DYNAMICAL ANALYSIS OF RESONANT TUNNELING IN PRESENCE OF A SELF CONSISTENT POTENTIAL DUE TO THE SPACE CHARGE

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ABSTRACT. *The resonant tunneling of electrons through a double barrier is analyzed from a dynamical point of view. When a self consistent potential, representing the effect of the electrostatic feedback induced by the charge trapped in the well, is taken into account, the non linearity of the transmission process can lead to oscillations of the transmitted fluxes. This behavior is shown to depend sensitively on the energy spread of the incident electron distribution and on the intensity of the electrostatic feedback.*

INTRODUCTION

In recent years there has been renewed interest in the phenomenon of resonant tunneling (RT) through double barriers. This interest has been greatly stimulated by the ability to synthesize double barriers with precisely tailored potentials using epitaxial crystal growth techniques such as molecular beam epitaxy (MBE).

Following the first demonstration of RT through semiconductor double barriers[1], in recent years many groups have studied the physics and device application of RT in semiconductor nanostructures[2]. MBE allows one to control the layer thickness and tune its composition down to the atomic scale (1-2 monolayers). This unique capability makes it possible to investigate fundamental questions on RT through simple model potentials by varying the barrier and well parameters (e.g. height, thickness or barrier phase area). Such questions include the tunneling times and the time constant required to establish the steady state resonant transmission[3-4], the influence of scattering[5] and the effect of charge accumulation in the well on the time dynamics of the process. The latter is still poorly understood; investigations so far have been limited to measurements of the charge density dynamically stored in the well under stationary or quasi-steady state conditions, and of its escape time following photoexcitation of electron hole pairs in the well[6]. It has also been pointed out and demonstrated that the dynamical storage of electrons in the well leads to bistability in the current voltage characteristics[7].

In a recent paper[8] we have investigated for the first time the RT time dynamics of wave packets 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 intriguing nonlinear oscillations of the stored charge and on the transmitted and reflected fluxes. The latter are shown to depend sensitively on the

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electrostatic feedback induced by the self-consistent potential and on the spread of the incident electron distribution with respect to the resonance width.

THE MODEL

From a mesoscopic point of view the modelling of the RT of electrons through a heterostructure as the evolution of a wave packet impinging on a fixed one-dimensional double barrier is only a crude approximation. More realistically, during the evolution of the tunneling process, accumulation of charge carriers takes place within the resonant well. A dynamical analysis of RT must thus consider the evolution of a many particle system. In the spirit of a Hartree-like approximation[9], we may assume the mean field equation:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) + \int W(t,t';x,x')|\psi(x',t')|^2 dt'dx'\right]\psi(x,t) \qquad (1)$$

In this simplified model the fermion nature of the carriers, as well as higher-dimensionality effects, e.g. elastic scattering with momentum transfer in the plane perpendicular to the symmetry axe of the potential, are ignored. In absence of an applied electric field, the external potential, $V(x)$, is assumed, as customary, to be a step function:

$$V(x) = V_0[\theta(x-a)\theta(b-x) + \theta(x-c)\theta(d-x)] \qquad (2)$$

with $a < b < c < d$ and where $\theta(x)$ is the Heaviside function.

The nucleus $W(t,t';x,x')$ is modelled assuming that memory effects can be neglected, i.e. $W \propto \delta(t-t')$. This implies that the repulsive potential due to the charge trapped in the well acts instantaneously on the wave packet. The approximation is good since the characteristic interaction time $(d-a)/s$, where s is the speed of light in the medium, is much less than the relevant tunneling time. Moreover it is reasonable to represent the global repulsive feedback effect, induced by the charge localized in the well, by a shift of the bottom of the well to higher energy, i.e.:

$$\int W(t,t';x,x')|\psi(x',t')|^2 dt'dx' = V_Q(t)\theta(x-b)\theta(c-x) \qquad (3)$$

with

$$V_Q(t) \equiv \alpha V_0 \frac{Q(t)}{Q_0} \qquad (4)$$

$Q(t)$ 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 wave packet, assumed localized around $x_0 < a$:

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

Note that Q_0 introduces an artificial dependence of the potential (4) on the initial conditions. We use this parameterization as it makes easier the comparison between different numerical simulations. The parameter α in Eq. (3) can be varied to reproduce phenomenologically the response of the medium in the well to the charge trapped in it.

