ac Conductance of a Double-Barrier Resonant Tunneling System under a dc-Bias Voltage

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An analytical path-integral method based on the nonequilibrium Green's function is developed to investigate the linear response of a double-barrier resonant-tunneling system under a small ac signal which is superimposed upon a dc bias. When the dc-bias voltage is zero, our calculated ac conductance reduces back to that of a recent Kubo-formula study. When the system is biased at the negative differential resistance point, both the real (negative) conductance and imaginary part of admittance are derived. Comparisons with previous numerical study and experiments are discussed.

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Since its conception by Tsu and Esaki[1] and the experimental realization by Sollner *et al.*,[2] the double-barrier resonant-tunneling system (DBRTS) has been the focus of intense experimental and theoretical investigations.[3-15] On one hand, this is due to its technological importance. On the other hand, DBRTS provides us with an ideal prototype system where nonequilibrium and quantum effects of a small-sized open system may become significant. The steady-state properties[1-7,11,12] of DBRTS are mainly characterized by an I-V curve shown in Fig. 1 where a regime of pronounced negative differential resistance (NDR) appears. Of particular importance is the time-dependent behavior[4,6,8-10,13-15] of such a system. Specifically, the frequency-dependent response of DBRTS to a small ac signal $u(t) \sim u_0 e^{-i\Omega t}$ superimposed upon a dc-bias voltage V needs to be investigated by a fully time-dependent quantum-statistical treatment. Very recently, Jacoboni and Price have presented a study of frequency dependence of resonant-tunneling conductance[15] at zero bias $V=0$ (see point a in Fig. 1), which is based upon the Kubo current-current correlation formula. In an earlier work Frensley[13] presented a numerical study of the frequency-dependent admittance $Y(\Omega)$ of DBRTS biased in the NDR region (see point n in Fig. 1). By numerically solving the Liouville equation for the Wigner distribution function, he was able to calculate both the negative conductance $\sigma(\Omega)$ [real part of $Y(\Omega)$] and the imaginary part of the admittance. While his result for negative conductance is consistent with experimental data,[2,3] the imaginary part of the admittance is 5 orders of magnitude too small to explain the inductance measured.[3,13] In this Letter we present the first analytical approach to the ac response of a DBRTS under a dc-bias voltage. When the bias voltage is set to zero our results for the conductance practically reduce back to the Kubo-formula results of Jacoboni and Price.[15] When the system is biased at NDR, both the conductance and the imaginary part of admittance obtained in the present study are consistent with the main features of the existence experiments.[2,3]

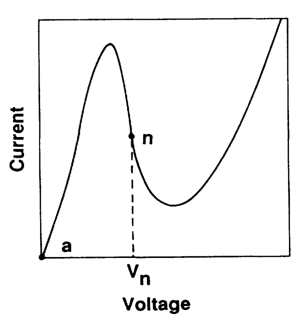

FIG. 1. A typical (qualitative) current-voltage characteristic of DBRTS. a, zero biased; n, biased so that the resonance level is equal to the conduction-band bottom of the emitter electrode.

In order to describe the properties of the DBRTS which is an open system of quantum size, we employ the nonequilibrium Green's-function technique with help of the Feynman path-integral theory.[16] As is well known for numerous systems,[16,17] the path-integral theory is the most elegant way to treat the effect of two electrodes (reservoirs) upon the quantum-well electronic state. The nonequilibrium retarded (advanced) Green's function G_r (G_a) describes the spectrum and dissipation of tunneling electrons; the distribution Green's function $G^<$ carries the distribution information. In Ref. 14, we have derived the nonequilibrium Green's functions for a DBRTS under a given dc-bias voltage V. In the following discussion, we first study the linear response of the nonequilibrium Green's functions due to a small ac signal voltage $u(t)$ superimposed on V. Then we shall calculate the induced ac current from which the conductance and the imaginary part of the admittance will be easily obtained.

