

# TRANSMISSION OF WAVE PACKETS THROUGH OPEN MESOSCOPIC SYSTEMS

*N. Ivanov\* and V. Skalozub*

*Dnipropetrovsk National University, 49010, Dnipropetrovsk, Ukraine*

(Received October 31, 2011)

Tunneling of the wave packets having rectangular and Gaussian forms through a quantum diode is investigated. By using the potential of the system the S-matrix for this structure is obtained and the analytic expressions describing the form of the transmitted pulse are calculated. These analytic solutions are compared with the numeric ones. An excellent coincidence is detected. The time-delay for the Gaussian pulse tunneling through the quantum dot is investigated in details.

PACS: 03.65.Pm, 03.65.Ge, 61.80.Mk

## 1. INTRODUCTION

The S-matrix formalism is commonly used in scattering theory for describing an association between a state after interaction with the one before interaction. This object contains a complete information on a system. For calculation of the S-matrix elements, either a perturbation theory is used or the methods based on studying of the S-matrix general characteristics are applied. The method for calculation of S-matrix elements was worked out in Ref. [1]. This approach is based on the establishing of the relationship between the final state and the state before interaction, presented in terms of the solutions for the Lippmann-Shwinger equation with a perturbed potential. By splitting a system potential in the perturbed and unperturbed parts and finding Green's functions for the former part, one can construct a solution. It gives a possibility to find the R-matrix of the scattering system. After that, using the relation between R- and S-matrices, one is able to determine the values of the scattering matrix elements.

The common feature of quantum dots, double-well diodes, quantum tunneling transistors is the existence of potential wells with discrete energy levels. At the same time, this results in the resonance conductivities of these systems. The problem of the time-delay determination (for pulse tunneling) is very important (see Refs. [2, 4]). Its solution, in particular, gives a possibility to find out for which parameters of the pulse or a quantum system the speed of the tunneling becomes maximal. Also it gives an opportunity for miniaturization and increasing the productivity of the microcircuit with quantum elements.

It is reasonable to begin with determining the characteristics of a wave packet best related with the quantum system. The approach applied here is based on the S-matrix formalism and modified saddle

point method developed in Refs. [1, 3]. It completely formalizes the solution of the wave packet tunneling problem and gives a possibility to define the form and the time-delay for arbitrary-form wave packets tunneling through a quantum system with resonance levels. The parameters of tunneling have to be expressed in terms of the incident pulse.

Using the approach of Ref. [5] let us obtain the S-matrix for the diode, which energy potential is represented in Fig. 1.

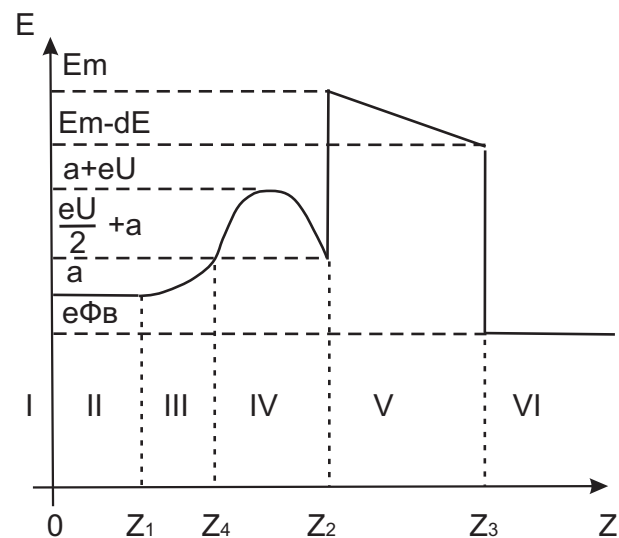


Fig. 1. Potential energy of diode

At first, we represent the potential eliminating the perturbation parts (from  $z_1$  to  $z_3$ ). Then we obtain the form of the diode potential (Fig. 2),

In this way we split the potential in the perturbed  $\Delta V(z)$  and unperturbed  $V_0(z)$  parts, respectively. The wave functions for the scattering state coming from the left are:

