinitesimal.

In the path-integral formalism, the quantum statistical average over the nonequilibrium ensemble for this DBRTS can be expressed as[20,21]

$$\langle\cdots\rangle=\int[da^{\dagger}_k][da_k]\int[db^{\dagger}_k][db_k]\int[dc^{\dagger}][dc](\cdots)e^{i\int_p[L(t)-H'(t)]dt}\ , \tag{2.19}$$

where

$$L(t)=\sum_k a^{\dagger}_k(t)(i\partial_t)a_k(t)+\sum_k b^{\dagger}_k(t)(i\partial_t)b_k(t)+c^{\dagger}(t)(i\partial_t)c(t)-H(t) \tag{2.20}$$

is the Lagrangian of the DBRTS without the ac signal $u(t)$. $\int_p dt=\int_{-\infty}^{+\infty}dt_+ +\int_{+\infty}^{-\infty}dt_-=\eta_\alpha\int_{-\infty}^{+\infty}dt_\alpha$ is the time integration along the closed time path. Since the closed-time-path action $\int_p L(t)dt$ contains only bilinear terms of the a_k and b_p variables, these variables can be eliminated exactly in the following path-integration formula by carrying out the Gaussian functional integrations of them:[20,21]

$$\begin{aligned}&\int[da^{\dagger}_k][da_k]\int[db^{\dagger}_k][db_k]\int[dc^{\dagger}][dc]O[c,c^{\dagger};a_k,a^{\dagger}_k;b_p,b^{\dagger}_p]e^{i\int_p L(t)dt}\\&=\int[dc^{\dagger}][dc]O\left[c,c^{\dagger};i\frac{\delta}{\delta(T_{Lk}c^{\dagger})},-i\frac{\delta}{\delta(T^*_{Lk}c)};i\frac{\delta}{\delta(T^*_{Rp}c^{\dagger})},-i\frac{\delta}{\delta(T_{Rp}c)}\right]e^{iI_{\rm eff}[c,c^{\dagger}]}\\&\equiv\left\langle O\left[c,c^{\dagger};i\frac{\delta}{\delta(T_{Lk}c^{\dagger})},-i\frac{\delta}{\delta(T^*_{Lk}c)};i\frac{\delta}{\delta(T^*_{Rp}c^{\dagger})},-i\frac{\delta}{\delta(T_{Rp}c)}\right]\right\rangle_{\rm eff}\ ,\end{aligned} \tag{2.21}$$

where $\delta/\delta(\cdots)$ is the functional derivative. $O[\cdots]$ is an arbitrary functional of c, a_k, and b_p Grassman variables. $I_{\rm eff}$ is the effective action of tunneling electrons:

$$I_{\rm eff}=\int_p dtc^{\dagger}(t)(i\partial_t-\varepsilon_c)c(t)-\int_p dt\int_p dt'c^{\dagger}(t)\left[\sum_k|T_{Lk}|^2A(k,t-t')+\sum_p|T_{Rp}|^2B(p,t-t')\right]c(t') \tag{2.22}$$

including the quantum influence of reservoir (electrode) couplings. Therefore the effect of the density matrices of the two electrodes [see Eq. (2.4)] are incorporated into their propagators $A_{\alpha\beta}$ and $B_{\alpha\beta}$ ($A^{<}$ carries distribution f_L and $B^{<}$ carries f_R).

For later discussion, we present here four equations of functional integrations involving only one of the a_k and b_p variables:

$$\int[da^{\dagger}_k][da_k]\int[db^{\dagger}_k][db_k]\int[dc^{\dagger}][dc](\cdots)a_k(t)e^{i\int_p L(i)dt}=\int_p dsT^*_{Lk}A(k,t-s)\int[dc^{\dagger}][dc](\cdots)c(s)e^{iI_{\rm eff}[c,c^{\dagger}]}\ , \tag{2.23}$$

$$\int[da^{\dagger}_k][da_k]\int[db^{\dagger}_k][db_k]\int[dc^{\dagger}][dc](\cdots)a^{\dagger}_k(t)e^{i\int_p L(t)dt}=\int_p dsT_{Lk}A(k,s-t)\int[dc^{\dagger}][dc](\cdots)c^{\dagger}(s)e^{iI_{\rm eff}[c,c^{\dagger}]}\ , \tag{2.24}$$

$$\int[da^{\dagger}_k][da_k]\int[db^{\dagger}_k][db_k]\int[dc^{\dagger}][dc](\cdots)b_p(t)e^{i\int_p L(t)dt}=\int_p dsT_{Rp}B(p,t-s)\int[dc^{\dagger}][dc](\cdots)c(s)e^{iI_{\rm eff}[c,c^{\dagger}]}\ , \tag{2.25}$$

$$\int[da^{\dagger}_k][da_k]\int[db^{\dagger}_k][db_k]\int[dc^{\dagger}][dc](\cdots)b^{\dagger}_p(t)e^{i\int_p L(t)dt}=\int_p dsT^*_{Rp}B(p,s-t)\int[dc^{\dagger}][dc](\cdots)c^{\dagger}(s)e^{iI_{\rm eff}[c,c^{\dagger}]}\ . \tag{2.26}$$