A DBRTS can be represented by the following one-dimensional many-body Hamiltonian[7,12,14] $H+H'$:

$$H=\sum_k \epsilon_k^L a_k^\dagger a_k + \epsilon_c c^\dagger c + \sum_p \epsilon_p^R b_p^\dagger b_p + \sum_k (T_{Lk} c^\dagger a_k + T_{Lk}^* a_k^\dagger c) + \sum_p (T_{Rp} b_p^\dagger c + T_{Rp}^* c^\dagger b_p) , \quad (1)$$

$$H'(t) = c^\dagger c[-\alpha e u(t)] + \sum_p b_p^\dagger b_p [-eu(t)] , \quad (2)$$

with a_k ($a_k^\dagger$), c ($c^\dagger$), and b_p ($b_p^\dagger$) being, respectively, the annihilation (creation) operators of electrons (fermions) in the left electrode, in the central quantum well, and in the right electrode. $\epsilon_c = \epsilon_0 - \alpha eV$ (α is structure dependent, $\alpha \simeq 0.5$ for a symmetrical structure) is the resonance level as affected by the dc bias. $\epsilon_k^L = k^2/2m$ and $\epsilon_p^R = p^2/2m - eV$ are the single-particle energy of the left and right electrodes, respectively. 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 energy starting point is arbitrary, e.g., it can also be chosen as the conduction-band bottom of the right electrode or the resonance level, but the physical result remains invariant.) The fourth and the fifth terms of Eq. (1) 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 effect of the bias V. $H'(t)$ is the perturbation due to the ac signal $u(t)$ which is superimposed upon 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 follows:

$$\rho = \exp\left[-\beta \sum_k (\epsilon_k^L - \mu_L) a_k^\dagger a_k\right] \rho_c \times \exp\left[-\beta \sum_p (\epsilon_p^R - \mu_R) b_p^\dagger b_p\right], \tag{3}$$

where $1/\beta$ is the temperature of the system. The left- and right-electrode systems are separate 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 which still needs 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, it also allows us to work out analytically the statistical average with a nonequilibrium density matrix as shown in Eq. (3) 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 thermocounterparts.[16,18]

The nonequilibrium steady-state solution of this tunneling problem without the ac signal $u(t)$ has been presented in Ref. 14. The retarded and advanced Green's functions for the central quantum-well electrons were found to be

$$G_{r(a)}(\omega) = [\omega - \epsilon_c + (-1) i\gamma(\omega)]^{-1}. \tag{4}$$

The distribution Green's function $G^<(t_1 - t_2) = i\langle c^\dagger(t_2) c(t_1)\rangle$ is given by

$$G^<(\omega) = F(\omega)[G_r(\omega) - G_a(\omega)], \tag{5}$$

where $F(\omega)$ is the nonequilibrium distribution function of tunneling electrons,

$$F(\omega) = [\gamma_L(\omega) f_L(\omega) + \gamma_R(\omega) f_R(\omega)]/\gamma(\omega), \tag{6}$$

with $\gamma(\omega) = \gamma_L(\omega) + \gamma_R(\omega)$ being the resonance-level broadening due to the tunneling coupling: $\gamma_L(\omega) = \sum_k |T_{Lk}|^2 \pi\delta(\omega - \epsilon_k^L)$ and $\gamma_R(\omega) = \sum_p |T_{Rp}|^2 \pi\delta(\omega - \epsilon_p^R)$. $f_L(\omega)$ and $f_R(\omega)$ are the Fermi-Dirac distribution functions of the two electrode subsystems with chemical potentials μ_L and μ_R. When a small ac signal $u(t)$ is applied, the system will have a linear response with respect to the above-described nonequilibrium steady state.

In the presence of a time-dependent field, the electric current flowing into the quantum well $I_L(t) = -ie\langle [H, \sum_k a_k^\dagger(t) a_k(t)]_- \rangle$ is not equal to that flowing out of the well $I_R(t) = ie\langle [H, \sum_p b_p^\dagger(t) b_p(t)]_- \rangle$ and the accumulation of electrons in the well occurs. The terminal current in accordance with the Ramo-Shockley theorem[13,15,19] is given by $I = (I_L + I_R)/2$:

$$I(t) = -\frac{ie}{2}\left\langle \sum_k [T_{Lk} c^\dagger(t) a_k(t) - T_{Lk}^* a_k^\dagger(t) c(t)] + \sum_p [T_{Rp} b_p^\dagger(t) c(t) - T_{Rp}^* c^\dagger(t) b_p(t)] \right\rangle. \tag{7}$$

