Time-dependent approach to resonant tunneling and inelastic scattering

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A time-dependent approach is applied to the resonant-tunneling problem. The time dependence of the accumulated charge and the tunneling current are calculated. Special attention is given to the effect of inelastic scattering on the resonant-tunneling process. The coherent and incoherent contributions to the total current are found, and are shown to modify it, sometimes in an unexpected manner.

The tunneling of carriers through potential barriers is a very important and well-studied quantum-mechanical phenomenon. It is remarkable, however, that the process of penetration through double-potential barriers—resonant tunneling—received almost no attention until the seminal work of Tsu and Esaki,[1] which has stimulated intensive theoretical and experimental work on the subject. Nevertheless, some fundamental questions concerning the nature of carriers transport by resonant tunneling remain to be settled. Two such questions are the role played by inelastic scattering and the time evolution of the process.

Usually resonant tunneling is treated in a time-dependent framework using the transfer-matrix technique.[2-4] This approach starts with a free wave at infinity impinging on a double-barrier potential that traps it in the region between the two barriers. The trapped wave undergoes multiple reflections off the two barriers. As a result the total transmission probability peaks at certain energies which correspond to the quasistationary states of the double-barrier potential. The accounting of multiple reflections in this framework is a rather delicate procedure, especially when inelastic processes randomize the phases between them. Furthermore, it is hard to reconstruct the time development of the system. Therefore, there are conflicting descriptions of the transport through the structure,[2-5] and different predictions regarding some measurable quantities, like the charge buildup due to the carrier trapping.[5-8]

Actually, the resonant state resembles a bound state more than a scattering state. In fact, the bound-state wave function in the potential well between the two barriers already includes all multiple reflections of the trapped wave. It is therefore very attractive to build up the resonant state from the bound-state wave functions rather than from free waves propagating back and forth, thus avoiding the need to account for the multiple-reflections terms. Such an approach has been proposed in Refs. 9–11 for treating the decay of a quasistationary state, and indeed was shown to be much simpler for applications than other techniques. An advantage of this approach is that it also directly reproduces the time dependence of a system during the tunneling process.

In this paper we extend this time-dependent approach to the resonant-tunneling problem. We find the time dependence of the accumulated charge and the tunneling current. Special attention is given to the role of inelastic processes which cause the phase randomization in the resonant tunneling. We calculate explicitly the coherent and incoherent contributions to the total current and show that these inelastic processes always increase the total current through the structure.

To demonstrate this approach we start with the problem of tunneling from a narrow quantum well to continuum through a single potential barrier, Fig. 1. The quantum well, on the left side, contains only one level and the continuum is represented by a large well to the right which contains very dense levels, such that when $L_R \to \infty$, we have a true continuum. We have shown[9,10] that the time evolution of the system can be expressed in terms of an effective wave function $\psi(t)=(b_0(t),\mathbf{b}_R(t))$. Here $b_0(t)$ is the probability amplitude to find the system at time t in the energy level E_0 corresponding to the eigenstate $\Phi_0(x)$ of the narrow-well Hamiltonian, where the barrier thickness is taken to be infinite. The vector $\mathbf{b}_R(t)=(b_R^1,\ldots,b_R^n)$, where b_R^j is similarly defined as the probability amplitude to find the system at time t in the energy level E_R^j corresponding to the eigenstate $\chi_j(x)$ of the right large well Hamiltonian, where the barrier thickness is again infinite. Then the time dependence of ψ is given by the following effective Schrödinger equation:

$$i\frac{d}{dt}\begin{bmatrix} b_0(t) \\ \mathbf{b}_R(t)\end{bmatrix} = \begin{bmatrix} E_0 & \underline{\Omega}_R \\ \underline{\Omega}_R^\dagger & \underline{H}_R \end{bmatrix} \begin{bmatrix} b_0(t) \\ \mathbf{b}_R(t)\end{bmatrix}, \tag{1}$$

where $(\underline{H}_R)_{ij}=E_R^j\delta_{ij}$, $\underline{\Omega}_R=(\Omega_R^1,\ldots,\Omega_R^n)$ is a row matrix, and $\underline{\Omega}_R^\dagger$ is the transposed (column) matrix. Ω_R^j is the coupling between the level E_0 in the narrow well and the level E_R^j in the right well. For $E_R^j=E_0$ the coupling Ω_R^j is given by[9]