III. TRANSIENT RESPONSE

In this section we examine the transient response process of a DBRTS when a step bias voltage $V(t)=\theta(t)V$ is imposed [$u(t)=0$]. We will examine the transient response of the Green's function and then demonstrate how the tunneling current evolves onto its steady-state limit. The time evolution of the system is mainly determined by the building up of a nonequilibrium distribution of tunneling electrons in the central quantum well and, therefore, the crucial time scale

of the problem will be the inverse of the resonance level width.

To derive the kinetic equations for $G_{\alpha\beta}$, we first take derivatives of Eq. (2.8) with respect to t_1 and t_2, respectively, and utilize the Hamiltonian in Eq. (2.2) and the Heisenberg equation to obtain a set of equations which involve the c variable as well as the a_k and b_k variables.

$$i\partial_{t_1}G_{\alpha\beta}(t_1,t_2)=\tfrac{1}{2}(\eta_\alpha+\eta_\beta)\delta(t_1-t_2)-i\varepsilon_c\langle T_p c_\alpha(t_1)c_\beta^\dagger(t_2)\rangle$$
$$-i\sum_k T_{Lk}\langle T_p a_{k\alpha}(t_1)c_\beta^\dagger(t_2)\rangle-i\sum_p T_{Rp}^*\langle T_p b_{p\alpha}(t_1)c_\beta^\dagger(t_2)\rangle\ , \tag{3.1}$$

$$i\partial_{t_2}G_{\alpha\beta}(t_1,t_2)=-\tfrac{1}{2}(\eta_\alpha+\eta_\beta)\delta(t_1-t_2)+i\varepsilon_c\langle T_p c_\alpha(t_1)c_\beta^\dagger(t_2)\rangle$$
$$+i\sum_k T_{Lk}^*\langle T_p c_\alpha(t_1)a_{k\beta}^\dagger(t_2)\rangle+i\sum_p T_{Rp}\langle T_p c_\alpha(t_1)b_{p\beta}^\dagger(t_2)\rangle\ . \tag{3.2}$$

Expressing the nonequilibrium ensemble average in the form of Eq. (2.19), the statistical average becomes a path integration. Then carry out the Gaussian functional integrations over a_k and b_k variables by using Eqs. (2.21)–(2.26). As a result, we have

$$i\partial_{t_1}G_{\alpha\beta}(t_1,t_2)=\tfrac{1}{2}(\eta_\alpha+\eta_\beta)\delta(t_1-t_2)+\varepsilon_c G_{\alpha\beta}(t_1,t_2)+\sum_k|T_{Lk}|^2\int dt' A_{a\nu}(k,t_1-t')\eta_\nu G_{\nu\beta}(t',t_2)$$
$$+\sum_k|T_{Rk}|^2\int dt' B_{\alpha\nu}(k,t_1-t')\eta_\nu G_{\nu\beta}(t',t_2)\ , \tag{3.3}$$

$$-i\partial_{t_2}G_{\alpha\beta}(t_1,t_2)=\tfrac{1}{2}(\eta_\alpha+\eta_\beta)\delta(t_1-t_2)+\varepsilon_c G_{\alpha\beta}(t_1,t_2)+\sum_k|T_{Lk}|^2\int dt' G_{\alpha\nu}(t_1,t')\eta_\nu A_{\nu\beta}(k,t'-t_2)$$
$$+\sum_k|T_{Rk}|^2\int dt' G_{\alpha\nu}(t_1,t')\eta_\nu B_{\nu\beta}(k,t'-t_2)\ . \tag{3.4}$$

It should be emphasized here that the Green's functions $A_{\alpha\beta},B_{\alpha\beta}$ for the left and right lead electrons are equilibrium functions and thus are time translationally invariant while Green's functions $G_{\alpha\beta}$ are not. The relative time $t=(t_1-t_2)$ dependence of $G_{\alpha\beta}(t_1,t_2)$ describes the spectrum of the quantum-well electrons, while its $T=(t_1+t_2)/2$ dependence corresponds to the transient evolution of their state. Therefore, in the following discussion we use (t,T) variables for $G(t_1,t_2)\equiv G(t,T)$. Fourier transforming the t variable in $G(t,T)$ yields $G(\omega,T)$.

