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Nonlinear feedback oscillations in resonant tunneling through double barriers

C. Presilla
Scuola del Dottorato di Ricerca in Fisica dell' Universitá "La Sapienza," Roma, Italy 00185 and Dipartimento di Fisica dell' Universitá, Perugia, Italy 06100

G. Jona-Lasinio
Dipartimento di Fisica dell' Universitá "La Sapienza," Roma, Italy 00185

F. Capasso
AT&T Bell Laboratories, 600 Mountain Avenue, Murray Hill, New Jersey 07974

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We analyze the dynamical evolution of the resonant tunneling of an ensemble of electrons through a double barrier in the presence of the self-consistent potential created by the charge accumulation in the well. The intrinsic nonlinearity of the transmission process is shown to lead to oscillations of the stored charge and of the transmitted and reflected fluxes. The dependence on the electrostatic feedback induced by the self-consistent potential and on the energy width of the incident distribution is discussed.

In recent years there has been renewed interest in the phenomenon of resonant tunneling (RT) through double barriers. The unique capabilities of molecular-beam epitaxy make it possible to investigate fundamental questions on RT through simple man-made potentials by controlling the barrier and well parameters (e.g., height, thickness, or barrier phase area) down to the atomic scale.[1]

In this paper we investigate the dynamics of RT of ballistic electrons in the presence of the potential created by the charge trapped within the well.[2] This problem is interesting not only from a technological point of view but also as a test of quantum-mechanical nonequilibrium situations in which many particles are involved.

The model we propose tries to describe the following situation. A group of electrons is created within a contact layer and launched towards embedded layers forming a double-barrier potential. The charge dynamically trapped by the resonance will produce a reaction field which modifies the time evolution of the system. An exact treatment of such a problem looks very complicated. We assume a decoupling between the longitudinal (in the direction x of motion perpendicular to the double barrier) and transverse degrees of freedom. This is a common assumption in treating tunneling phenomena. It makes the problem one dimensional and allows the following factorization of the wave function:

$$\Psi(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N;t) = \Phi(x_1,x_2,\ldots,x_N;t)\,\Omega(y_1,z_1,y_2,z_2,\ldots,y_N,z_N;t)\,, \tag{1}$$

where $\mathbf{x}\equiv(x,y,z)$ are the coordinates of each electron and t represents the time. We remark that antisymmetry of Ψ is established if we take, for example, Φ symmetric and Ω antisymmetric in their arguments. The experimental set-up we have in mind ideally puts all the electrons in the same high-energy longitudinal state while the transverse degrees of freedom are essentially decoupled.[1] Therefore the choice (1) with Φ symmetric is the only possibility. In other words, the transverse degrees of freedom ensure that the Pauli principle is obeyed.

Finally, we assume the electrons in the group at the initial time are uncorrelated, which corresponds to a choice of Φ as a product state of single-particle states $\psi(x,0)$. At this point theorem 5.7 of Ref. 3 guarantees in the mean-field approximation (which is reasonable due to the large number of electrons involved) that the state Φ remains a product state during its evolution and allows us to write the following self-consistent equation for $\psi(x,t)$:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) + \int W(t,t';x,x')|\psi(x',t')|^2 dt'dx'\right)\psi(x,t)\,. \tag{2}$$

The external potential $V(x)$ is assumed, as customary, to be composed of step functions (no electric field is applied):

$$V(x) = V_0[\Theta(x-a)\Theta(b-x)+\Theta(x-c)\Theta(d-x)]\,, \tag{3}$$

with $a<b<c<d$ and where $\Theta(x)$ is the Heaviside function. The kernel $W(t,t';x,x')$ is modeled assuming that memory effects can be neglected, i.e., $W\propto\delta(t-t')$. We represent the global repulsive feedback effect, induced by the charge localized in the well, by a shift of the bottom of the well to a higher energy, $V_Q(t)$, proportional to the charge, i.e.:

$$\int W(t,t';x,x')|\psi(x',t')|^2 dt'dx' \equiv \alpha V_0\frac{Q(t)}{Q_0}\Theta(x-b)\Theta(c-x)\,. \tag{4}$$

$Q(t)$ is the charge localized in the well at time t and Q_0 is a normalization charge which depends on the shape of the initial state, assumed localized around x_0:

$$Q(t)\equiv\int_b^c dx'|\psi(x',t)|^2,$$
$$Q_0\equiv\int_{x_0-(c-b)/2}^{x_0+(c-b)/2} dx'|\psi(x',0)|^2. \quad (5)$$

Q_0 introduces an artificial dependence of Eq. (2) on the initial condition. We have used this parametrization to make the comparison of different numerical simulations easier. The parameter α in Eq. (4) can be varied to reproduce phenomenologically the response of the medium to the charge trapped in the well and the characteristics of the incident electron group, i.e., its areal density n_s. It is proportional to $e^2 n_s/CV_0$, where e is the electronic charge and C is the double barrier capacitance per unit area.