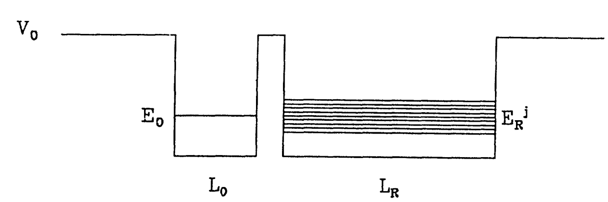

FIG. 1. Tunneling from the quasistationary level E_0 to continuum.

$$\Omega_R^j=\frac{\alpha}{m}\Phi_0(x_0)\chi_j(x_0)\ , \tag{2}$$

where x_0 is some point between the wells (the final result is not sensitive to the choice of x_0), and $\alpha=[2m(V_0-E_0)]^{1/2}$. If $E_R^j\neq E_0$ there is an additional correction term proportional to the integral over the overlap of Φ_0 and χ_j. It is of the order $\varepsilon\Omega_R^j/V_0$, where $\varepsilon=E_R^j-E_0$. If $\varepsilon\sim\Omega_R^j$ this term can be neglected. Note that we have adapted units where $\hbar=1$.

Solving Eq. (1) (by employing the Laplace transformation) one obtains in the continuum limit ($L_R\to\infty$) that the probability to find the system in the small well decreases exponentially: $|b_0(t)|^2=\exp(-\Gamma_0 t)$, with the exponential factor $\Gamma_0=2\pi[\Omega_R(E_0)]^2\rho_R(E_0)$, where $\rho_R(E)$ is the density of states in the right well, and $\Omega_R(E_0)\equiv\Omega_R^j$ for $E_R^j=E_0$, Eq. (2).

Let us now apply our approach to the problem of resonant tunneling through the double-barrier potential, Fig. 2(a). As before we represent the continuum at the two sides by two large wells, which contain a dense spectrum of energy levels, E_L^j and E_R^k for the left and right wells, respectively. The narrow quantum well, which is formed between the two barriers, contains only one level, E_0. As in the previous case the time dependence is given by an effective Schrödinger equation

$$i\frac{d}{dt}\begin{bmatrix}\mathbf{b}_L(t)\\ b_0(t)\\ \mathbf{b}_R(t)\end{bmatrix}=\begin{bmatrix}\underline{H}_L & \underline{\Omega}_L^\dagger & 0\\ \underline{\Omega}_L & E_0 & \underline{\Omega}_R\\ 0 & \underline{\Omega}_R^\dagger & \underline{H}_R\end{bmatrix}\begin{bmatrix}\mathbf{b}_L(t)\\ b_0(t)\\ \mathbf{b}_R(t)\end{bmatrix}. \tag{3}$$

Comparing Eq. (3) to Eq. (1) we see the additional terms related to the left (L) well: $\mathbf{b}_L=(b_L^1,\dots,b_L^n)$ is the probability amplitude to find the system in the left well, $(\underline{H}_L)_{ij}=E_L^j\delta_{ij}$, and $\underline{\Omega}_L=(\Omega_L^1,\dots,\Omega_L^n)$ represents the coupling between the levels E_L^j in the left well and the level E_0 in the narrow well.

Consider the electrons initially localized in the left well with the occupation function $f(E_L^j)$. First we look for the charge accumulated in the small well during the tunneling. We denote $B_{j,0}(t)$ as the probability amplitude for an electron which was initially in the left well at the level j, to be found in the narrow well at time t. [$B_{j,0}(t)=b_0(t)$ is the solution of Eq. (3) with the initial condition $b_L^i(0)=\delta_{ij}$, $b_0(0)=0$, $b_R^i=0$.] We can easily show that the accumulated charge in the narrow well at time t is given by

$$\sigma(t)=\frac{qm}{\pi}\sum_j f(E_L^j)(E_F-E_L^j)|B_{j,0}(t)|^2\ , \tag{4}$$

where q and m are the electron charge and mass, and E_F is the Fermi energy. The factor $m(E_F-E_L^j)/\pi$ appears from the integration over the transverse electron momenta. Replacing the sum by an integral for the dense electron states [$\sum_j\to\int\rho(E)dE$] one obtains from Eqs. (3) and (4)

$$\sigma(t)=\frac{qm}{2\pi^2}\int_0^{E_F}dE\,f(E)(E_F-E)\frac{\Gamma_L}{(E-E_0)^2+\gamma^2}\times\{1-2\cos[(E_0-E)t]e^{-\gamma t}+e^{-2\gamma t}\}\ . \tag{5}$$

Here $\gamma=\Gamma/2$, where

$$\Gamma=\Gamma_L+\Gamma_R=2\pi[\Omega_L^2(E_0)\rho_L(E_0)+\Omega_R^2(E_0)\rho_R(E_0)] \tag{6}$$

is the total width of the quasistationary state E_0 due to tunneling into the left and right large wells. The energy shift is included into E_0, and we assumed that $\Omega(E)$ and $\rho(E)$ vary slowly near the resonance.