Making use of the relations between G_r, G_a, $G^<$, and $G_{\alpha\beta}$ as described in the preceding section [Eqs. (2.13)–(2.16)], we could get kinetic equations for G_r, G_a, and $G^<$. Then changing the variables (t_1,t_2) to (t,T) and taking the Fourier transform of the t variable, we arrive at the following results:

$$(\omega-\varepsilon_c)G_{r(a)}(\omega)=1+\left[\sum_k|T_{Lk}|^2A_{r(a)}(k,\omega)+\sum_k|T_{Rk}|^2B_{r(a)}(k,\omega)\right]G_{r(a)}(\omega)\ , \tag{3.5}$$

$$i\frac{d}{dT}G^<(\omega,T)=\left[\sum_k|T_{Lk}|^2[A_r(k,\omega)-A_a(k,\omega)]+\sum_k|T_{Rk}|^2[B_r(k,\omega)-B_a(k,\omega)]\right]$$
$$\times G^<(\omega,T)-[G_r(\omega)-G_a(\omega)]\left[\sum_k|T_{Lk}|^2A^<(k,\omega)+\sum_k|T_{Rk}|^2B^<(k,\omega)\right]\ . \tag{3.6}$$

Equation (3.5) yields the information of spectrum and dissipation:

$$G_{r(a)}(\omega)=\frac{1}{\omega-\varepsilon_c'+(-)i\gamma(\omega)}\ , \tag{3.7}$$

where ε_c' is the renormalized resonant level and

$$\gamma(\omega)=\gamma_L(\omega)+\gamma_R(\omega) \tag{3.8}$$

is its width and

$$\gamma_L(\omega)=\frac{i}{2}\sum_k|T_{Lk}|^2[A_r(k,\omega)-A_a(k,\omega)]\ , \tag{3.9}$$

$$\gamma_R(\omega)=\frac{i}{2}\sum_k|T_{Rk}|^2[B_r(k,\omega)-B_a(k,\omega)]\ . \tag{3.10}$$

The inverse of γ is the lifetime of the resonance state $\tau_R=1/\gamma(\varepsilon_c')$. τ_R here is found to be dependent upon the barrier profile via the relative position of ε_c, μ_L, and μ_R and via the tunneling coefficients in which the applied bias is included. The above result of the resonance level deduced from Eq. (3.5) does not have a dependence upon T since the resonance level only depends upon the barrier potential profile and the potential profile responds very fast to an applied bias voltage. This point has also been emphasized in Sec. II when we introduced the nonequilibrium density matrix in Eq. (2.4).

From Eq. (3.6), we have the following time-dependent solution, which characterizes the transient tunneling process:

$$G^<(\omega,T)=-\{F(\omega)-[F(\omega)-F_0(\omega)]e^{-2\gamma T}\}$$
$$\times[G_r(\omega)-G_a(\omega)] \tag{3.11}$$

with

$$F(\omega)=\frac{f_L(\omega)\gamma_L(\omega)+f_R(\omega)\gamma_R(\omega)}{\gamma(\omega)} \tag{3.12}$$

being a Fermi-Dirac-type distribution for the quantum-well electrons. In Eq. (3.11), $F_0(\omega)$ is the initial distribution. When a dc bias is applied at $T=0$, the two subsystems of lead electrons very soon reach their own new equilibrium states separately (with distribution f_L and f_R, respectively). The evolution of quantum-well electrons is determined here by the distribution Green's function $G^<$ given above. It takes a time $\tau_R=1/\gamma$ for the transient part of Eq. (3.11) to die out after which the quantum-well electrons arrive at a steady state with nonequilibrium distribution $F(\omega)$.

Just after a bias voltage V is applied at $t=0$, the current flowing into the quantum well $I_L=\langle\hat{I}_L(t)\rangle$,

$$\hat{I}_L(t)\equiv -ie\left[H,\sum_k a_k^\dagger(t)a_k(t)\right] \tag{3.13}$$

is not equal to that flowing out of the well $I_R=\langle\hat{I}_R(t)\rangle$,

$$\hat{I}_R(t)\equiv ie\left[H,\sum_k b_k^\dagger(t)b_k(t)\right] \tag{3.14}$$

during the building up of electrons in the well. However, when a steady transport state is established after a certain long time, I_L and I_R should reach the same limit. Using Eq. (2.2) to make the commutators and Eqs. (2.19) and (2.21) to carry out the path integrals, we have the following time-dependent current (I_R as an example) expressed in terms of the nonequilibrium Green's functions discussed above:

$$I_R(t)=e\sum_k |T_{Rk}|^2\int_0^\infty dt'[B_r(k,t-t')G^<(t',t)-G^<(t,t')B_a(k,t'-t) +B^<(k,t-t')G_a(t'-t)-G_r(t-t')B^<(k,t'-t)] . \tag{3.15}$$