The one-particle state which is the initial condition in our mean-field equation [Eq. (2)] has been chosen to be a Gaussian-shaped superposition of plane waves with mean momentum $\hbar k_0$:

$$\psi(x,0)=\frac{1}{\sqrt{\sigma\sqrt{\pi}}}\exp\left[-\frac{1}{2}\left(\frac{x-x_0}{\sigma}\right)^2+ik_0x\right] \quad (6)$$

with energy spread [energy full width at half maximum of the square modulus of the Fourier transform of (6)] $\Gamma_0=2\sqrt{\ln 2}\hbar^2k_0/m\sigma$. x_0 is chosen so that at the initial time no appreciable charge sits in the well, i.e., $Q(0)=0$.

The solution of the differential equation [(2)–(5)] with the initial condition (6) has been achieved by a numerical integration on a two-dimensional lattice.[4] Assuming for the barrier and well widths the values $b-a=d-c=20a_0$ and $c-b=15a_0$ ($a_0\simeq 0.529$ Å, being the Bohr radius) and for the barrier height 0.3 eV and using for m the free-electron mass, the potential $V(x)$ exhibits a single resonance in the transmission coefficient at energy $E_R\simeq 0.15$ eV, the shape of which is well approximated by a Lorentzian of full width $\Gamma_R\simeq 5$ meV. The choice of these parameters was a compromise between the requirement of standard technological values and that of reasonable computation times. The electron mass was set to its free value to avoid the complications of a space-variable effective mass.

The mean energy of the incoming state has been chosen so as to satisfy the resonance condition $\hbar^2k_0^2/2m=E_R$. Finally, the normalized charge in the well, $Q(t)/Q_0$, has been plotted as a function of time. The results for different choices of the parameter α are shown in Figs. 1–4 in the case of states with energy spread larger, of the order of, and smaller than the resonance width.

Figure 1 represents the scattering of a wave packet on the fixed double barrier (linear Schrödinger equation). When the packet is energetically much wider than the resonance, the buildup and the decay of the charge are asymmetric, the decrease following[5] the law $\exp(-t/\tau)$ with $\tau=\hbar/\Gamma_R$ (decay of a Lorentzian-shaped quantum state). On the other hand, for a wave packet narrower than the resonance, the charge presents a symmetric behavior, like the law $\exp\{-[(t-t_0)/\tau]^2\}$, where $\tau=\sigma/v_0=2\sqrt{\ln 2}\hbar/\Gamma_0$,

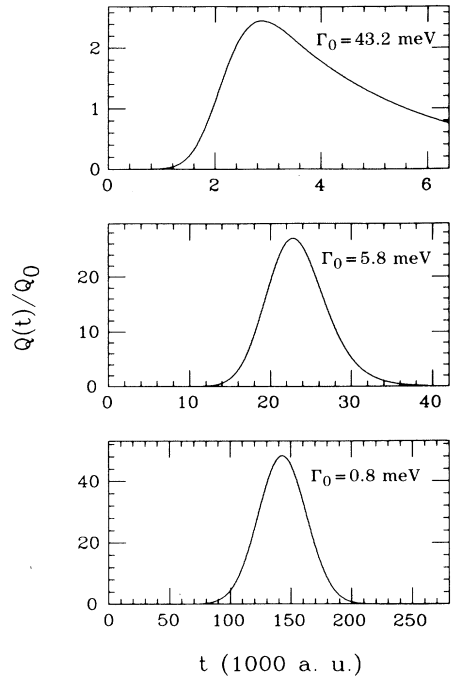

FIG. 1. Time development of the normalized charge trapped in the well in the case of the linear Schrödinger equation, i.e., $\alpha=0$, for incident states with energy spread much wider ($\Gamma_0=43.2$ meV), of the same order of ($\Gamma_0=5.8$ meV), and much smaller ($\Gamma_0=0.8$ meV) than the resonance width ($\Gamma_R\simeq 5$ meV). An atomic unit of time corresponds to 4.83×10^{-17} s.