To find the current we use the following procedure: We first calculate the probability amplitude $B_{j,k}(t)$ for transition from the level E_L^j in the left well to the level E_R^k in the right well. Then we calculate the accumulated charge $Q_R(t)$ in the right well according to Eq. (4), where the amplitude $B_{j,0}$ is replaced by $B_{j,k}$, and we sum on all j's and k's. The current which flows in the right well is defined as $J(t)=dQ_R(t)/dt$. Carrying out the calculations we get

$$J(t)=\frac{qm}{2\pi^2}\int_0^{E_F}dE\,f(E)(E_F-E)\frac{\Gamma_L\Gamma_R}{(E-E_0)^2+\gamma^2}\times\{1-2\cos[(E_0-E)t]e^{-\gamma t}+e^{-2\gamma t}\}\ . \tag{7}$$

It can be seen that in the limit of $t\to\infty$, Eq. (7) coincides with the result for the current obtained in the transfer-matrix approach.[4]

If all the levels in the left well are populated [$f(E)=1$], and the resonant level E_0 is not close to the integration limits, one can integrate Eqs. (5) and (7) and obtain the accumulated charge and current densities

$$\sigma(t)=\frac{qm(E_F-E_0)}{\pi}\frac{\Gamma_L}{\Gamma}(1-e^{-\Gamma t})\ , \tag{8a}$$

$$J(t)=\frac{qm(E_F-E_0)}{\pi}\frac{\Gamma_L\Gamma_R}{\Gamma}(1-e^{-\Gamma t})\ . \tag{8b}$$

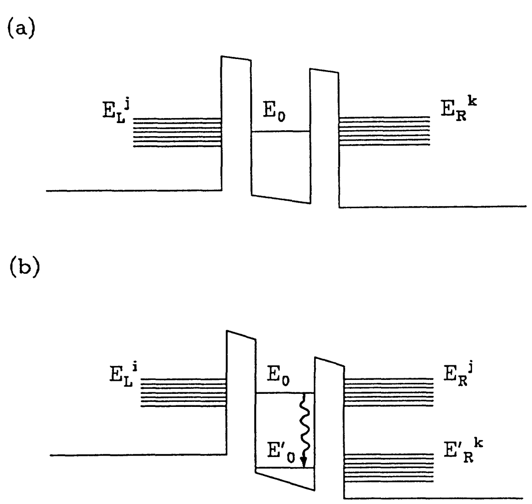

FIG. 2. Resonant tunneling through the double-barrier potential (a) without and (b) with inelastic scattering.

It is interesting to note that the time development of the system is governed by the total decay width of the level E_0. However, the ratio between $\sigma(t)$ and $J(t)$, which is commonly assumed[7,8] to be the total tunneling time $1/\Gamma$ is in fact given by $\sigma/J=1/\Gamma_R$, i.e., it is related to the exit barrier only. This was indeed observed in recent experiment.[12]

We now apply our technique to analysis of the interesting problem of the effect of inelastic scattering on the resonant-tunneling process. To approach this problem it is very important to find a model which on the one hand is quite general to bear essential features of inelastic events and on the other hand can be tested experimentally. Such a model is shown in Fig. 2(b). Here the narrow well contains two levels, an upper one E_0 and a lower one E_0'. An electron which tunnels from the large left well into the upper level E_0 can either relax inelastically into the lower state and then tunnel out into the right well, or tunnel out directly into the right well. We shall assume in the following that the inelastic process is phonon emission, but the analysis holds for any inelastic process. Similar to the previous case the time behavior of the system is given by an effective Schrödinger equation[10,11]