After substitution of the Green's functions into Eq. (3.15), we arrive at the final result

$$I_R(T)=I\left[1+\frac{F_0-F}{f_L-f_R}\frac{\gamma}{\gamma_L}e^{-2\gamma T}\right] \quad \text{for } T\gg\tau_{\text{lead}} . \tag{3.16}$$

Following the same procedure, we could derive an expression for $I_L(T)$,

$$I_L(T)=I\left[1+\frac{F-F_0}{f_L-f_R}\frac{\gamma}{\gamma_R}e^{-2\gamma T}\right] \quad \text{for } T\gg\tau_{\text{lead}} . \tag{3.17}$$

In Eqs. (3.16) and (3.17), τ_{lead} is the response time of the electrodes which is assumed to be much shorter than $1/\gamma$. I is steady state tunneling current

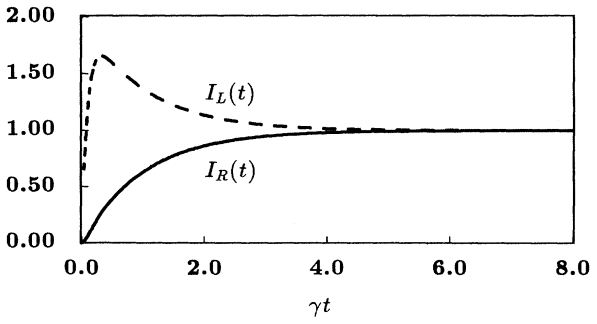

FIG. 2. Transient behavior of tunneling current $I_L(t)$ and $I_R(t)$. I_L and I_R are normalized by I. $\gamma_L=\gamma_R$ after the bias is switched on. Initially before the bias is applied the Fermi level of the electrodes is below the resonance level so that $F_0=0$.

$$I=e\int\frac{d\omega}{2\pi}\frac{2[f_L(\omega)-f_R(\omega)]}{(\omega-\varepsilon_c')^2+\gamma^2}4\gamma_L\gamma_R . \tag{3.18}$$

Obviously, it takes a time $\tau_R=1/\gamma$ for $I_R(t)$ and $I_L(t)$ to reach their steady-state limit I if $F_0\neq F$, i.e., the initial distribution of electrons in the quantum well is not the very nonequilibrium steady-state distribution F. If initially the Fermi level of the two electrodes is below the resonance level before the bias is applied, then the initial distribution $F_0=0$ and $I_L(t)$ and $I_R(t)$ will have an overshoot and undershoot transient behavior, respectively, as shown in Fig. 2.

IV. FREQUENCY RESPONSE

In the presence of a time-dependent field $u(t)$, the electric currents flowing into the quantum well and flowing out of the well $I_L(t)$ and $I_R(t)$ are not in balance. The terminal current is given by $I=(I_L+I_R)/2$, in accordance with the Ramo-Shockley theorem[22]

$$I(t)=-\frac{ie}{2}\left\langle\sum_k[T_{Lk}c^\dagger(t)a_k(t)-T_{Lk}^*a_k^\dagger(t)c(t)] +\sum_p[T_{Rp}b_p^\dagger(t)c(t)-T_{Rp}^*c^\dagger(t)b_p(t)]\right\rangle , \tag{4.1}$$

where $\langle\cdots\rangle$ is defined as in Eq. (2.19). In order to calculate the ac current $i(t)$ induced by the small signal $u(t)$, we expand the functional integral in Eq. (4.1) as defined by Eq. (2.19) to the linear order in H' [thus linear in $u(t)$]. Then it is straightforward to obtain the following linear-response result for $i(t)$:

$$i(t)=\frac{e^2}{4\pi}\int dt'\Pi_r(t-t')u(t') , \tag{4.2}$$

where Π_r is a retarded correlation function and its closed-time-path form is

$$\Pi_{\alpha\beta}(t-t')=2\pi\left\langle \left[\sum_k [T_{Lk}c^\dagger(t)a_k(t)-T^*_{Lk}a^\dagger_k(t)c(t)] + \sum_p [T_{Rp}b^\dagger_p(t)c(t)-T^*_{Rp}c^\dagger(t)b_p(t)] \right]_\alpha \left[\alpha c^\dagger(t')c(t')+\sum_p b^\dagger_p(t')b_p(t') \right]_\beta \right\rangle . \tag{4.3}$$

