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Time delay of wave packets during their tunnelling through a quantum diode

N.A. Ivanov, V.V. Skalozub

Abstract. **A modified saddle-point method is used to investigate the process of propagation of a wave packet through a quantum diode. A scattering matrix is constructed for the structure in question. The case of tunnelling of a packet with a Gaussian envelope through the diode is considered in detail. The time delay and the shape of the wave packet transmitted are calculated. The dependence of the delay time on the characteristics of the input packet and the internal characteristics of the quantum diode is studied. Possible applications of the results obtained are discussed.**

Keywords: *quantum diode, tunnelling, delay time of a wave packet.*

1. Introduction

The problem of the wave packet tunnelling through open quantum systems with resonance levels is one of difficult problems that has not been solved yet in nanophysics (see, for example, [1–5]). The main difficulty here is the need to take into account the impact of internal characteristics of quantum systems and the parameters of the input pulse on the process of signal propagation. Therefore, most developed approaches were not universal and could be applied only to study the tunnelling of a packet with a particular form of the envelope and a narrow class of systems with a similar geometry. Thus, propagation through a system with a 'narrow' and a 'broad' resonance levels was considered separately, i.e., a common approach to the description of the problem was absent.

The problem of tunnelling of wave packets through resonant quantum systems is not trivial, which is due to the presence of quantum and boundary effects associated with the superposition of incident and reflected wave functions. These effects are observed when signals propagate through such structures as double-barrier diodes, quantum tunnelling transistors and open heterostructures. These systems are widely used in modern micro- and nanoelectronics. Currently, a large number of modern scientific investigations are devoted to this issue. In a number of studies [6–8] we have developed a modified quasi-classical method that makes it possible to study analytically in the general form the process of wave packet tunnelling through a resonant quantum system. The approach is based on two main ideas: description of the system parameters in terms of the input packet (thereby eliminating the need to consider separately the cases of 'narrow' and 'broad' resonance levels) and use of a modified steepest-descent method. A quantum system is described by constructing a corresponding scattering matrix S, which allows one to introduce dimensionless variables corresponding to arbitrary quantum systems and wave packets.

The S-matrix formalism is widely used for establishing correspondence between the final states of the system, arising after the interaction, and the states that preceded them. The scattering matrix is given by a set of levels (channels) through which the tunnelling occurs. It contains all information about the behaviour of the system if we know not only the numerical values, but also the analytic properties of its elements; in particular, its poles determine the bound states of the system (i.e., discrete energy levels). To calculate the matrices use is made of the methods of the matrix element analysis or perturbation theory.

The poles of the S-matrix play an important role in the tunnelling process. They determine the existence of resonant levels in scattering structures. Consequently, for a detailed study of the scattering process it is needed to construct the corresponding scattering matrix and specify the characteristics of the input packet. The calculation of S-matrix elements can rely on a method based on the solution of the Lippmann–Schwinger equations for a given scattering potential [9, 10].

The initial scattering potential is represented as a superposition of unperturbed and perturbed parts. After finding Green's function for the first part the solution can be generalised to the case of a total potential. The next step is to calculate the R-matrix and to find the scattering matrix elements using the known formula for the relationship between these matrices. This approach is transparent and fully formalises the calculation of the scattering matrix to the case of an arbitrary potential.

The existence of potential wells with discrete energy levels is a common feature of such objects as quantum dots, two-barrier diodes and quantum tunnelling transistors. It is assumed that such structures have a similar resonant conductivity. That is why the analytical determination of the delay time during the propagation of the wave packets in the systems of this type is a very important problem [5, 11, 12]. In particular, its solution helps to choose the best parameters of the systems or packets at which the signal transmission speed is maximal. This points towards a further miniaturisation and increase in the performance of chips with quantum elements.

In this paper, we apply the method described above to calculate the scattering matrix of the quantum diode used in electronic devices. In addition, we calculate the delay time for a Gaussian wave packet at its entry to the input. The delay

N.A. Ivanov, V.V. Skalozub Oles Honchar Dnipropetrovsk National University, prosp. Gagarina 72, 49010 Dnepropetrovsk, Ukraine; e-mail1: rokosovskij@mail.ru, skalozubv@daad-alumni.de

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times for other packets can be calculated similarly based on the results obtained (e.g., in the case of a rectangular wave packet [7]).

