Nonlinear resonant tunneling in systems coupled to quantum reservoirs

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An adiabatic approximation in terms of instantaneous resonances is developed to study the steady-state and time-dependent transport of interacting electrons in biased resonant-tunneling heterostructures. The resulting model consists of quantum reservoirs coupled to regions where the system is described by nonlinear ordinary differential equations and has a general conceptual interest. [S0163-1829(97)04311-7]

The mathematical method recently proposed in Ref. 1 provides a significant advance in the solution of time-dependent scattering problems for Schrödinger equations with nonlinearities concentrated near the resonances of the corresponding potential. The method consists in the separation of the original system in two coupled subsystems through the splitting of the wave function in two components. In this way, we can separately study the simple problem of a reservoirlike subsystem having only extended states and couple its solution to the other subsystem having resonance states. The solution of this second problem is then simplified by an adiabatic approximation in terms of instantaneous resonances.

The situation investigated in Ref. 1 depicts ballistic transport in a double-barrier heterostructure, i.e., the scattering of a wave-packet on a double-barrier potential. The nonlinearity, concentrated in the well between the barriers, is due to the interaction of the electrons represented by the wave packet (mean field). Here, we generalize the approach[1] to the case of biased heterostructures where a band of scattering states are to be considered. For these systems, hysteresis in the current-voltage characteristics has been observed[2] and recognized as a consequence of the mutual interaction of the electrons trapped in the resonance.[2,3] We show that the approach[1] allows us to quantitatively reproduce experimental results like[4] and predict new time-dependent properties. Although illustrated in the case of heterostructures, these results are very general and have applications in fields like the theory of electric systems[5] and nonlinear optics.[6,7]

Let us consider a heterostructure whose conduction band edge profile consists of two barriers of height V_0 located in $[a,b]$ and $[c,d]$ with $a<b<c<d$ along the growth direction x. Translational invariance is assumed in the plane parallel to the junctions. Suppose that a bias energy ΔV is applied between the emitter ($x<a$) and collector ($x>d$) regions uniformly doped with net donor concentration n_D. At thermal equilibrium with temperature T, transport is due to a band of scattering states with Fermi energy $E_F=(3\pi^2 n_D)^{2/3}$ [we use everywhere effective atomic units $\hbar=2m^*=1$ and $e^2/\varepsilon=2a_B^{-1}$, where m^* is the electron effective mass, ε the dielectric constant, and $a_B=\hbar^2\varepsilon/(m^*e^2)$ the effective Bohr radius]. Due to the translational invariance in the plane parallel to the junctions, the single-electron scattering state at energy E along the x direction is described by the one-dimensional Schrödinger equation,

$$[-i\partial_t-\partial_x^2+V_{\rm cb}(x)+U(\phi,x)]\phi(x,t,E)=0, \qquad (1)$$

where $V_{\rm cb}(x)$ is the steplike conduction band edge profile and $U(\phi,x)$ takes into account the applied bias and, at the Hartree level, the electron-electron interaction. Assuming ideal metallic behavior in the emitter and collector regions, i.e., neglecting the formation of accumulation and depletion layers, $U(\phi,x)$ can be obtained as a solution of the Poisson equation,

$$\partial_x^2 U(\phi,x)=-8\pi a_B^{-1}\int dE\; g(E)|\phi(x,t,E)|^2, \qquad (2)$$

with boundary conditions $U(\phi,a)=0$, $U(\phi,d)=-\Delta V$. The parallel degrees of freedom are considered through

$$g(E)=\frac{\Theta(E)}{2\pi}[k_BT\ln(1+e^{(E-E_F)/k_BT})+E_F-E], \qquad (3)$$

where the Heaviside function $\Theta(E)$ limits the integration in (2) to energies above the bottom of the emitter conduction band, $E=0$, as correct for $E_F\ll\Delta V$.