In Eq. (4.3), $\langle \cdots \rangle$ represents the path integral in Eq. (2.19) with $H'=0$. Carrying out the path integrations in Eq. (4.3) will enable us to find the desired admittance $Y(\Omega)$: $i(\Omega)=Y(\Omega)u(\Omega)$, as a function of frequency Ω, i.e.,

$$Y(\Omega)=\frac{e^2}{4\pi}\Pi_r(\Omega) . \tag{4.4}$$

Since

$$\Pi_r(t-t')=\tfrac{1}{2}\xi_\alpha\eta_\beta\Pi_{\alpha\beta}(t-t') \tag{4.5}$$

is a retarded function, its Fourier transform $\Pi_r(\Omega)$ and thus $Y(\Omega)$ will be analytical in the upper half plane of the complex variable Ω. Consequently, the conductance $\sigma(\Omega)=\mathrm{Re}Y(\Omega)$ and the imaginary admittance $\mathrm{Im}Y(\Omega)$ can be related through the Kronig-Kramers relations.

In order to calculate the correlation function Π in Eq. (4.3), we utilize Eq. (2.21) to eliminate the a_k and b_p variables and then carry out the path integrations of the c variable. As the result, we have

$$\begin{aligned}\Pi_{\alpha\beta}(t-t')=2\pi\alpha\eta_\nu\int ds \Big[& A_{\alpha\nu}(t-s)G_{\nu\beta}(s-t')G_{\beta\alpha}(t'-t)-G_{\alpha\beta}(t-t')G_{\beta\nu}(t'-s)A_{\nu\alpha}(s-t) \\ & +G_{\alpha\beta}(t-t')G_{\beta\nu}(t'-s)B_{\nu\alpha}(s-t)-B_{\alpha\nu}(t-s)G_{\nu\beta}(s-t')B_{\beta\alpha}(t'-t) \\ & +G_{\alpha\nu}(t-s)\sum_p B_{\nu\beta}(p,s-t')|T_{Rp}|^2B_{\beta\alpha}(p,t'-t) \\ & -\sum_p B_{\alpha\beta}(p,t-t')|T_{Rp}|^2B_{\beta\nu}(p,t'-s)G_{\nu\alpha}(s-t)\Big] \\ +2\pi\eta_\mu\eta_\nu\eta_\rho\int ds_1\int ds_2\int ds_3 & \\ \times\Big[& A_{\alpha\mu}(t-s_1)G_{\mu\nu}(s_1-s_2)\sum_p B_{\nu\beta}(p,s_2-t')|T_{Rp}|^2B_{\beta\rho}(p,t'-s_3)G_{\rho\alpha}(s_3-t) \\ & -G_{\alpha\mu}(t-s_1)\sum_p B_{\mu\beta}(p,s_1-t')|T_{Rp}|^2B_{\beta\nu}(p,t'-s_2)G_{\nu\rho}(s_2-s_3)A_{\rho\alpha}(s_3-t) \\ & +G_{\alpha\mu}(t-s_1)\sum_p B_{\mu\beta}(p,s_1-t')|T_{Rp}|^2B_{\beta\nu}(p,t'-s_2)G_{\nu\rho}(s_2-s_3)B_{\rho\alpha}(s_3-t) \\ & -B_{\alpha\mu}(t-s_1)G_{\mu\nu}(s_1-s_2)\sum_p B_{\nu\beta}(p,s_2-t')|T_{Rp}|^2B_{\beta\rho}(p,t'-s_3)G_{\rho\alpha}(s_3-t)\Big] .\end{aligned} \tag{4.6}$$

In Eq. (4.6),

$$A_{\alpha\beta}(t)\equiv\sum_k|T_{Lk}|^2A_{\alpha\beta}(k,t),\quad B_{\alpha\beta}(t)\equiv\sum_p|T_{Rp}|^2B_{\alpha\beta}(p,t) . \tag{4.7}$$

Next we use the relations in Eqs. (2.13)–(2.16) to express the retarded correlation Π_r in terms of the retarded, advanced, and distribution Green's functions. In such a substitution procedure, the following four relations are repeatedly utilized. The first one is

$$\tfrac{1}{2}\xi_\alpha\eta_\beta C_{\alpha\beta}(t-t')D_{\beta\alpha}(t'-t)=C^<(t-t')D_a(t'-t)+C_r(t-t')D^<(t'-t) , \tag{4.8}$$

where C and D could be combinations of Green's functions A, B, and G. For the combination defined as

$$C_{\alpha\beta}(t-t')\equiv\int ds_1\int ds_2\cdots\int ds_n C^{(1)}_{\alpha\mu}(t-s_1)\eta_\mu C^{(2)}_{\mu\nu}(s_1-s_2)\eta_\nu\cdots\eta_\rho C^{(n)}_{\rho\beta}(s_n-t') ,$$

we have the three more identities:

$$\begin{aligned}C^<(t-t')=\int ds_1\cdots\int ds_n[& C^{(1)<}(t-s_1)C^{(2)}_a(s_1-s_2)\cdots C^{(n)}_a(s_n-t') \\ & +C^{(1)}_r(t-s_1)C^{(2)<}(s_1-s_2)\cdots C^{(n)}_a(s_n-t') \\ & +\cdots+C^{(1)}_r(t-s_1)C^{(2)}_r(s_1-s_2)\cdots C^{(n)<}(s_n-t')] ,\end{aligned} \tag{4.9}$$

$$C_r(t-t')=\int ds_1\cdots\int ds_n[C_r^{(1)}(t-s_1)C_r^{(2)}(s_1-s_2)\cdots C_r^{(n)}(s_n-t')]\ , \tag{4.10}$$

$$C_a(t'-t)=\int ds_1\cdots\int ds_n[C_a^{(1)}(t'-s_1)C_a^{(2)}(s_1-s_2)\cdots C_a^{(n)}(s_n-t)]\ . \tag{4.11}$$

To prove these four identities [Eqs. (4.8)–(4.11)] is quite straightforward by using the basic relations in Eqs. (2.13)–(2.16). With the help of the above-mentioned relations, it is easy to show that each term of $\Pi_r(t-t')$ [see Eqs. (4.5) and (4.6)] has the common factor $\theta(t-t')$ coming either from $G_r(t-t')$ or from $G_a(t'-t)$, which explicitly confirms that $\Pi_r(t-t')$ is retarded and thus $\Pi_r(\Omega)$ is analytical in the upper half plane of complex Ω.

The Fourier transform $\Pi_r(\Omega)$ is found to be

$$\begin{aligned}\Pi_r(\Omega)=\alpha\int_{-\infty}^{\infty}d\omega\{&2i[\gamma_L(+)f_L(+)-\gamma_R(+)f_R(+)]G_a(+)G_a\\&-2i(\gamma_Lf_L-\gamma_Rf_R)G_r(+)G_r+[A_r(+)-A_a-B_r(+)+B_a][G^<(+)G_a+G_r(+)G^<]\}\\+\int_{-\infty}^{\infty}d\omega\{&G^<(+)\Gamma_a(\omega,\Omega)-G^<\Gamma_r(\omega,\Omega)-2i[\gamma_R(+)f_R(+)-\gamma_Rf_R]\frac{1}{\Omega}[G_r(+)-G_a]\\&-2i[\gamma_R(+)f_R(+)-\gamma_Rf_R]G_r(+)G_a\frac{1}{\Omega}[A_r(+)-A_a-B_r(+)+B_a]\\&+2i[\gamma_L(+)f_L(+)-\gamma_R(+)f_R(+)]G_a(+)G_a\Gamma_a(\omega,\Omega)-2i(\gamma_Lf_L-\gamma_Rf_R)G_r(+)G_r\Gamma_r(\omega,\Omega)\\&+\Gamma_a(\omega,\Omega)G^<(+)G_a[A_r(+)-A_a-B_r(+)+B_a]\\&+\Gamma_r(\omega,\Omega)G_r(+)G^<[A_r(+)-A_a-B_r(+)+B_a]\}\ ,\end{aligned} \tag{4.12}$$

where $\gamma_{L(R)}(+)$ and $\gamma_{L(R)}$, etc., stand for, respectively, $\gamma_{L(R)}(\omega+\Omega)$ and $\gamma_{L(R)}(\omega)$, etc., Γ_r and Γ_a are introduced as

$$\Gamma_r(\omega,\Omega)\equiv\sum_p B_r(p,\omega+\Omega)|T_{Rp}|^2B_r(p,\omega)\ , \tag{4.13}$$

$$\Gamma_a(\omega,\Omega)\equiv\sum_p B_a(p,\omega+\Omega)|T_{Rp}|^2B_a(p,\omega)\ . \tag{4.14}$$

In deriving Eq. (4.12), we have also used

$$A^<(\omega)=2if_L(\omega)\gamma_L(\omega),\quad B^<(\omega)=2if_R(\omega)\gamma_R(\omega)\ , \tag{4.15}$$

$$\sum_p B^<(p,\omega+\Omega)|T_{Rp}|^2B_a(p,\omega)=-\frac{2i}{\Omega}f_R(\omega+\Omega)\gamma_R(\omega+\Omega)\ , \tag{4.16}$$

$$\sum_p B_r(p,\omega+\Omega)|T_{Rp}|^2B^<(p,\omega)=\frac{2i}{\Omega}f_R(\omega+\Omega)\gamma_R(\omega+\Omega)\ . \tag{4.17}$$

Equation (4.12) is our central result for the frequency response characteristics. Using the nonequilibrium steady-state Green's functions derived in Eqs. (3.7) and (3.11) and Eqs. (2.17) and (2.18) to carry out the frequency integrations, we can obtain the final expressions of conductance $\sigma(\Omega)$ and imaginary admittance $\mathrm{Im}Y(\Omega)$ for various cases.