The initial wave packet has been chosen to be a gaussian shaped superposition of plane waves with mean momentum $\hbar k_0$:

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

σ gives the entity of localization in x-space of the packet. Its Fourier transform,

$$\tilde{\psi}(k,0) = \sqrt{\frac{\sigma}{\sqrt{\pi}}} \exp\left[-\frac{1}{2}\left(\frac{k-k_0}{\sigma^{-1}}\right)^2 - ix_0(k-k_0)\right] \tag{7}$$

gives the energy spread Γ_0 (full width at half maximum of the square modulus of (6)) of the packet: $\Gamma_0 = 2\sqrt{\ln 2}\ \hbar^2 k_0/m\sigma$. x_0 is chosen so that, at the initial time, the wave packet is very distant from the double barrier and no appreciable charge sits in the well, i.e. $Q(0) = 0$.

NUMERICAL SOLUTION

The solution of the differential equation (1-5) with the initial condition (6) has been achieved by a numerical integration on a two-dimensional lattice. As in the case of the standard Schrödinger equation, it is convenient to use a finite-difference temporal-evolution operator in the Cayley form[10,11], which has the advantage of preserving the norm of $\psi(x,t)$. This is a conserved quantity if the nucleus in (1) is real. The finite-difference version of Eq. (1) reduces to a linear tridiagonal system which can be solved to obtain $\psi(x,t+\Delta t)$ from $\psi(x,t)$ considered as known. Starting from Eq. (6) the wave function is calculated step by step at any point of the chosen lattice.

The computation time imposes some restrictions on the choice of the potential parameters in (2). This time, in fact, grows almost quadratically with the spatial width σ of the wave packet. The analysis of a wave packet with energy spread much smaller than the resonance width, becomes, then, impracticable if the resonance width is too small. Here we report the results of Ref. 8 where a compromise between standard technological values and reasonable computation times has been achieved assuming for the barrier and well widths the values $b - a = d - c = 10.6$ Å and $c - b = 7.9$ Å and for the barrier height $0.3\ eV$ and where for m the free electron mass has been used . With these parameters 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 at half maximum $\Gamma_R \simeq 5\ meV$. The electron mass was set to its free value to avoid the complications of a space variable effective mass.

An example of the above dynamical analysis is shown in Fig. 1 in the case of linear RT, i.e. for $\alpha = 0$. The starting wave function, Eq. (6), has been chosen so as to satisfy the resonance condition, e.g. $\hbar^2 k_0^2/2m = E_R$. The wave function at later times has been then calculated and its square modulus is plotted, at different times. All the relevant quantities, such as the normalized charge in the well, $Q(t)/Q_0$, or the transmitted flux at a given point, can be extracted from this analysis because the wave function $\psi(x,t)$ is known.

From now on, we concentrate on the analysis of the charge dynamically trapped in the well. Some results, for different choices of the parameter α, are shown in Fig. 2 in the case of wave-packets with energy-spread much larger, of the order of and much smaller compared with the resonance width.

The case $\alpha = 0$ represents the scattering of a wave packet on the potential of Eq. (2) (linear Schrödinger equation). When the packet is energetically much wider than the resonance ($\Gamma_0 = 43.2\ meV$) the building up and the decay of the charge are asymmetric, the decay following[10] the law $exp(-t/\tau)$ with $\tau = \hbar/\Gamma_R$. This is the decay law of a quantum state whose spectral decomposition in plane waves has a lorentzian shape. On the other hand, for a wave packet narrower than the resonance ($\Gamma_0 = 0.8\ meV$) the charge presents a symmetric behavior governed by the law $exp[-((t-t_0)/\tau)^2]$ where $\tau = \sigma/v_0 = 2\sqrt{\ln 2}\ \hbar/\Gamma_0$, $t_0 \simeq [(b+c)/2 - x_0]/v_0$ and $v_0 = \hbar k_0/m$ (free evolution of a gaussian-shaped quantum state for negligible time-spreading). This latter result is not surprising, since now the wave packet traverses the double barrier almost undistorted because every Fourier component sees a nearly unity transmission coefficient. In the case of a wave-packet with energy-spread comparable to the resonance width the evolution of the trapped charge interpolates between these two extreme behaviors.

When the non linear term is effective, i.e. $\alpha \neq 0$, the evolution of the trapped charge changes drastically and oscillations can appear. This phenomenon has been suggested for the first time by Ricco and Azbel[3]. Their reasoning was very simple. At the initial time no charge is present in the well, the wave packet is 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 more complicated. For example, the conclusion by Ricco and Azbel that the above effect should be maximal for monochromatic waves is not correct.