In general, the solution of (2) cannot be handled analytically. We will suppose that, due to the accumulation of electrons in the well with sheet density

$$s(\phi)=\int dE\; g(E)\int_{(a+b)/2}^{(c+d)/2}dx\,|\phi(x,t,E)|^2, \qquad (4)$$

ideal metallic behavior in the well $[b,c]$ and ideal insulating behavior in the barriers $[a,b]$ and $[c,d]$ hold. Then the total potential $V_{\rm cb}+U$ in (1) is better rewritten as $V+W$, where

$$V(x)=[V_0-\Delta V(x-a)/\ell]\ 1_{[a,b]}(x)-\Delta V(b-a)/\ell 1_{[b,c]}(x)+[V_0-\Delta V(b-a+x-c)/\ell]1_{[c,d]}(x)-\Delta V\ 1_{[d,+\infty[}(x) \quad (5)$$

gives the band profile modified by the external bias and

$$W(s,x)=8\pi a_B^{-1}\ s(\phi)\{(x-a)(d-c)/\ell 1_{[a,b]}(x)+(b-a)(d-c)/\ell 1_{[b,c]}(x)+(b-a)(d-x)/\ell 1_{[c,d]}(x)\} \quad (6)$$

depends on the wave function ϕ through the sheet density of electrons in the well $s(\phi)$. Here $\ell=b-a+d-c$ and $1_{[x_0,x_1]}(x)$ is 1 if $x\in[x_0,x_1]$ and 0 otherwise.

Following Ref. 1, we will solve (1) with the potential (5) and (6) in two steps. Let $V_{\rm fill}(x)=V(x)+V_0 1_{[b,c]}(x)$ be the potential obtained by filling the well $[b,c]$. First we solve

$$[-i\partial_t-\partial_x^2+V_{\rm fill}(x)+W(s,x)]\tilde{\mu}(x,t,E)=0 \quad (7)$$

and then we look for ϕ in the form $\phi=\tilde{\mu}+\tilde{\nu}$ where $\tilde{\nu}(x,t,E)$ should solve

$$[-i\partial_t-\partial_x^2+V(x)+W(s,x)]\tilde{\nu}=V_0\ \ 1_{[b,c]}(x)\tilde{\mu}. \quad (8)$$

Substituting (1) with (7) and (8) corresponds to decomposing the original system in quantum reservoirs coherently coupled to a small subsystem. The wave function $\tilde{\mu}$ describes an electron at energy E which is delocalized in the emitter and collector regions (reservoirs) and has an exponentially small probability to be found in the forbidden region $[a,d]$. The wave function $\tilde{\nu}$ describes the same electron in the double-barrier region and is driven by the value of $\tilde{\mu}$ in the well $[b,c]$. Due to the quasilocalization of $\tilde{\nu}$ in $[b,c]$, we have $\phi\simeq\tilde{\mu}$ in the reservoirs and $\phi\simeq\tilde{\nu}$ in the well, with an error which is exponentially small in the limit of wide barriers.[1]

Equation (7) can be solved by evaluating the instantaneous eigenstates of the potential $V_{\rm fill}+W$. We put $\tilde{\mu}(x,t,E)=\exp(-iEt)\mu(x,t,E)$ and suppose that ΔV and s are slowly varying functions of time so that also $\mu(x,t,E)$ is slowly varying in time. In the emitter region $x<a$ we take $\mu(x,t,E)=\mu(x,E)$ as the sum of a left- and right-going plane wave at energy E and propagate this expression to the adjacent regions by requiring μ to be of class C^1. For wide barriers we can use a WKB expansion for the potential $V_{\rm fill}+W$ and explicitly evaluate μ in the region $[b,c]$ which is of interest for solving (8).