In the path-integral formalism,[17,18] quantum-statistical average can be expressed as[14,16]

$$\langle (\cdot) \rangle = \mathrm{Tr}[\rho(\cdot)] = \int [da_k^\dagger][da_k] \int [db_p^\dagger][db_p] \int [dc^\dagger][dc] (\cdot) \exp\left[i \int_p dt [L(t) - H'(t)] \right], \tag{8}$$

where

$$L(t) = \sum_k a_k^\dagger(t) i\partial_t a_k(t) + \sum_p b_p^\dagger(t) i\partial_t b_p(t) + c^\dagger(t) i\partial_t c(t) - H(t) \tag{9}$$

is the Lagrangian of the total system without ac perturbation H' and $\int_p dt = \int_{-\infty}^{+\infty} dt_+ + \int_{+\infty}^{-\infty} dt_-$ is integration along the closed time path.[14,18] In order to calculate the ac current $i(t)$ induced by the small signal $u(t)$, we expand the functional integral in Eq. (7) as defined by Eq. (8) to the linear order in H' [thus linear in $u(t)$]. Then it is straightforward to obtain the following linear-response result for $i(t)$,

$$i(t) = -\frac{ie}{2}\int [da_k^\dagger][da_k]\int [db_p^\dagger][db_p]\int [dc^\dagger][dc](-i)\int_p dt' \left(\sum_k [T_{Lk}c^\dagger(t)a_k(t) - T^*_{Lk}a_k^\dagger(t)c(t)] + \sum_p [T_{Rp}b_p^\dagger(t)c(t) - T^*_{Rp}c^\dagger(t)b_p(t)]\right) \times H'(t')\exp\left[i\int_p dt\, L(t)\right]. \quad (10)$$

Carrying out the path integrations in Eq. (10) enables us to find the desired admittance $Y(\Omega)$ as a function of frequency Ω: $i(\Omega)=Y(\Omega)u(\Omega)$, which can be expressed in terms of the nonequilibrium steady-state Green's functions. The detailed calculation and the general expression for $Y(\Omega)$ are rather lengthy and shall be presented in a later publication. However, when the temperature is zero and the system is biased at some special points (for example, points a and n in Fig. 1), the expressions for the conductance $\sigma(\Omega)=\mathrm{Re}Y(\Omega)$ and for the imaginary part of the admittance may become rather simple. For instance, with 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., $\epsilon_c=\mu_L=\mu_R$, the conductance and the imaginary part of the admittance can be shown to reduce to the following compact forms:

$$\frac{\sigma(\Omega)}{|\sigma(0)|} = \frac{(16\gamma_L\gamma_R+\Omega^2)\gamma^3}{4\gamma_L\gamma_R(\Omega^2+4\gamma^2)\Omega}\tan^{-1}\left(\frac{\Omega}{\gamma}\right) + \frac{(\gamma_L-\gamma_R)^2\gamma^2}{4\gamma_L\gamma_R(\Omega^2+4\gamma^2)}\ln\left(1+\frac{\Omega^2}{\gamma^2}\right), \quad (11)$$

$$\frac{\mathrm{Im}Y(\Omega)}{|\sigma(0)|} = \frac{(16\gamma_L\gamma_R+\Omega^2)\gamma^3}{8\gamma_L\gamma_R(\Omega^2+4\gamma^2)\Omega}\ln\left(1+\frac{\Omega^2}{\gamma^2}\right) - \frac{(\gamma_L-\gamma_R)^2\gamma^2}{2\gamma_L\gamma_R(\Omega^2+4\gamma^2)}\tan^{-1}\left(\frac{\Omega}{\gamma}\right). \quad (12)$$

In Eqs. (11) and (12) and in the following, $\gamma=\gamma(\epsilon_c)$ and $\gamma_{L(R)}=\gamma_{L(R)}(\epsilon_c)$. The numerical results for Eqs. (11) and (12) are shown in Fig. 2. There the solid curve, which corresponds to the frequency-dependent conductance [Eq. (11)], coincides exactly with that of a Kubo-formula study.[15] 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. 2 with the increasing frequency. The characteristic frequency for this behavior is given by the resonance-level broadening $\Omega_0=2\gamma$. When $\Omega > \Omega_0$, tunneling electrons will not be able to follow the applied field and the tunneling current vanishes.