2. *S*-matrix for perturbed potentials

In this section we present all the information necessary to calculate the scattering matrix (all the calculations are given in [10]). Here and below the level width is expressed in the widths of the packet, the time – in the packet durations, coordinates – in the characteristic dimensions of the signal.

According to the approach applied, we divide the system potential $V(z)$ in the perturbed $[\Delta V(z)]$ and unperturbed $[V_0(z)]$ parts, as shown in Fig. 1:

$$V(z) = \Delta V(z) + V_0(z). \tag{1}$$

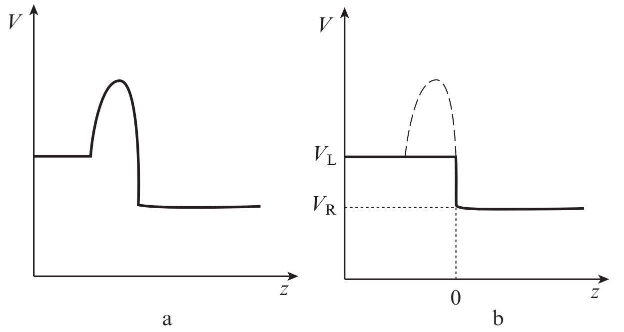

Figure 1. (a) Total potential of the system and (b) its representation as a sum of the unperturbed (solid curve) and perturbed (dashed curve) parts.

The scattering process can be described by a stationary Schrödinger equation

$$\left[\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2} - V_0(z) + v\right]\Psi(z,v) = \Delta V(z)\,\Psi(z,v). \tag{2}$$

Such an inhomogeneous equation can be solved using the Green function for the unperturbed part, which is the solution of the equation:

$$\left[\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2} - V_0(z) + v\right]\Gamma(z,z',v) = \delta(z - z'). \tag{3}$$

Its solution for a wave moving from the left ($z' < 0$) has the form

$$\Gamma(z,z',v) = \frac{m^*}{\mathrm{i}k_L\hbar^2}\left\{\exp[-\mathrm{i}k_L(z - z')] + \frac{k_L - k_R}{k_L + k_R}\exp[-\mathrm{i}k_L(z + z')]\right\},\ z < z',$$

$$\Gamma(z,z',v) = \frac{m^*}{\mathrm{i}k_L\hbar^2}\left\{\exp[\mathrm{i}k_L(z - z')] + \frac{k_L - k_R}{k_L + k_R}\exp[-\mathrm{i}k_L(z + z')]\right\},\ z' < z < 0, \tag{4}$$

$$\Gamma(z,z',v) = \frac{2m^*}{(\mathrm{i}k_L + \mathrm{i}k_R)\hbar^2}\exp[\mathrm{i}(k_R z - k_L z')],\ z > 0,$$

and for a wave moving from the right ($z' > 0$) has the form

$$\Gamma(z,z',v) = \frac{2m^*}{(\mathrm{i}k_L + \mathrm{i}k_R)\hbar^2}\exp[\mathrm{i}(k_R z' - k_L z)],\ z < 0,$$

$$\Gamma(z,z',v) = \frac{m^*}{\mathrm{i}k_R\hbar^2}\left\{\exp[\mathrm{i}k_R(z - z')] + \frac{k_R - k_L}{k_L + k_R}\exp[-\mathrm{i}k_R(z + z')]\right\},\ 0 < z < z', \tag{5}$$

$$\Gamma(z,z',v) = \frac{m^*}{\mathrm{i}k_R\hbar^2}\left\{\exp[\mathrm{i}k_R(z - z')] + \frac{k_R - k_L}{k_L + k_R}\exp[\mathrm{i}k_R(z + z')]\right\},\ z' < z.$$