Equation (8) can be simplified by developing $\tilde{\nu}$ into the instantaneous eigenstates of the potential $V+W$ and keeping only the contributions from the discrete resonant states.[1] In the case of a single resonant state we put $\tilde{\nu}(x,t,E)=\exp(-iEt)z(t,E)e(s,x)$ where $e(s,x)$ is the (ground) resonant state of the potential $V+W$ with complex eigenvalue $\lambda(s)=E_R(s)-i\Gamma(s)/2$

$$[-\lambda(s)-\partial_x^2+V(x)+W(s,x)]e(s,x)=0. \quad (9)$$

The eigenfunction $e(s,x)$ is of class L^2 on the contour $\gamma\equiv(e^{i\theta}]-\infty,0]+a)\cup[a,d]\cup(d+e^{i\theta}[0,+\infty[)$ for θ conveniently chosen[8] and satisfies $\int_\gamma dx\ e(s,x)^2=1$, $\int_\gamma dx\ e(s,x)\ \partial_s e(s,x)=0$. Multiplying (8) with e and integrating over γ, we get

$$\partial_t z(t,E)=i[E-\lambda(s)]z(t,E)+\mathcal{B}(s,E), \quad (10)$$

with the driving term given by $\mathcal{B}(s,E)=iV_0\int_b^c dx\ \mu(x,t,E)e(s,x)$ and the sheet density (4) reduced, with small error, to

$$s=\int dE\ g(E)|z(t,E)|^2\equiv\|z(t)\|^2. \quad (11)$$

Explicit expressions of $\lambda(s)$ and $e(s,x)$ can be found within the same WKB approximation used for evaluating μ.[9] For later use we note that $E_R(s)=E_R^0+\eta s$, where $E_R^0=E_0-\Delta V(b-a)/\ell$, E_0 being the (ground) eigenstate of the potential $V_0[1_{]-\infty,b]}(x)+1_{[c,+\infty[}(x)]$ and $\eta=8\pi a_B^{-1}(b-a)(d-c)/\ell=e^2/(C_e+C_c)$, C_e and C_c being the emitter and collector capacitance per unit area, respectively. Moreover, $\Gamma(s)=\Gamma_e(s)+\Gamma_c(s)$, Γ_e and Γ_c being the contributions to the resonance width given by the emitter and collector barriers, respectively.

The original problem (1) is reduced to solving the system (10) with the condition (11). Let us first consider the stationary solutions

$$z(E)=\frac{\mathcal{B}(s,E)}{-\Gamma(s)/2+i[E-E_R(s)]}. \quad (12)$$

Equation (11) gives a self-consistency condition for $s=\|z\|^2$. Assuming that $|\mathcal{B}(s,E)|^2$ is a smooth function of E and $\Gamma(s)\ll E_F$, a Dirac δ approximation can be used to get

$$s=f(s)\equiv 2\pi g(E_R(s))|\mathcal{B}(s,E_R(s))|^2\Gamma(s)^{-1}. \quad (13)$$

The function $f(s)$ vanishes everywhere except for $0\leq E_R(s)\leq E_F$ where, for $E_F\ll V_0$ we have $2\pi|\mathcal{B}(s,E_R(s))|^2\simeq\Gamma_e(s)$. Equation (13) is then equivalent to $s\Gamma(s)=g(E_R(s))\Gamma_e(s)$ which has a simple interpretation in terms of charge conservation. In the steady state, the current of electrons injected from the emitter into the well, $g(E_R(s))\Gamma_e(s)$, equilibrates the escaping current, $s\Gamma(s)$. The latter current increases with increasing the sheet density of electrons in the well, s, while the former vanishes at both $E_R(s)=0$ (square root singularity) and $E_R(s)\simeq E_F$. Therefore, Eq. (13) has only one solution for $E_R^0\geq 0$ and may have three for $E_R^0<0$. For $E_R^0\gtrsim E_F$ the unique solution vanishes and for $E_R^0<0$ the couple of nonvanishing solutions is to be searched in the interval $-E_R^0/\eta\leq s\lesssim(-E_R^0+E_F)/\eta$.