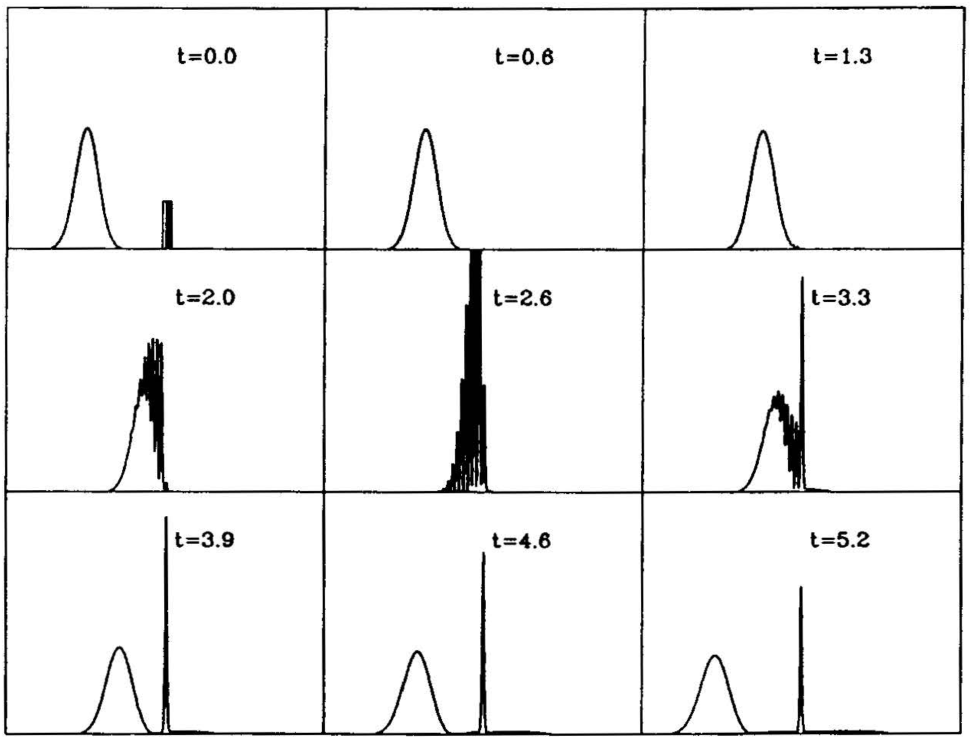

FIGURE 1. *Example of time evolution of a wave packet impinging on a resonant double barrier. The position probability density,* $|\psi(x,t)|^2$*, is shown in each box at the indicated time (in* 10^3 *atomic units). The conversion of the atomic units of time to seconds is 1 a.u.* $\simeq 4.83\ 10^{-17}$ *s. The wave packet is moving from left to right against the double barrier positioned as indicated in the box at* $t = 0$*. The packet fulfills the resonance condition* $\hbar^2 k_0^2/2m = E_R$ *but has an energy spread,* $\Gamma_0 = 43.2$ *meV, much greater than the resonance width,* $\Gamma_R = 5$ *meV, and, as a consequence, is almost completely reflected.*