For the Schrödinger equation in the absence of perturbation

$$\left[-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2} + V_0(z) - v\right]\Psi_0^{L(R)}(z,v) = 0 \tag{6}$$

we obtain the following solutions: for a wave propagating from the right

$$\Psi_0^L(z,v) = \exp(\mathrm{i}k_L z) + \frac{k_L - k_R}{k_L + k_R}\exp(-\mathrm{i}k_L z),\ z < 0,$$

$$\Psi_0^L(z,v) = \frac{2k_L}{k_L + k_R}\exp(\mathrm{i}k_R z),\ z > 0, \tag{7}$$

and for a wave propagating from the left

$$\Psi_0^R(z,v) = \frac{2k_R}{k_L + k_R}\exp(-\mathrm{i}k_L z),\ z < 0,$$

$$\Psi_0^R(z,v) = \exp(-\mathrm{i}k_R z) - \frac{k_L - k_R}{k_L + k_R}\exp(\mathrm{i}k_R z),\ z > 0. \tag{8}$$

The initial equation can be reduced to an equivalent integral equation using Green's function $\Gamma(z,z',v)$:

$$\Psi(z,v) = \Psi_0(z,v) + \int_{-b_L}^{b_R} dz'\,\Gamma(z,z',v)\Delta V(z')\,\Psi(z',v), \tag{9}$$

where $\Psi_0(z,v)$ is the solution to the Schrödinger equation in the absence of perturbation. For $z < -b_L$ we obtain

$$\Psi^L(z,v) = A^L(v)\exp(\mathrm{i}k_L z) + B^L(v)\exp(-\mathrm{i}k_L z), \tag{10}$$

where $A^L(v) = 1$;

$$B^L(v) = \frac{k_L - k_R}{k_L + k_R} + \frac{m^*}{\mathrm{i}\hbar^2 k_L}\int_{b_L}^{0} dz'\left[\exp(\mathrm{i}k_L z') + \frac{k_L - k_R}{k_L + k_R}\exp(-\mathrm{i}k_L z')\right]\Delta V(z')\,\Psi^L(z',v) + \frac{2m^*}{\mathrm{i}\hbar^2(k_L + k_R)}\int_0^{b_R} dz'\,\exp(\mathrm{i}k_R z')\Delta V(z')\,\Psi^L(z',v). \tag{11}$$

For $z > b_R$ we have

$$\Psi^{\mathrm{L}}(z,v) = C^{\mathrm{L}}(v)\exp(\mathrm{i}k_{\mathrm{R}}z) + D^{\mathrm{L}}(v)\exp(-\mathrm{i}k_{\mathrm{R}}z), \quad (12)$$

where $D^{\mathrm{L}} = 0$;

$$C^{\mathrm{L}}(v) = \frac{2k_{\mathrm{L}}}{k_{\mathrm{L}} + k_{\mathrm{R}}} + \frac{m^*}{\mathrm{i}\hbar^2 k_{\mathrm{R}}}\int_{b_{\mathrm{L}}}^{0}\mathrm{d}z'\Big[\exp(-\mathrm{i}k_{\mathrm{R}}z')$$

$$+\frac{k_{\mathrm{R}} - k_{\mathrm{L}}}{k_{\mathrm{L}} + k_{\mathrm{R}}}\exp(\mathrm{i}k_{\mathrm{R}}z')\Big]\Delta V(z')\,\Psi^{\mathrm{L}}(z',v)$$

$$+\frac{2m^*}{\mathrm{i}\hbar^2(k_{\mathrm{L}} + k_{\mathrm{R}})}\int_{0}^{b_{\mathrm{R}}}\mathrm{d}z'\exp(\mathrm{i}k_{\mathrm{R}}z')\Delta V(z')\,\Psi^{\mathrm{L}}(z',v). \quad (13)$$

The corresponding result for Ψ^{R} will be as follows: for $z > b_{\mathrm{R}}$

$$\Psi^{\mathrm{R}}(z,v) = C^{\mathrm{R}}(v)\exp(\mathrm{i}k_{\mathrm{R}}z) + D^{\mathrm{R}}(v)\exp(-\mathrm{i}k_{\mathrm{R}}z), \quad (14)$$

where $D^{\mathrm{R}} = 1$;

$$C^{\mathrm{R}}(v) = \frac{k_{\mathrm{R}} - k_{\mathrm{L}}}{k_{\mathrm{L}} + k_{\mathrm{R}}} + \frac{m^*}{\mathrm{i}\hbar^2 k_{\mathrm{R}}}\int_{0}^{b_{\mathrm{R}}}\mathrm{d}z'\Big[\exp(-\mathrm{i}k_{\mathrm{R}}z')$$