In terms of applied bias, multiple solutions of (13) can be obtained for $\Delta V>E_0\ell/(b-a)$. The range of ΔV values for which three solutions exist depends on the amplitude of the function f. If the emitter barrier is more opaque than the collector one, f is suppressed by the factor $\Gamma_e/\Gamma_c\ll 1$ and we always have only one solution.

The solutions of (13) can be characterized in terms of stability. This is particularly important in view of a comparison with steady-state experiments where only stable solutions are measured. By studying the eigenvalues of the linearization of the vector field defined by the r.h.s. of (10) one can demonstrate that a solution of (13) is stable (unstable)

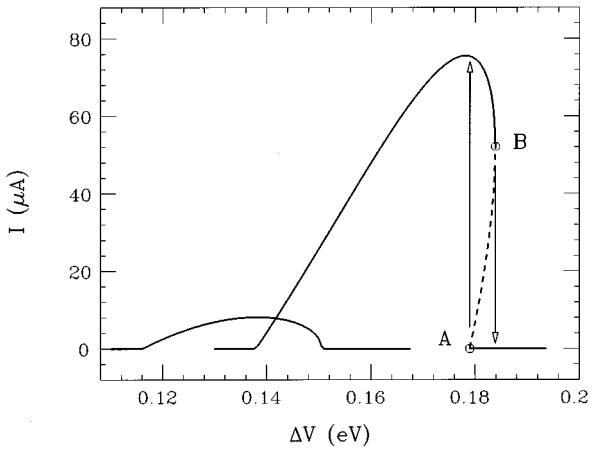

FIG. 1. Theoretical steady-state current-voltage characteristic for the GaAs-$Al_xGa_{1-x}As$ heterostructure experimentally investigated in[4] under forward (right-most curve) and reverse (left-most curve) bias. In the reverse bias case we permuted the barriers instead of making ΔV (and I) negative. In the forward bias case the dashed line is an unstable steady-state solution and arrows indicate the transition expected at the bistability thresholds A and B by decreasing or increasing the bias, respectively. The relevant parameters are $n_D=2\times10^{17}$ cm^{-3}, $T=1$ K, $A=2\times10^{-5}$ cm^2, $m^*=0.067m$, where m is the free electron mass, $\varepsilon=11.44$, $V_0=0.34$ eV, $b-a=9.0$ nm, $c-b=5.6$ nm, and $d-c=10.7$ nm Ref. 10.

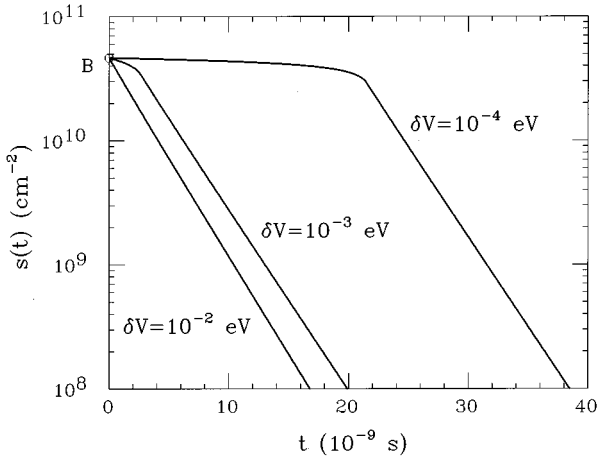

FIG. 2. Sheet density of electrons in the well $s(t)$ after an instantaneous increase δV of the bias from point B of Fig. 1.

when $\partial_s f(s)<1$ (>1).[9] The trivial solution $s=0$, when it exists, is, therefore, a stable one. When three solutions exist, two of them, the largest and the smallest one, are stable while the intermediate one is unstable.

