NONLINEAR FEEDBACK OSCILLATIONS
IN RESONANT TUNNELING THROUGH DOUBLE BARRIERS

C. Presilla
Scuola del Dottorato di Ricerca in Fisica dell’ Universitá “La Sapienza”, Roma, I 00185
and
Dipartimento di Fisica dell’ Universitá, Perugia, I 06100

G. Jona-Lasinio
Dipartimento di Fisica dell’ Universitá “La Sapienza”, Roma, I 00185
and

F. Capasso
AT&T Bell Laboratories, 600 Mountain avenue, Murray Hill, N J 07974

Abstract

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.

P.A.C.S. numbers: 03.65.-w, 73.40Gk
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\cite{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 barriers\cite{2}. This problem is interesting not only from a technological point of view but also as a test of quantum mechanical non-equilibrium situations in which many particles are involved.

The model we propose tries to describe the following situation. A bunch of electrons is created within a contact layer and launched towards embedded semiconductor 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 transversal 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:

$$\Psi(x_1, x_2, \ldots, x_N; t) = \Phi(x_2, \ldots, x_N; t) \Omega(y_1, y_2, \ldots, y_N; t)$$ (1)

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

Finally we assume the electrons in the bunch at the initial time uncorrelated which corresponds to a choice of $\Phi$ 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 $\Phi$ remains a product state during its evolution and allows us to write the following self-consistent equation for $\psi(x, t)$:

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

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

$$V(x) = V_0 [\theta(x - a)\theta(b - x) + \theta(x - c)\theta(d - x)] \quad (3)$$

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. $W \propto \delta(t - t')$. 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.:

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

$Q(t)$ 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 $x_0$:

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

$Q_0$ introduces an artificial dependence of the Eq. (2) on the initial condition. We have used this parameterization to make the comparison of different numerical simulations easier.
The parameter $\alpha$ 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 electron bunch, e.g. its areal density.

The 1-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 $\hbar k_0$:

$$\psi(x, 0) = \frac{1}{\sqrt{\sigma \sqrt{\pi}}} \exp \left[ -\frac{1}{2} \left( \frac{x - x_0}{\sigma} \right)^2 + ik_0 x \right]$$

(6)

with energy spread (energy full width at half maximum of the square modulus of the Fourier transform of (6)) $\Gamma_0 = 2\sqrt{\ln 2} \ \hbar^2 k_0 / m \sigma$. $x_0$ 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 \cite{4}. Assuming for the barrier and well widths the values $b-a = d-c = 20 \ a_0$ and $c-b = 15 \ a_0$ ($a_0 \approx 0.529 \ \text{Å}$ 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 $E_R \approx 0.15 \ eV$, the shape of which is well approximated by a lorentzian of full width $\Gamma_R \approx 5 \ meV$. 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 incoming state mean-energy has been chosen so as to satisfy the resonance condition $\hbar^2 k_0^2 / 2m = E_R$. 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 $\alpha$ 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.

The Fig. 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 building up and the decay of the charge are asymmetric, the decreasing 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 \(\exp\left[-((t - t_0)/\tau)^2\right]\), 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). 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 with 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 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.

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 non-linear term, $\alpha$, 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 $\alpha$ 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 $\alpha$ and $\sigma$. 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 with each other by the 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, $\gamma$, of the asymptotically transmitted charge $Q_T$:

$$Q_T(V_Q) = \int_{-\infty}^{+\infty} dk \, |\tilde{\psi}(k,0)|^2 \, |t_{V_Q}(k)|^2$$  \hspace{1cm} (7)

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

$$\frac{V_Q}{\alpha V_0} = \frac{\gamma Q_T(V_Q)}{Q_0}$$  \hspace{1cm} (8)