$$+\frac{k_{\mathrm{R}} - k_{\mathrm{L}}}{k_{\mathrm{L}} + k_{\mathrm{R}}}\exp(\mathrm{i}k_{\mathrm{R}}z')\Big]\Delta V(z')\,\Psi^{\mathrm{R}}(z',v)$$

$$+\frac{2m^*}{\mathrm{i}\hbar^2(k_{\mathrm{L}} + k_{\mathrm{R}})}\int_{b_{\mathrm{L}}}^{0}\mathrm{d}z'\exp(-\mathrm{i}k_{\mathrm{L}}z')\Delta V(z')\,\Psi^{\mathrm{R}}(z',v), \quad (15)$$

and for $z < -b_{\mathrm{L}}$

$$\Psi^{\mathrm{R}}(z,v) = A^{\mathrm{R}}(v)\exp(\mathrm{i}k_{\mathrm{L}}z) + B^{\mathrm{R}}(v)\exp(-\mathrm{i}k_{\mathrm{L}}z), \quad (16)$$

where $A^{\mathrm{R}} = 0$;

$$B^{\mathrm{R}}(v) = \frac{2k_{\mathrm{R}}}{k_{\mathrm{L}} + k_{\mathrm{R}}} + \frac{m^*}{\mathrm{i}\hbar^2 k_{\mathrm{L}}}\int_{b_{\mathrm{L}}}^{0}\mathrm{d}z'\Big[\exp(\mathrm{i}k_{\mathrm{L}}z')$$

$$+\frac{k_{\mathrm{R}} - k_{\mathrm{L}}}{k_{\mathrm{L}} + k_{\mathrm{R}}}\exp(-\mathrm{i}k_{\mathrm{L}}z')\Big]\Delta V(z')\,\Psi^{\mathrm{R}}(z',v)$$

$$+\frac{2m^*}{\mathrm{i}\hbar^2(k_{\mathrm{L}} + k_{\mathrm{R}})}\int_{0}^{b_{\mathrm{R}}}\mathrm{d}z'\exp(\mathrm{i}k_{\mathrm{R}}z')\Delta V(z')\,\Psi^{\mathrm{R}}(z',v). \quad (17)$$

We have obtained the wavefunctions Ψ^{R} and Ψ^{L} describing the states, which are to the right and to the left of the investigated structure. The input signal and its reflected part of the wavefunctions are described by equations (2) and (4) and the parts of the propagated signal are described by expressions (3) and (5), respectively. Thus we can determine the coefficients of transmission (C^{L}, B^{R}) and reflection (B^{L}, C^{R}) of the wavefunctions Ψ^{R} and Ψ^{L}. These values may be regarded as elements of transmission/reflection (TR) matrix:

$$\mathrm{TR} = \begin{vmatrix} B^{\mathrm{L}} & B^{\mathrm{R}} \\ C^{\mathrm{L}} & C^{\mathrm{R}} \end{vmatrix}. \quad (18)$$

Using the eigenstate matrix we can obtain the R-matrix (see, for example, [5]) of the system:

$$R = \Psi'(z,v)\,\Psi^{-1}(z,v). \quad (19)$$

After that, using the relations between R- and S-matrices we can calculate the later:

$$S = [R\Psi^+ - (\Psi^+)']^{-1}[R\Psi^- - (\Psi^-)'], \quad (20)$$

where Ψ^+ and Ψ^- are the divergent and convergent parts of the corresponding wave packets [10, 12].

3. Investigation of a quantum diode

Let us apply the above-developed approach to the calculation of the scattering matrix of the structure, the potential of which is shown in Fig. 2 – a real quantum diode finding wide application in modern electronics. Figure 3 shows one of the possible representations of the unperturbed part of this potential. According to the approach developed, we solve the Schrödinger equation for the unperturbed part and obtain the wave functions for each interval discussed. Next, using the sowing conditions, we find the amplitudes of the wave functions and the corresponding Green functions. We do not find it necessary to present the expressions derived in the body of this paper, because they are quite bulky and can be easily calculated by using known mathematical packages. Substituting