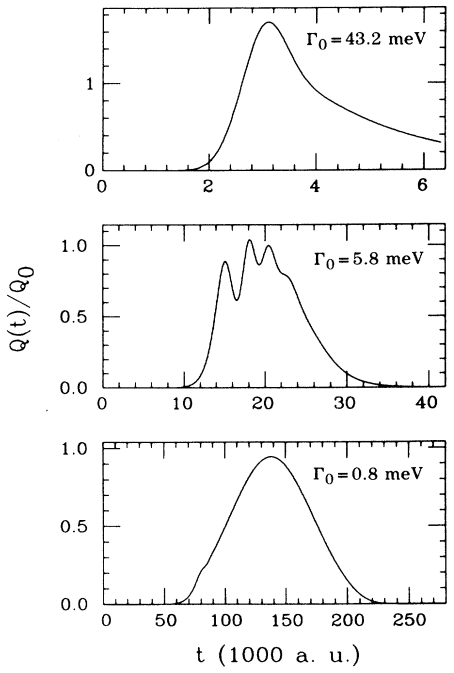

FIG. 2. As Fig. 1 but in the case of effective nonlinearity in the Schrödinger equation with $\alpha=0.1$.

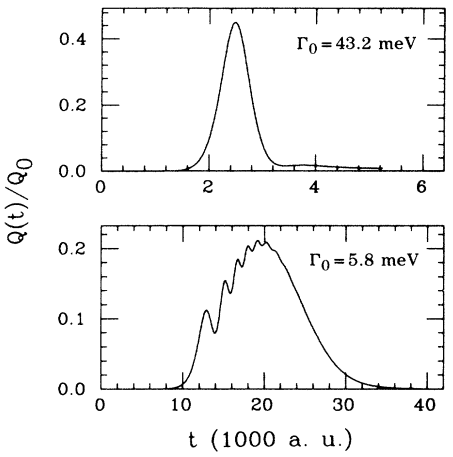

FIG. 3. As Fig. 2 but with $\alpha=1$. The case with $\Gamma_0=0.8$ meV is not shown.

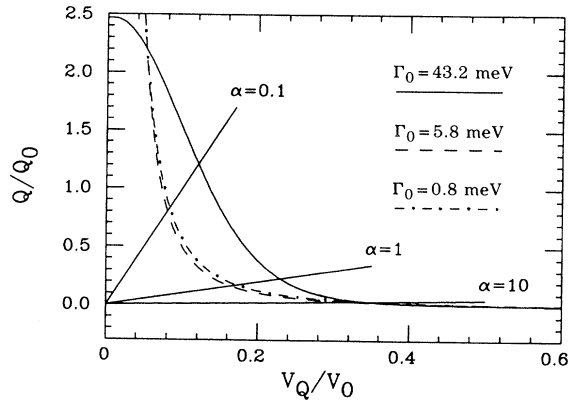

FIG. 5. Self-consistent estimate of the time-averaged normalized charge trapped in the well for different values of the parameters α and Γ_0.

$t_0 \simeq |(b+c)/2 - x_0|/v_0$, and $v_0 = \hbar k_0/m$ (free evolution of a Gaussian-shaped quantum state for negligible time spreading). The latter result is not surprising, since now the packet traverses the double barrier almost undistorted. In the case of a state energy spread comparable to the resonance width, the evolution of the trapped charge interpolates between these two extreme behaviors.

When the nonlinear term is effective, i.e., $\alpha \neq 0$, the evolution of the trapped charge changes drastically and oscillations can appear. This phenomenon has been qualitatively anticipated by Ricco and Azbel.[6] Their reasoning was very simple. At the initial time no charge is present in the well, the electrons are moving towards the double barrier and the resonance condition is fulfilled. When some charge penetrates into the well, the modification of the potential destroys the resonance condition. As a consequence the quantity of trapped charge has a maximum followed by a decrease. The resonance condition tends to be restored and a new cycle begins. However, as it will appear in the following, the nonlinearity makes the interpretation of the phenomenon significantly more complicated. For example, the conclusion by Ricco and Azbel that the above effect should be maximal for monochromatic states is not correct.

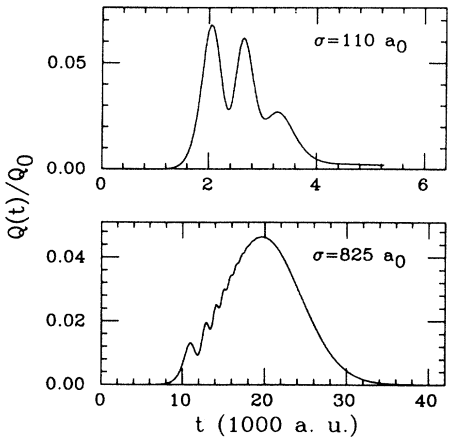

FIG. 4. As Fig. 3 but with $\alpha=10$.