The two sides of this equation are plotted in Fig. 5 for different values of $\alpha$ and $\sigma$; 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 $\gamma$ is fixed by imposing that for $\alpha = 0$ the results of Fig. 1 are reproduced. As expected it is
of the order of unity. Fig. 5 predicts correctly the time-averaged obtained from Fig.s 2-4. We also notice that for very large \( \alpha \) 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 reasonable for states narrower in energy than the resonance width). For the process (b) a reasonable time scale is \( \hbar / \Gamma_{VQ} \), where \( \Gamma_{VQ} \) is the energy spread of the function to be integrated in Eq. (7) (spectral decomposition of the charge present in the well). Oscillations are then expected if a substantial crossover of \( \Gamma_{VQ} \) and \( \Gamma_0 \) 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 \( \Gamma_{VQ} \) rises from, approximatively, \( \Gamma_0 \Gamma_R / \sqrt{\Gamma_0^2 + \Gamma_R^2} \) at \( V_Q = 0 \), to a maximum greater than \( \Gamma_0 \) (position and amplitude of the maximum are roughly proportional to \( \Gamma_0 / \Gamma_R \)) and, eventually, decreases to \( \Gamma_0 \). As a consequence when \( \Gamma_0 \ll \Gamma_R, \Gamma_{VQ} \) is very close to \( \Gamma_0 \) and independent of \( V_Q \). No oscillations are possible in this case for any value of \( \alpha \). On the other hand, when \( \Gamma_0 \geq \Gamma_R, \Gamma_{VQ} \) crosses \( \Gamma_0 \) at a some \( V_Q \); oscillations are then realized for a sufficiently high value of \( \alpha \). This critical value of \( \alpha \) increases with the ratio \( \Gamma_0 / \Gamma_R \). These predictions agree quantitatively with the results of the simulations reported above.

The effects we have discovered exhibit a considerable stability under modifications of the model for example in the direction of a more realistic choice of the self-consistent potential. A deeper analysis of the problem, together with an investigation on the possibility
of an experimental study, is matter for a forthcoming publication.

Acknowledgments

We thank F. Marchesoni, L. A. Pastur and F. Sacchetti for their helpful suggestions and comments.
References

[1] For a review see F. Capasso and S. Datta, Phys. Today, 43 (2), 74, (1990) and Physics of Quantum Electron Devices, F. Capasso, ed., Springer-Verlag, New York, Heidelberg (1990)

[2] M. Tsuchiya, T. Matsusue and H. Sakaki, Phys. Rev. Lett. 59, 2356 (1987); J. F. Young, B. M. Wood, G. C. Aers, R. L. S. Devine, H. C. Liu, D. Landheer, M. Buchanan, A. S. Springthorpe and P. Mandeville, Phys. Rev. Lett. 60, 2085 (1988); V. S. Goldman, D. C. Tsui and J. E. Cunningham, Phys. Rev. Lett. 58, 1256 (1987)

[3] H. Spohn, Rev. Mod. Phys. 53, 569 (1980)

[4] A. Goldberg, H. M. Schey and J. L. Schwartz, Am. J. Phys. 35, 177 (1967); W. H. Press, B. P. Flannery, S. A. Teukolsky and W. T. Vetterling, Numerical Recipes: the Art of Scientific Computing (Cambridge University Press, Cambridge 1986)

[5] S. Collins, D. Lowe and J. R. Barker, J. Phys. C 20, 6233 (1987); A. Grincwajg, On the time dependence of double barrier resonant tunneling (Diploma thesis at the Chalmers University of Technology, Göteborg 1986)

[6] B. Ricco and M. Ya. Azbel, Phys. Rev. B 29, 1970 (1984)
Figure Captions

Fig. 1 Time development of the normalized charge trapped in the well in the case of linear Schrödinger equation, i.e. $\alpha = 0$, for states with energy spread much wider ($\sigma = 110\ a_0$ and $\Gamma_0 = 43.2\ meV$), of the same order of ($\sigma = 825\ a_0$ and $\Gamma_0 = 5.8\ meV$) and much smaller ($\sigma = 5775\ a_0$ and $\Gamma_0 = 0.8\ meV$) than the resonance width ($\Gamma_R \simeq 5\ meV$). An atomic unit of time corresponds to $4.83\ 10^{-17}$ seconds and the Bohr radius $a_0$ is 0.529 Å.

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

Fig. 3 As Fig. 2 but with $\alpha = 1$. The case with $\sigma = 5775\ a_0$ is not shown.

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

Fig. 5 Self-consistent estimate of the time-averaged normalized charge trapped in the well for different values of the parameters $\alpha$ and $\sigma$. 