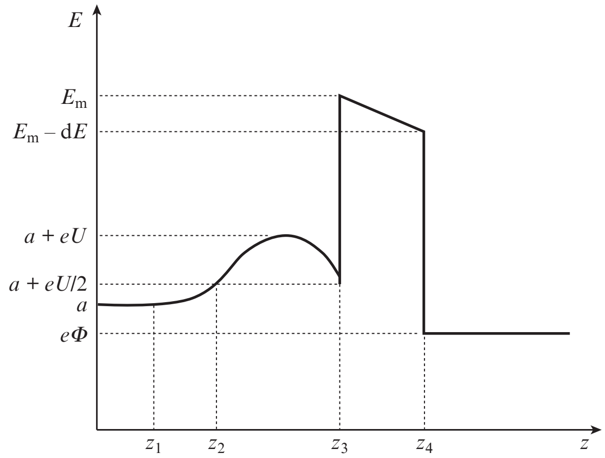

Figure 2. Potential energy in the diode under study.

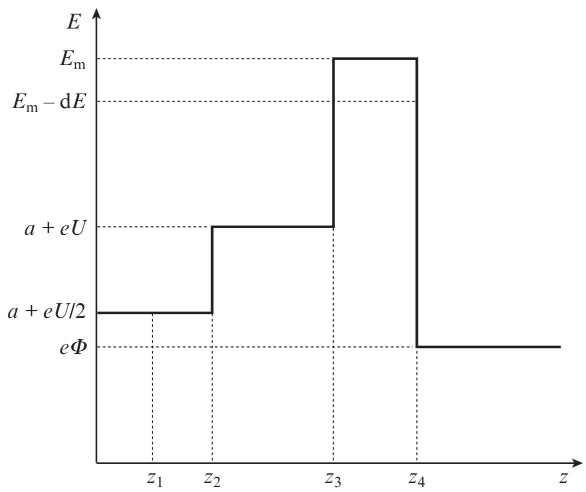

Figure 3. Representation of the potential in the absence of perturbation.

these expressions in (2), we find the reflection and transmission coefficients for the case of the perturbed potential, which, in turn, are solutions to the Lippmann–Schwinger equations in the next interpretation. The wavefunctions of the initial state and the wavefunctions obtained after the scattering process differ by the presence of an additional component, the existence of which is associated with the perturbation $\Delta V_1(z)$ in the interval $(z_1; z_2)$, the perturbation $\Delta V_2(z)$ in the interval $(z_2; z_3)$, etc. After the wavefunctions for each interval are found, we can construct a matrix $\hat{\Psi}$ of the eigenvalues of the wavefunction and the matrix

$$R = \hat{\Psi}'\hat{\Psi}^{-1}. \tag{21}$$

Now according to (20) we find the corresponding scattering matrix. This result can be used to describe the process of propagation of a Gaussian wave packet through the diode under study.

We will describe the input wave packet by the equation:

$$\Psi(k) = \exp\left[-\frac{1}{2}a^2(k-k_0)^2\right], \tag{22}$$

where a is the width of the packet. The calculation is performed using the dimensionless variables introduced in [6]. From the boundary conditions we find the saddle points of the integral expression given in [7], assuming that the packet will be observed after a sufficiently long period of time. The wave packet transmitted through the system is represented as a superposition of packets for all saddle points satisfying the boundary conditions. Once this packet is calculated, it is possible to find the argument of the wavefunction. This argument is related to the argument of the wavefunction of the input packet and only differs from it by some phase factor which depends on the kinetic energy of the input packet, the potential energy barrier and delay time. Hence, the delay time is calculated as a derivative of the argument of the wavefunction in energy (see, for example, [5]):