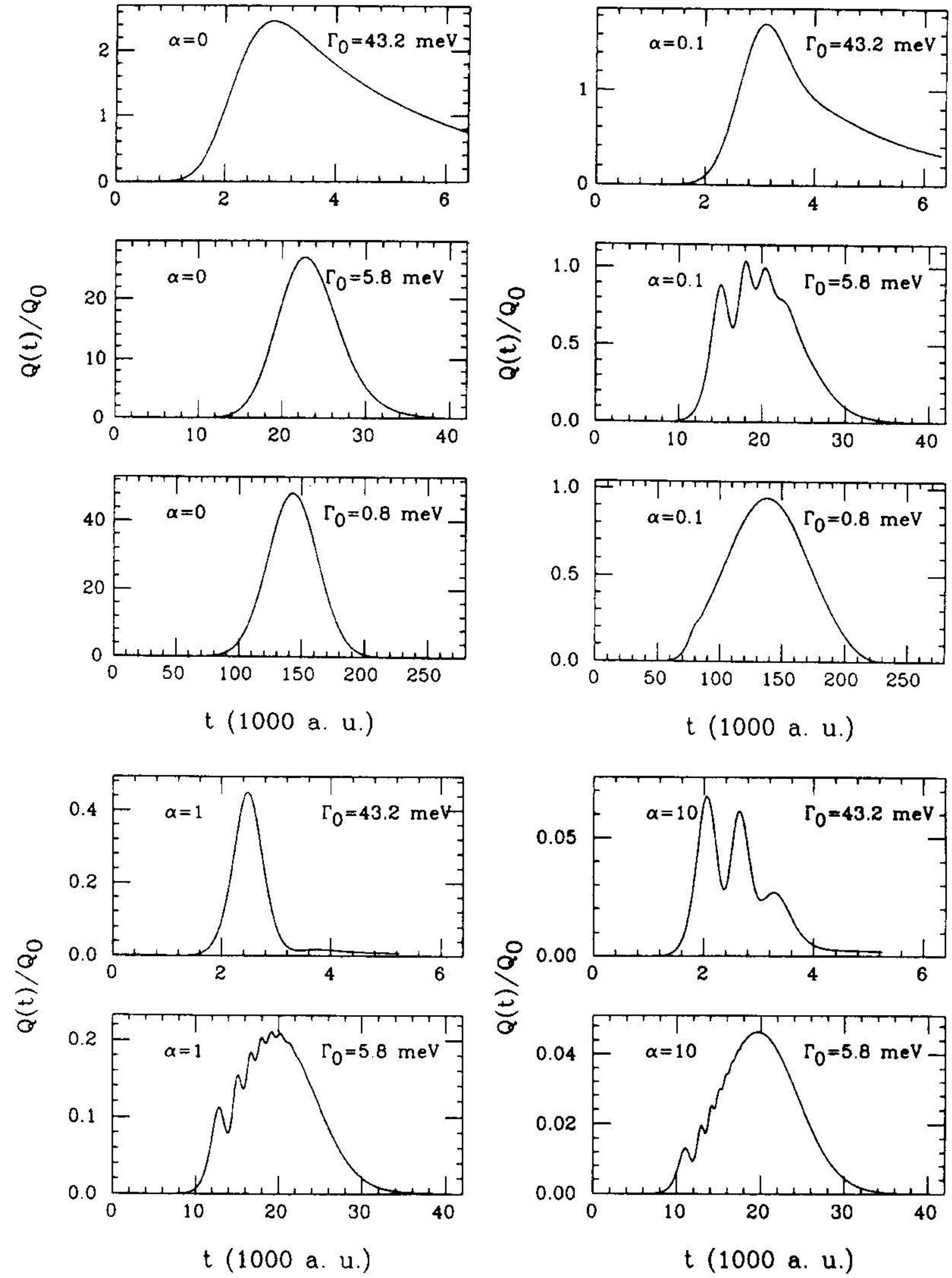

FIGURE 2. *Time development of the normalized charge trapped in the well for wave packets with energy spread much wider ($\Gamma_0 = 43.2$ meV), of the same order of ($\Gamma_0 = 5.8$ meV) and much smaller ($\Gamma_0 = 0.8$ meV) than the resonance width ($\Gamma_R \simeq 5$ meV). The results are shown for various values of the feedback intensity parameter, α.*

ANALYSIS OF THE RESULTS

A detailed analysis of our global numerical simulations for different values of α and σ suggests the following observations. Oscillations are present, for appropriate values of the strength of the non linear term, α, only when the energy spread of the wave packet is wider or comparable to the resonance width. No oscillations are seen for a nearly monochromatic wave-packet ($\Gamma_0 = 0.8\ meV$). 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 trapped charge as a function of the parameters α and Γ_0. We reduce the question to a stationary problem concentrating on 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 time averaged quantities denoted by $\bar{V}_Q$ and Q. Let us suppose, now, that we have a time independent situation with the bottom of the well at the level V_Q. As can be shown by explicit calculations, the charge Q present in the well is a fraction γ of the asymptotically transmitted charge Q_T[12]:

$$Q_T(V_Q) = \int_{-\infty}^{+\infty} dk\ |\tilde{\psi}(k,0)|^2\ |t_{V_Q}(k)|^2 \tag{8}$$

where $|t_{V_Q}(k)|^2$ is the transmission coefficient of the depicted potential. Eq. (8) can be inserted in the time-averaged version of Eq. (4) to obtain a self consistent relationship for V_Q (or Q):

$$\frac{V_Q}{\alpha V_0} = \frac{\gamma Q_T(V_Q)}{Q_0} \tag{9}$$

The two sides of this equation are plotted in Fig. 3 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 that for $\alpha = 0$ the corresponding numerical results of Fig. 2 are reproduced. As expected it is of the order of unity. When $\alpha \neq 0$ Fig. 3 predicts correctly the time-averaged charges obtained from Fig. 2.