Considerations analogous to those made for s hold for the steady-state collector current $I/e=As\ \Gamma_c(s)$, proportional to the number of electrons in the well, As, A being the transverse area of the heterostructure, and to collector escape rate $\Gamma_c(s)$. In Fig. 1 we show $I(\Delta V)$ evaluated for the asymmetric double-barrier heterostructure experimentally investigated in Ref. 4. In agreement with the above discussion and with the experimental findings, no multiple solutions are obtained in the left-most curve (reverse bias case) of Fig. 1 when the emitter barrier is wider than the collector one. On the other hand, a bistability region extending between points A and B is observed in the forward bias case.

The above results can be generalized to include the effect of inelastic processes if we change $\Gamma\to\Gamma+\Gamma_i$ in Eq. (12), where $\Gamma_i=\Gamma_{ie}+\Gamma_{ic}$ is the total width representing collector and emitter inelastic decay channels.[11] The collector current becomes $I/e=As[\Gamma_c(s)+\Gamma_{ic}]$. However, if $\Gamma+\Gamma_i\ll E_F$, Eq. (13) still holds so that for $\Gamma_c\simeq\Gamma$ $(\Gamma_{ic}\simeq\Gamma_i)$, as in the case of Fig. 1, the value of I is independent of the ratio Γ_i/Γ.

Now we turn to the time-dependent transport properties. According to (10) and (11), we have

$$\partial_t s(t)=-\Gamma(s(t))s(t)+2\mathrm{Re}\langle z|\mathcal{B}\rangle, \tag{14}$$

where $\langle u|v\rangle\equiv\int dE\ g(E)\overline{u(E)}v(E)$. The last term in (14) can be expressed in terms of $s(t)$ by using the formal solution of (10)

$$\begin{aligned} z(t,E)=&\,e^{\int_0^t dt'\{-(1/2)\,\Gamma(s(t'))+i[E-E_R(s(t'))]\}}z(0,E)\\ &+\int_0^t dt'\,e^{\int_{t'}^t dt''\{-(1/2)\,\Gamma(s(t''))+i[E-E_R(s(t''))]\}}\\ &\times\mathcal{B}(s(t'),E). \end{aligned} \tag{15}$$

The first term in (15) vanishes exponentially and can be neglected after a time $t\gg2/\Gamma$. In the second term, an analogous exponential factor selects the contributions for $t-t'\lesssim2/\Gamma$ as the dominant ones so that the lower integration bound can be safely changed into $-\infty$ for $t\gg2/\Gamma$. In this case, $2\mathrm{Re}\langle z|\mathcal{B}\rangle$ can be approximated with

$$\begin{aligned} &2\mathrm{Re}\int_{-\infty}^t dt'\,e^{\int_{t'}^t dt''[-(1/2)\Gamma(s(t''))+iE_R(s(t''))]}\mathcal{F}(g|\mathcal{B}|^2)(t-t')\\ &\simeq2\mathrm{Re}\int_{-\infty}^t dt'\,e^{iE_R(s(t))(t-t')}\mathcal{F}(g|\mathcal{B}|^2)(t-t')\\ &=2\pi g(E_R(s(t)))|\mathcal{B}(s(t),E_R(s(t)))|^2, \end{aligned} \tag{16}$$

where $\mathcal{F}(g|\mathcal{B}|^2)$ is the Fourier transform obtained by performing the energy integral in the scalar product and the approximation in the third line is valid for Γ and $\partial_t s(t)$ small. With this result Eq. (14) becomes

$$\partial_t s(t)=-\Gamma(s(t))[s(t)-f(s(t))]. \tag{17}$$

As Eq. (13), this is a conservation law for the charge trapped in the well. The steady-state solutions, $\partial_t s=0$, of (17) coincide with those defined by (13) and also their attractive nature agrees with the stability condition discussed above.