$$i\frac{d}{dt}\begin{bmatrix}\mathbf{b}_L(t)\\ b_0(t)\\ \mathbf{b}_R(t)\\ \mathbf{c}_0(t)\\ \mathbf{c}_R(t)\end{bmatrix}=\begin{bmatrix}\underline{H}_L & \underline{\Omega}_L^\dagger & 0 & 0 & 0\\ \underline{\Omega}_L & E_0 & \underline{\Omega}_R & \underline{\Omega}_{\text{ph}} & 0\\ 0 & \underline{\Omega}_R^\dagger & \underline{H}_R & 0 & 0\\ 0 & \underline{\Omega}_{\text{ph}}^\dagger & 0 & E_0'\underline{I}+\underline{H}_{\text{ph}} & \underline{\Omega}_R'\odot\underline{I}\\ 0 & 0 & 0 & \underline{\Omega}_R'^\dagger\odot\underline{I} & \underline{H}_R'+\underline{H}_{\text{ph}}\end{bmatrix}\begin{bmatrix}\mathbf{b}_L(t)\\ b_0(t)\\ \mathbf{b}_R(t)\\ \mathbf{c}_0(t)\\ \mathbf{c}_R(t)\end{bmatrix}, \tag{9}$$

where $c_0\equiv\{c_0^l\}$ and $c_R\equiv\{c_R^{k,l}\}$ are the probability amplitudes to find the electron at the level E_0' in the narrow well and at the level $E_R'^k$ in the right well, respectively, where the phonon $|l\rangle$ with the energy ε_l is emitted. $\underline{\Omega}_{\text{ph}}\equiv\{\Omega_{\text{ph}}^l\}$ couples the two levels of the narrow well by the emission of a phonon $|l\rangle$, and is given by $\Omega_{\text{ph}}^{(l)}=\langle\Phi_0',l|V_{\text{ph}}|\Phi_{0,}0\rangle$, where V_{ph} represents the electron-phonon interaction. [The transitions $\langle\Phi_0',k|V_{\text{ph}}|\Phi_0',k'\rangle$ which influence the final result only to the third order of V_{ph} are neglected in Eq. (9).] $\underline{H}_{\text{ph}}$ and $\underline{H}_R'$ are diagonal matrices with the matrix elements ε_l and $E_R'^k$, respectively, and $\underline{I}$ is the unit matrix. The submatrix $\underline{\Omega}'_R\odot\underline{I}$ is obtained from the unit matrix by replacing each diagonal element by $\underline{\Omega}_R'=(\Omega_R'^1,\ldots,\Omega_R'^n)$, and represents the coupling of the levels E_0' and $E_R'^k$ by tunneling [Eq. (2)].

Notice that Eq. (9) takes into account only the *dominant inelastic* processes (the relaxation to the level E_0') in which the electron *remains* in the quantum well. Another process is the so-called phonon-assisted tunneling, where the electron emits a phonon and makes a transition from the narrow-well state $|\Phi_0,0\rangle$ to a continuum state $|\chi_j,l\rangle$. This process is very weak since it is proportional to $\langle\chi_j,l|V_{\text{ph}}|\Phi_0,0\rangle\sim\Omega_R\Omega_{\text{ph}}$ and we neglect it. In fact, it was considered in detail in Ref. 4 and was shown to have no effect on the total current.

Solving Eq. (9) with the same procedure as in the previous case we can determine the accumulated charge and the tunneling current in this system. The current $J(t)$ through the structure can be written as $J(t)=J_1(t)+J_2(t)=(dQ_1/dt)+(dQ_2/dt)$, where Q_1 and Q_2 are the charges accumulated in the right well due to tunneling from the levels E_0 and E_0', respectively. For a case where all the levels in the left well are populated $[f(E_L)=1]$ one obtains

$$J_1(t)=\frac{qm(E_F-E_0)}{\pi}\frac{\Gamma_L\Gamma_R}{\Gamma_T}(1-e^{-\Gamma_T t}), \tag{10a}$$

$$J_2(t)=\frac{qm(E_F-E_0)}{\pi}\frac{\Gamma_L\Gamma_{\text{ph}}}{\Gamma_T}\times\left[1-\frac{\Gamma_T e^{-\Gamma_R' t}-\Gamma_R' e^{-\Gamma_T t}}{\Gamma_T-\Gamma_R'}\right], \tag{10b}$$

where $\Gamma_T=\Gamma_L+\Gamma_R+\Gamma_{\text{ph}}$. Here $\Gamma_{\text{ph}}=2\pi|\Omega_{\text{ph}}^{(l)}|^2\rho_{\text{ph}}(\varepsilon_l)$ is the inelastic width, $\rho_{\text{ph}}(\varepsilon)$ is the density of photon states, and $\varepsilon_l=E_0-E_0'$. Therefore, the total steady-state current at $t\to\infty$ is given by