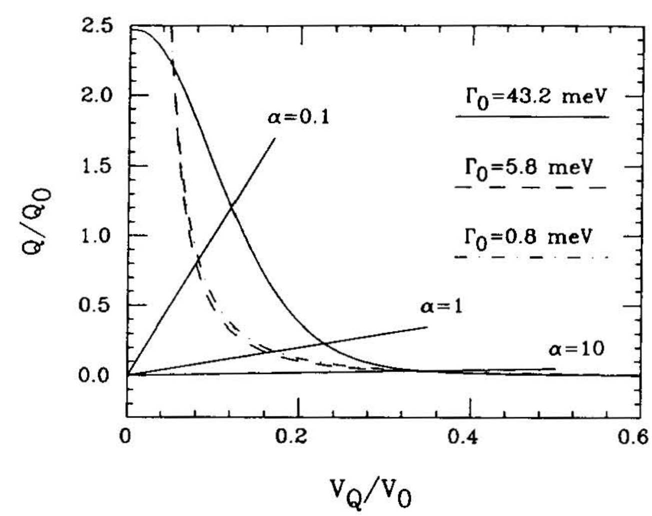

FIGURE 3. *Self-consistent estimate of the mean normalized charge trapped in the well for different values of the parameters α and Γ_0.*

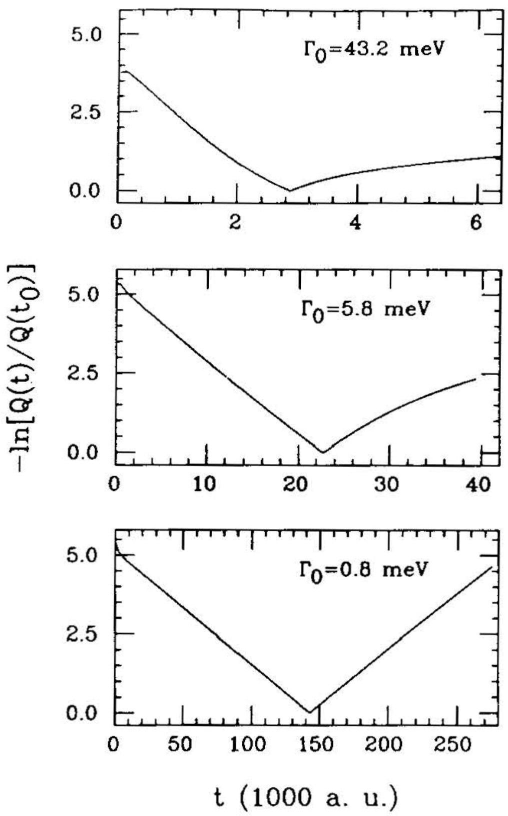

FIGURE 4. *Estimate of the well filling up rate from the results of Fig. 2 for $\alpha = 0$; t_0 is the instant at which the charge trapped in the well is at its maximum value, $Q(t_0)$. For the case $\Gamma_0 = 0.8$ meV, the plot is well represented by the law $|t - t_0|/\tau$ with $\tau = 2\sqrt{\ln 2}\hbar/\Gamma_0$. In the other cases only the leading edge of the wave-packet ($t < t_0$) is approximatively fitted by this law.*

Let us now interpret the oscillating behavior. We 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 characteristic time scale can be deduced by studying the rising of the trapped charge in Fig. 2 at $\alpha = 0$. The question is simple for a wave packet with energy spread much narrower than the resonance width. In this case $Q(t)$ strictly follows, as explained, the law $Q(t) \simeq Q(t_0) \exp[-((t-t_0)/\tau)^2]$ with $\tau = 2\sqrt{\ln 2}\, \hbar/\Gamma_0$. For packets with greater energy spread this law remains approximatively valid when $t < t_0$, as shown in Fig. 4. As a consequence, $\Gamma_0/\hbar$ is a reasonable rate of the process *a)* in all the cases. For the process *b)* a reasonable rate is $\Gamma_{V_Q}/\hbar$, where Γ_{V_Q} is the energy spread of the function $|\widetilde{\psi}(k,0)|^2\ |t_{V_Q}(k)|^2$. In fact, as shown by Eq. (8), it represents the spectral decomposition of the charge trapped in the well. The shape of Γ_{V_Q} as a function of V_Q is shown in Fig. 5 for various choices of Γ_0. Γ_{V_Q} rises from, approximatively, $\Gamma_0\Gamma_R/\sqrt{\Gamma_0^2+\Gamma_R^2}$ at $V_Q = 0$ to a maximum greater than Γ_0 and, eventually, decreases to Γ_0.