Close to a bistability threshold, the dynamics of certain nonliner optical systems has been shown to be characterized by a quasistationary transient followed by a fast evolution.[6,7] As we will discuss in a moment, this behavior is typical of any rate equation of the form $\partial_t s=h(s,\delta V)$ where δV is the control parameter of a bistability threshold. An example for our heterostructure is shown in Fig. 2. At time $t=0$ the system is in the threshold stable steady-state B of Fig. 1 when the bias is instantaneously increased by an amount δV. For δV smaller than a critical value, we observe a quasistationary

$s(t)$ which decreases linearly at small times and, after a time τ, vanishes in a nearly exponential way. The border between these two regimes is given by the condition $E_R(s(\tau))=0$. Indeed, when the resonant energy $E_R(s)$ becomes smaller than the emitter band edge the filling current, $\Gamma(s)f(s)$, vanishes and (17) has the solution $s(t)\propto\exp[-\int^t dt'\Gamma(s(t'))]$. The nearly exponential decay is established from the beginning if $\delta V \gtrsim E_R(s(0))$. For $\delta V < E_R(s(0))$ and $t \lesssim \tau$, $s(t)$ is in a quasi-stationary regime which is characterized only by the fact that the starting point, $s(0)$, is a threshold stable steady state. Indeed, for $s(t)-s(0)$ and δV small in this case we must have $h(s,\delta V)\simeq -q[s(t)-s(0)]^2-p\,\delta V$ with $q,p>0$, independently of $h(s,\delta V)$. Integrating, we get $s(t)=s(0)-\sqrt{\delta V p/q}\tan(\sqrt{qp\,\delta V}t)$ which has linear behavior for small t. In the case of Eq. (17), the condition $E_R(s(\tau))=0$ and the approximate evaluation of q and p at $T=0$ K give

$$\tau \simeq \frac{4E_R(s(0))}{\eta s(0)\Gamma_c}\sqrt{\frac{E_R(s(0))}{\delta V}}\ \arctan\left(\sqrt{\frac{E_R(s(0))}{4\,\delta V}}\right), \tag{18}$$

where $E_R(s(0))\simeq E_F\Gamma_c/(2\Gamma)[1+2\pi\Gamma/(\eta\Gamma_e)]^{-1}$ and $s(0)\simeq[E_F-E_R(s(0))]\Gamma_e/(2\pi\Gamma)$. When $\delta V \ll E_R(s(0))$, we have $\tau\sim\delta V^{-1/2}$ as shown in Fig. 3 where we compare (18) with τ obtained by numerically integrating (17).[12] For $E_R(s(0))\ll E_F$, the temperature dependence of (18) is easily obtained by substituting the Fermi energy with the effective value $\tilde{E}_F=E_F+k_BT\ln[1+\exp(-E_F/k_BT)]$. The survival time increases by increasing T and for $\delta V \ll E_R(s(0))$ we have $\tau\sim\tilde{E}_F^{1/2}$.

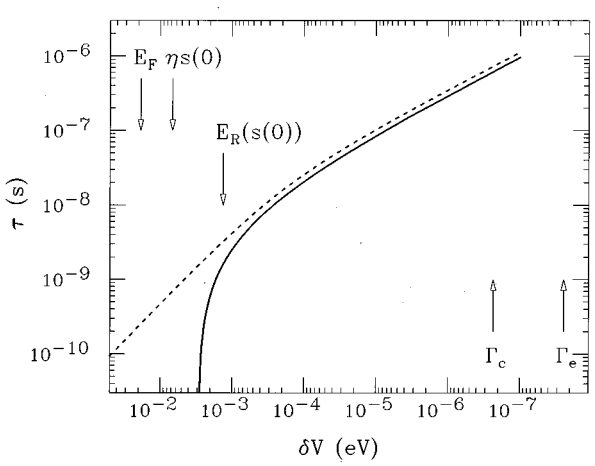

FIG. 3. Survival time of the quasistationary solutions of Fig. 2 *versus* δV (solid line). The dashed line is Eq. (18). Arrows indicate the relevant energy scales.

The phenomenon discussed above may be exploited for device applications like those suggested for optical systems.[6] More complex time-dependent features are expected in heterostructures with many resonances[9] or in superlattices.[13]

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