When the temperature $1/\beta=0$, the dc bias $V=0$ (point a in Fig. 1) and for a system whose resonance level is equal to the Fermi level of the two electrodes, i.e., $\varepsilon_c=\mu_L=\mu_R$, the distribution of tunneling electrons $F(\omega)=f_L(\omega)=f_R(\omega)=\theta(\varepsilon_c-\omega)$. Approximately, $\gamma_L(\omega)$ and $\gamma_R(\omega)$ are assumed to be constants γ_L and γ_R, respectively. Further carrying out the ω integrations in Eq. (4.12), the conductance and the imaginary part of the admittance can be shown to have the following compact forms:

$$\frac{\sigma(\Omega)}{|\sigma(0)|}=\frac{(16\gamma_L\gamma_R+\Omega^2)\gamma^3}{4\gamma_L\gamma_R(\Omega^2+4\gamma^2)\Omega}\tan^{-1}\left[\frac{\Omega}{\gamma}\right]+\frac{(\gamma_L-\gamma_R)^2\gamma^2}{4\gamma_L\gamma_R(\Omega^2+4\gamma^2)}\ln\left[1+\frac{\Omega^2}{\gamma^2}\right]\ , \tag{4.18}$$

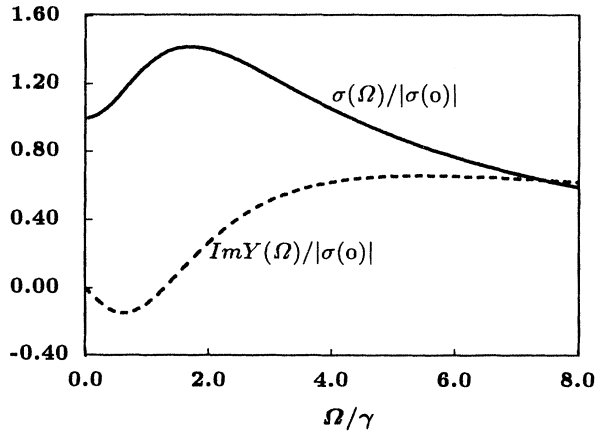

FIG. 3. Frequency-dependent conductance and imaginary part of admittance of the DBRTS with zero bias. The system is asymmetrical so that $\gamma_L=0.9\gamma$, $\gamma_R=0.1\gamma$.

$$\frac{\mathrm{Im}Y(\Omega)}{|\sigma(0)|}=\frac{(16\gamma_L\gamma_R+\Omega^2)\gamma^3}{8\gamma_L\gamma_R(\Omega^2+4\gamma^2)\Omega}\ln\left[1+\frac{\Omega^2}{\gamma^2}\right]-\frac{(\gamma_L-\gamma_R)^2\gamma^2}{2\gamma_L\gamma_R(\Omega^2+4\gamma^2)}\tan^{-1}\left[\frac{\Omega}{\gamma}\right]. \quad (4.19)$$

The numerical results for Eqs. (4.18) and (4.19) are shown in Fig. 3. In response to an applied ac voltage, the electrons tunnel into the center well from one electrode and tunnel out of it into the other electrode. This response decreases monotonically as shown in Fig. 3 with the increasing frequency when $\Omega>\Omega_0$. The characteristic frequency for this behavior is given by the resonance level broadening $\Omega_0=2\gamma$. When $\Omega\gg\Omega_0$, tunneling electrons will not be able to follow the applied field and the tunneling current becomes vanishing. For an asymmetrical system such as that shown in Fig. 3 ($\gamma_L=9\gamma_R$), the low-frequency conductance shows a capacitance behavior since the terminal current is mainly controlled by one (left) barrier, which is in good agreement with a Kubo formula study (third reference of Ref. 14).

Also at zero temperature, when the DBRTS is biased at V_n (point n in Fig. 1) so that the resonance level is equal to the conduction-band bottom, i.e., $\varepsilon_c=\varepsilon^L_{k=0}=0$, and $\gamma_L(\omega)$ and $\gamma_R(\omega)$ can be approximated as $\gamma_L\theta(\omega)$ and γ_R, respectively. Since $\mu_L\gg0$ and $\mu_R\ll0$, the distribution functions $f_L\simeq1$, $f_R\simeq0$, and $F(\omega)\simeq\gamma_L(\omega)/\gamma(\omega)$. With these approximations, the negative conductance $\sigma(\Omega)$ and imaginary part of the admittance $\mathrm{Im}Y(\Omega)$ are derived from Eq. (4.12) to have the following expressions:

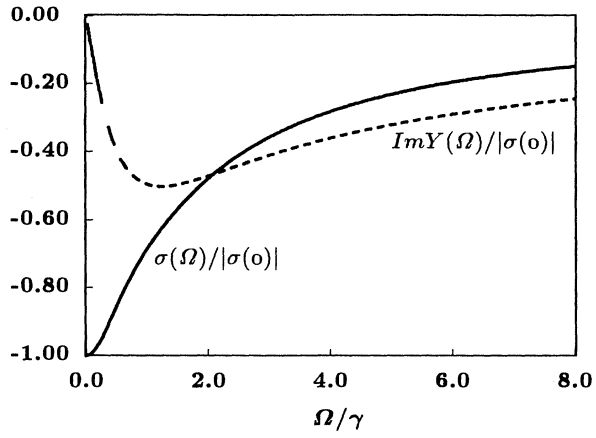

FIG. 4. Frequency-dependent conductance and imaginary part of admittance of the DBRTS biased at NDR ($V=V_n$ so that $\varepsilon_c=\varepsilon^L_{k=0}=0$). The system is asymmetrical and it becomes symmetrical when biased: $\gamma_L=\gamma_R=0.5\gamma$.

$$\frac{\sigma(\Omega)}{|\sigma(0)|}=-\frac{\gamma_R+\xi(\gamma+\gamma_R)}{4\gamma_R}\frac{\gamma}{\Omega}\tan^{-1}\left[\frac{\Omega}{\gamma}\right]+\frac{\xi\gamma}{8\gamma_R}\ln\left[1+\frac{\Omega^2}{\gamma^2}\right]-\frac{\gamma+\xi(\gamma+\gamma_R)}{4\gamma_R}\frac{\gamma}{\Omega}\tan^{-1}\left[\frac{\Omega}{\gamma_R}\right]+\frac{\xi\gamma}{8\gamma_R}\ln\left[1+\frac{\Omega^2}{\gamma_R^2}\right], \quad (4.20)$$

$$\frac{\mathrm{Im}Y(\Omega)}{|\sigma(0)|}=-\frac{\gamma_R+\xi(\gamma+\gamma_R)}{4\gamma_R}\frac{\gamma}{2\Omega}\ln\left[1+\frac{\Omega^2}{\gamma^2}\right]+\frac{\xi\gamma}{4\gamma_R}\tan^{-1}\left[\frac{\Omega}{\gamma}\right]-\frac{\gamma+\xi(\gamma+\gamma_R)}{4\gamma_R}\frac{\gamma}{2\Omega}\ln\left[1+\frac{\Omega^2}{\gamma_R^2}\right]+\frac{\xi\gamma}{4\gamma_R}\tan^{-1}\left[\frac{\Omega}{\gamma_R}\right], \quad (4.21)$$

with

$$\xi=\frac{2\gamma_R^2-\gamma_L(\gamma+\gamma_R)}{\Omega^2+(\gamma+\gamma_R)^2}. \quad (4.22)$$

For an asymmetrical DBRTS, if the right barrier is higher and/or thicker than the left one, $\gamma_L\gg\gamma_R$ at $V=0$. However, it may become symmetrical $\gamma_L=\gamma_R$ when a proper dc bias is applied. In Fig. 4 we plot the conductance and imaginary part of the admittance as functions of frequency Ω for such an asymmetrical structure. The differential conductance (negative) $\sigma(\Omega)$ rolls off with a characteristic frequency given by the width of the resonance level $\Omega_0=\gamma+\gamma_R$ and remains significantly negative until Ω equals approximately several Ω_0. This behavior agrees with a previous numerical investigation[14] and is consistent with the main feature of experiments.[2,13] The imaginary part of the admittance is shown as the dashed curve in Fig. 4, which matches the experimental results as far as its magnitude is concerned.[13]

V. CONCLUDING REMARKS

To conclude, we have presented a nonequilibrium-Green's-function treatment for the time-dependent properties of double-barrier resonant-tunneling systems. With the help of the Feynman path-integral theory, the tunneling couplings are treated exactly (nonperturbatively), which is essential to the resonant phenomena. The other essential of the problem, i.e., the nonequilibrium statistics, has also been well accounted for in this approach. The distribution of tunneling electrons in the central

quantum well, driven far from equilibrium by the bias, is determined by the couplings to the two reservoirs (electrodes) with different chemical potentials. Especially, in response to an oscillating voltage, the tunneling electrons oscillate into and out of the well and so does their distribution. The duration time for the tunneling electrons to follow the varying applied voltage yields a characteristic frequency given by the resonance level broadening at which the differential conductance begins to roll off. Finally the present time-dependent quantum statistical approach can be generalized to treat three-dimensional systems including both the elastic- and inelastic-scattering effects.

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