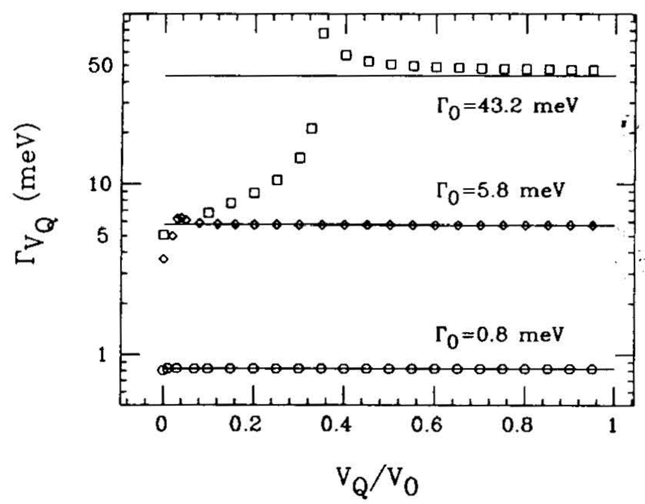

FIGURE 5. *Shape of Γ_{V_Q} as a function of V_Q for different values of the wave packet energy spread (squares: $\Gamma_0 = 43.2$ meV, lozenges: $\Gamma_0 = 5.8$ meV, circles: $\Gamma_0 = 0.8$ meV). Γ_{V_Q} asymptotically tends to the corresponding Γ_0 (solid lines). Γ_{VQ} and Γ_0 are proportional to the escape rate of the charge from the well and to the filling up rate of the well, respectively.*

The oscillating mechanism can be understood from the behavior of Γ_{VQ} as a function of the charge dynamically trapped in the well. At the initial time no charge sits in the well and $V_Q = 0$. The filling up rate is greater than the decay rate ($\Gamma_0 > \Gamma_{V_Q}$) and the charge in the well builds up. As the potential in the well, V_Q, increases the decay rate of the charge speeds up. At a critical value of V_Q, the decay rate becomes greater than the filling up rate ($\Gamma_{V_Q} > \Gamma_0$). The charge trapped in the well reaches a maximum and then decreases thus reducing V_Q. Another cycle can start again ($\Gamma_0 > \Gamma_{V_Q}$).

From Fig. 5 it is evident that when $\Gamma_0 \ll \Gamma_R$, Γ_{V_Q} is very close to Γ_0 and almost independent of V_Q. No oscillations are possible in this case for any value of α. On the other hand, when $\Gamma_0 \geq \Gamma_R$, Γ_{V_Q} crosses the value Γ_0 at an appropriate V_Q. Then oscillations are realized for a sufficiently high value of α. This critical value of α, is deduced by inserting the critical value of V_Q in Fig. 3. It increases with the ratio Γ_0/Γ_R in agreement with the numerical results.

CONCLUSIONS

We have proposed a model of resonant tunneling based on a non linear Schrödinger equation. This model shows dynamical oscillations in all relevant quantities, such as transmitted and reflected fluxes, for appropriate values of the feedback intensity α and for $\Gamma_0 \geq \Gamma_R$. The latter is a well satisfied condition in resonant tunneling experiments[2]. The fulfillment of the other condition is more subtle. Let us imagine that in the mean field limit the wave packet $\psi(x,t)$ describes the longitudinal motion of a bunch of electrons with transversal areal density eN/A, e being the electron charge. The model feedback potential of Eq. (4) can be then equated with the electrostatic potential energy difference between two charged sheets with charge areal density $eQ(t)N/A$ separated by a distance l of the order of $(b+c)/2 - a$. As a consequence we obtain, in the Gauss system, the estimate $\alpha = 4\pi e^2 l Q_0 N/(\epsilon V_0 A)$ where ϵ is the dielectric constant of the medium. In the case when $\Gamma_0 = 43.2\ meV$ the oscillating behavior occurs in the above simulations for $\alpha \geq 1$. For a typical value of the dielectric constant $\epsilon \simeq 13$ this implies $N/A \geq 10^{14} cm^{-2}$.

A tunneling experiment with time resolution in the femtosecond range could test the predictions of our model and perhaps exploit them from a device point of view. The present availability of femtosecond lasers and the possibility of changing the barrier parameters to increase the period of the oscillations should make the task of observing these effects realizable.

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