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., $\epsilon_c=\epsilon^L_{k=0}=0$, the negative conductance $\sigma(\Omega)$ and imaginary part of the admittance $\mathrm{Im}Y(\Omega)$ are derived to have the following expressions:

$$\frac{\sigma(\Omega)}{|\sigma(0)|} = -\frac{\gamma_R+\xi(\gamma+\gamma_R)}{4\gamma_R}\frac{\gamma}{\Omega}\tan^{-1}\left(\frac{\Omega}{\gamma}\right) + \frac{\xi\gamma}{8\gamma_R}\ln\left(1+\frac{\Omega^2}{\gamma^2}\right) - \frac{\gamma+\xi(\gamma+\gamma_R)}{4\gamma_R}\frac{\gamma}{\Omega}\tan^{-1}\left(\frac{\Omega}{\gamma_R}\right) + \frac{\xi\gamma}{8\gamma_R}\ln\left(1+\frac{\Omega^2}{\gamma_R^2}\right), \quad (13)$$

$$\frac{\mathrm{Im}Y(\Omega)}{|\sigma(0)|} = -\frac{\gamma_R+\xi(\gamma+\gamma_R)}{4\gamma_R}\frac{\gamma}{2\Omega}\ln\left(1+\frac{\Omega^2}{\gamma^2}\right) + \frac{\xi\gamma}{4\gamma_R}\tan^{-1}\left(\frac{\Omega}{\gamma}\right) - \frac{\gamma+\xi(\gamma+\gamma_R)}{4\gamma_R}\frac{\gamma}{2\Omega}\ln\left(1+\frac{\Omega^2}{\gamma_R^2}\right) + \frac{\xi\gamma}{4\gamma_R}\tan^{-1}\left(\frac{\Omega}{\gamma_R}\right), \quad (14)$$

with

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

It is easy to check that σ and $\mathrm{Im}Y$ in Eqs. (13) and (14) as well as in Eqs. (11) and (12) are related by the Hilbert transform (Kramers-Kronig relation). For a symmetrical DBRTS, one has $\gamma_L=\gamma_R$ at $V=0$. However, γ_R may become much larger than γ_L when a dc bias is applied. In Fig. 3 we plot the conductance and imaginary part of the admittance as functions of frequency Ω for such a symmetrical structure. The differential conductance (negative) $\sigma(\Omega)$ rolls off with a characteristic frequency given by the width of resonance level $\Omega_0=\gamma+\gamma_R$ and continues to be significantly negative until $\Omega\sim$ several Ω_0. (For example, for a symmetrical structure with parameters[2,10] barrier width 50 Å, well width

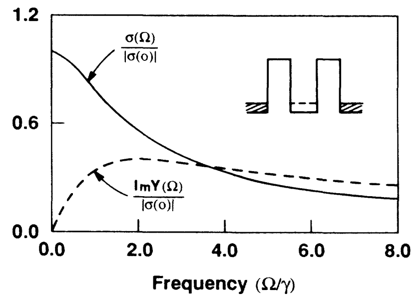

FIG. 2. Frequency-dependent conductance and imaginary part of admittance of DBRTS with zero bias. The system is symmetrical so that $\gamma_L = \gamma_R = 0.5\gamma$.

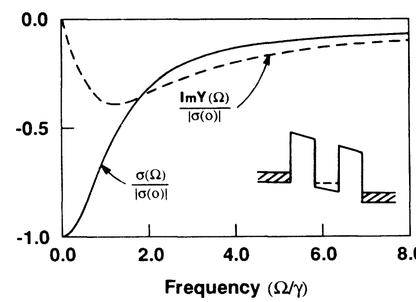

FIG. 3. Frequency-dependent conductance and imaginary part of admittance of DBRTS biased at NDR ($V = V_n$ so that $\epsilon_c = \epsilon_k^L{}_{=0} = 0$). The system is symmetrical and it becomes very asymmetrical when biased: $\gamma_L = 0.001\gamma$ and $\gamma_R = 0.999\gamma$.

50 Å, and barrier height 0.23 eV, Ω_0 is around 10^{12} $\sec^{-1}$.) This behavior agrees with a previous numerical investigation[13] and is consistent with the main feature of experiments (e.g., Refs. 2 and 3). The imaginary part of the admittance is shown as the dashed curve in Fig. 3, which matches with the experimental results[3,13] as far as its magnitude is concerned.

In conclusion, we have presented in this Letter the first analytical investigation of the frequency-dependent conductance and imaginary part of admittance of a DBRTS with zero bias and biased at NDR point. Our approach to this problem is based upon the Feynman path-integral theory and the nonequilibrium Green's-function method. It not only produces the frequency dependences of the conductances in agreement with previous numerical studies[13,15] and consistent with existent experiments,[2,3] it also consistently yields the imaginary part of the admittance which has not been successfully studied previously.

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