$$\Delta t = \frac{\mathrm{d}\arg\Psi}{\mathrm{d}E}. \tag{23}$$

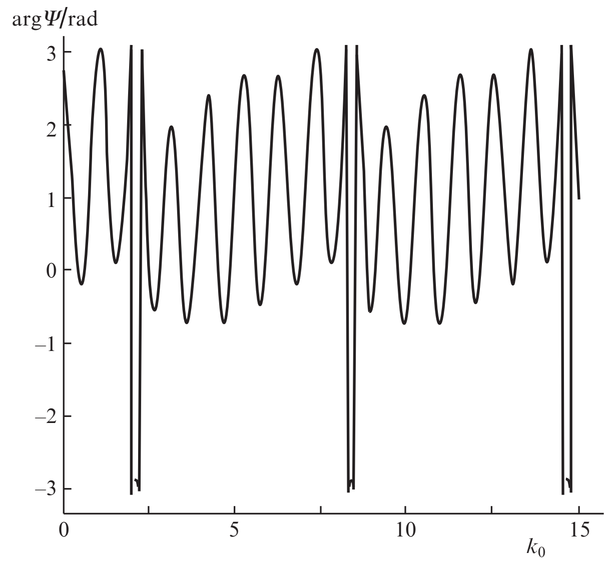

Figure 4. Argument of the packet wavefunction at $\Gamma = 1$ and wavenumbers $k_1 = 1$, $k_2 = 1$, $k_3 = 2$, $k_4 = 5$ and $k_5 = 1$, corresponding to the intervals on the z axis in Figs 2 and 3.

The argument of the wavefunction of a transmitted packet is presented in Fig. 4. The dependence of the delay time on the parameters of the system and momentum are presented in Figs 5 and 6. One can see that for some values of the input wave packet of the momentum, a minimum delay time is observed, which corresponds to the maximum speed of the packet tunnelling through the diode under consideration. A further change in the momentum does not reduce the delay time. When a certain value is reached, the increase in the momentum does not significantly affect the packet delay time.

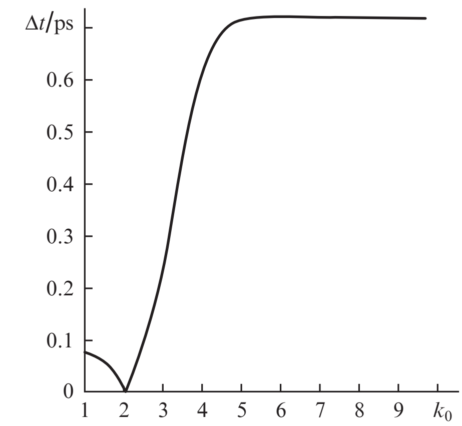

Figure 5. Packet delay time Δt for the system at $\Gamma = 1$ and wavenumbers $k_1 = 1$, $k_2 = 1$, $k_3 = 2$, $k_4 = 5$ and $k_5 = 1$.

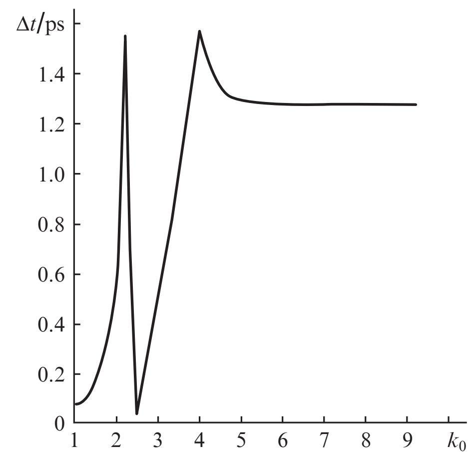

Figure 6. Packet delay time Δt for the system at $\Gamma = 1$ and wavenumbers $k_1 = 1$, $k_2 = 3$, $k_3 = 4$, $k_4 = 4$ and $k_5 = 1$.

4. Conclusions

We have investigated the delay time of packets in a quantum diode. We have studied in detail the propagation of a Gaussian wave packet through not a hypothetical but through a real resonant quantum structure used in practice. Calculations show that at some values of the system and packet parameters, one can observe total internal scattering. This means that the packet transmitted is absent, and the time delay is infinite.

A specific behaviour of the observed dependence of the tunnelling time on the parameters of the system and the packet can be used in practice. As mentioned in the Introduction, the problem of resonant tunnelling through an open quantum system has not been solved in general form. Therefore, the results obtained can be used in microelectronics for selecting the optimal packet parameters for the systems under consideration. The method developed is universal and allows one to study the tunnelling of the wave packets with different shapes of the envelope through random resonant quantum systems. A further application of this method is its generalisation to electromagnetic pulses and classical resonance systems. This issue will be addressed in our future work.

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