$$J=J_1+J_2=\frac{qm(E_F-E_0)}{\pi}\frac{\Gamma_L(\Gamma_R+\Gamma_{\text{ph}})}{\Gamma_T} \tag{11}$$

and is independent of the tunneling width Γ_R'. Note, however, that if $\Gamma_R'=0$ it follows from Eq. (10b) that $J_2(t)\equiv 0$. If the levels in the left well are not fully occupied we obtain a more general result

$$J=\frac{qm}{2\pi^2}\int_0^{E_F}dE\, f(E)(E_F-E)T(E), \tag{12}$$

where

$$T(E)=\frac{\Gamma_L(\Gamma_R+\Gamma_{\text{ph}})}{(E-E_0)^2+(\Gamma_T/2)^2} \tag{13}$$

is the total transmission through the structure. Comparing Eqs. (11) and (12) with Eqs. (7) and (8) in the limit of $t\to\infty$, one finds that inelastic processes modify the resonance current by replacing the outgoing width Γ_R by the total outgoing width $\Gamma_R+\Gamma_{\text{ph}}$.

Our analysis clarifies the essential nature of true phase randomizing inelastic events in electron transport. Furthermore, it can help us assess their influence on the total current in resonant tunneling. Let us first consider the surprising absence of Γ'_R dependence in Eqs. (11) and (12). It indicates that the total stationary current J does not depend on subsequent processes which happened after the electron relaxation to the level E'_0. The reason is the high density of final states of the electron-phonon system $\{c_0^l\}$, which makes the process irreversible and therefore disconnects the *inelastic flux* from the initial channel. This irreversibility is the essential characteristic of a true incoherent process. In fact, the emission of a phonon is just an example for any transition inside the well with a high density of final states, such as scattering by irregularities in the potential leading to energy transfer into transversal motion. It is remarkable, however, that the Γ'_R dependence does nevertheless appear in the transient behavior of the tunneling current $J(t)$, as is evident from Eqs. (10).

Let us assess the influence of inelastic processes on the total current. An important consequence of Eq. (13) is that the integrated transmission

$$\int T(E)dE = 2\pi \frac{\Gamma_L(\Gamma_R+\Gamma_{ph})}{\Gamma_L+\Gamma_R+\Gamma_{ph}} \tag{14}$$

[and hence the total current, Eq. (11)] *always increases* with Γ_{ph}. This finding is in contrast to a commonly assumed sum rule that the integrated transmission is independent of the inelastic width.[3] The difference originates from the phenomenological assumption of Ref. 3 that only the transmitted part of the inelastic processes should be included in the total transmission.[13]

Finally, to demonstrate the application of our analysis to the practical case of the double-barrier resonant-tunneling diode, let us consider two extreme cases, $\Gamma_{ph} \ll \Gamma_L, \Gamma_R$—the so-called coherent limit (J_{coh}), and $\Gamma_{ph} \gg \Gamma_L, \Gamma_R$—the so-called incoherent (sequential) limit (J_{inc}). It is evident from Eq. (11) that $J_{coh} \sim \Gamma_L\Gamma_R/(\Gamma_L+\Gamma_R)$, whereas J_{inc} is always $\sim\Gamma_L$. Therefore, when $\Gamma_R \gg \Gamma_L$, as is the case in the resonant-tunneling diode under bias, Fig. 2(b), $J_{coh} \approx J_{inc}$, and inelastic scattering does not change appreciably the total current. However, when $\Gamma_L \gg \Gamma_R$ we get that $J_{coh} \sim \Gamma_R$ while $J_{inc} \sim \Gamma_L$. It follows that even though the transmission peak $T(E_0)$ of Eq. (13) is strongly suppressed in the incoherent limit, the total current in that limit increases such that $J_{inc} \gg J_{coh}$. Such a considerable increase of the resonant-tunneling current in the presence of inelastic scattering can be verified experimentally.

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[13] If the total inelastic-scattering term [Eq. (6) of Ref. 3] is included, one gets an expression for T which is identical to our result for the symmetric barriers case, Eq. (12) ($\Gamma_R=\Gamma_L=\Gamma_e/2$, where Γ_e is the phenomenological elastic width of Ref. 3).