A detailed analysis of Figs. 2–4 (that are a sample of our global numerical work) suggests the following observations. Oscillations are present, for appropriate values of the strength of the nonlinear term α, only when the energy spread of the state is wider or comparable to the resonance width. No oscillations are seen for nearly monochromatic states. When α increases, the oscillations, if present, tend to increase in number but decrease in amplitude.

To understand these results, let us first interpret the dependence of the intensity of the trapped charge as a function of the parameters α and Γ_0. We simplify the question by considering a time average of the charge dynamically present inside the well. Since during the time evolution $V_Q(t)$ and $Q(t)$ are related to each other by Eq. (4), a similar relation has to hold between the relevant time-averaged quantities denoted by V_Q and Q. Let us suppose now that we have a time-independent situation with the bottom of the well at level V_Q. As can be shown by explicit calculations, the charge Q present in the well is a fraction γ of the transmitted charge Q_T:[5]

$$Q_T(V_Q) = \int_{-\infty}^{+\infty} dk\, |\tilde{\psi}(k,0)|^2 |t_{V_Q}(k)|^2 , \tag{7}$$

where $\tilde{\psi}(k,0)$ is the Fourier transform of (5) and $|t_{V_Q}(k)|^2$ is the transmission coefficient of the double barrier in the presence of a charge Q in the well. The time average of Eq. (4) can be combined with Eq. (7) to obtain a self-consistent relationship for V_Q (or Q):

$$\frac{V_Q}{\alpha V_0} = \frac{\gamma Q_T(V_Q)}{Q_0} . \tag{8}$$

The two sides of this equation are plotted in Fig. 5 for different values of α and Γ_0; their intersection points represent our estimate for the time-averaged normalized charge trapped in the well during the interaction of the packet with the double barrier. The factor γ is fixed by imposing the condition that for $\alpha=0$ the results of Fig. 1 are reproduced. As expected, it is of the order of unity. Figure 5 correctly predicts the time average obtained from

Figs. 2–4. We also notice that for very large α the charge tends to disappear due to the smallness of the transmitted amplitude.

We then try to understand the oscillating behavior. Let us assume that this phenomenon is due to the competition of two processes: (a) the filling up of the well by the incoming wave packet and (b) the natural decay of the trapped charge. For the process (a) the time scale is of the order of $\hbar/\Gamma_0$ (this estimate appears more accurate for states narrower in energy than the resonance width). For the process (b) a reasonable time scale is $\hbar/\Gamma_{V_Q}$, where Γ_{V_Q} is the energy spread of the function to be integrated in Eq. (7) (spectral decomposition of the transmitted charge). Oscillations are then expected if a substantial crossover of Γ_{V_Q} and Γ_0 is realized for the V_Q values reached during the time evolution. The analysis of the function $|\tilde{\psi}(k,0)|^2|t_{V_Q}(k)|^2$ shows that Γ_{V_Q} rises from, approximately, $\Gamma_0\Gamma_R/(\Gamma_0^2+\Gamma_R^2)^{1/2}$ at $V_Q=0$, to a maximum greater than Γ_0 (position and amplitude of the maximum are roughly proportional to Γ_0/Γ_R) and, eventually, decreases to Γ_0. As a consequence, when $\Gamma_0 \ll \Gamma_R$, Γ_{V_Q} is very close to Γ_0 and independent of V_Q. No oscillations are possible in this case for any values of α. On the other hand, when $\Gamma_0 \geq \Gamma_R$, Γ_{V_Q} crosses Γ_0 at some V_Q; oscillations are then realized for a sufficiently high value of α. This critical value of α increases with the ratio Γ_0/Γ_R. These predictions agree quantitatively with the results of the simulations reported above.

The geometry considered here can be implemented by ballistically launching electrons into a double barrier inserted in the thin (<1000 Å) base of a unipolar transistor.[7] The predicted range of oscillations (≤ 1 ps) should be detectable with electro-optical sampling techniques.[8]

[1]For a review, see F. Capasso and S. Datta, Phys. Today **43** (2), 74 (1990); B. K. Ferry, in *Physics of Quantum Electron Devices,* edited by F. Capasso (Springer-Verlag, New York, 1990), Chap. 4.

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