\*Corresponding author E-mail address: na\_ivanov@dsu.dp.ua

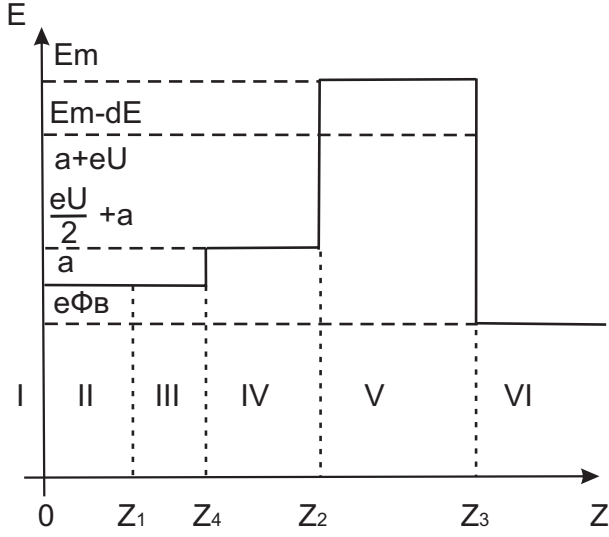


Fig. 2. Potential energy without perturbed parts

$$\begin{aligned}
\Psi_1^L &= e^{ik_1 z} + Ae^{-ik_1 z}, & z < 0, \\
\Psi_2^L &= Be^{ik_2 z} + Ce^{-ik_2 z}, & 0 < z < z_1, \\
\Psi_3^L &= De^{ik_3 z} + Ee^{-ik_3 z}, & z_1 < z < z_4, \\
\Psi_4^L &= Fe^{ik_4 z} + Ge^{-ik_4 z}, & z_4 < z < z_2, \\
\Psi_5^L &= He^{ik_5 z} + Ne^{-ik_5 z}, & z_2 < z < z_3, \\
\Psi_6^L &= Me^{ik_6 z}, & z_3 < z,
\end{aligned}$$

and for the one coming from the right are:

$$\begin{aligned}
\Psi_1^R &= e^{-ik_6 z} + A'e^{ik_6 z}, & z_3 < z, \\
\Psi_2^R &= B'e^{-ik_5 z} + C'e^{ik_5 z}, & z_2 < z < z_3, \\
\Psi_3^R &= D'e^{-ik_4 z} + E'e^{ik_4 z}, & z_4 < z < z_2, \\
\Psi_4^R &= F'e^{-ik_3 z} + G'e^{ik_3 z}, & z_1 < z < z_4, \\
\Psi_5^R &= H'e^{-ik_2 z} + N'e^{ik_2 z}, & 0 < z < z_1, \\
\Psi_6^R &= M'e^{-ik_1 z}, & z < 0.
\end{aligned}$$

Hence, by using the matching conditions we have found all the amplitudes for these states.

Then we obtain the Green-functions which are solutions of inhomogeneous Shrödinger equation

$$\left[ \frac{\hbar^2}{2m^*} \frac{d^2}{dz^2} - V_0(z) + v \right] \Gamma(z, z', v) = \delta(z - z') \quad (1)$$

for all of the potential sections ( $v$  is the particle energy). The solution for the Shrödinger equation with initial potential can be represented as the superposition of the unperturbed solution ( $\Psi_0 = \Psi_0(z, v)$ ) and the solution for the perturbation:

$$\Psi = \Psi_0 + \int dz' \Gamma_i(z, z', v) \Delta V(z') \Psi(z', v), \quad (2)$$

where  $i$  is a number of matching points and  $\Gamma_i(z, z', v)$  corresponds to a potential block Green-function. This equation represents the solution of the Lippmann-Schwinger equation. For each of this blocks we can obtained the transmission and reflection coefficients taking into account the consecutive order of matching points and the corresponding to them Green's functions. After that we use the well-known relationship between these coefficients and the S-matrix elements. In this way we find the S-matrix for the resonant system.

## 2. FORM OF THE TRANSMITTED WAVE-PACKET

The incident and outgoing pulses are bound by the next expression:

$$\Psi_a^{out} = \frac{1}{2\pi} \sum_b \int_{-\infty}^{\infty} \Psi_b^{in} S_{b,a} dk, \quad (3)$$

which is integrated over all the  $k$ -space. The parameters of the outgoing pulse wave function are:  $x$  is the coordinate variable,  $t$  is the time variable,  $k$  and  $k_0$  are momentum and center of incident wave packet in the momentum space.  $k_j$  are the positions of S-matrix poles. We consider the incident pulse width  $a$  in the real space and all calculations will be realized in terms of the unperturbed pulse.

Let us make use the next dimensionless variables:

$$\begin{aligned}
q' &= \frac{x}{a}; \quad \tau = \frac{t}{t_a}; \quad z = a(k - k_0); \quad l_j = ak_j; \\
\rho_j &= a \frac{\Gamma_j}{2}; \quad l_0 = ak_0.
\end{aligned}$$

Moreover, to simplify further expressions we introduce the parametrization:

$$\beta = \frac{1 + i\tau}{2}, \quad q_{0j} = l_0 - l_j + i\rho_j, \quad q = q' - l_0\tau. \quad (4)$$

Here, the coordinate variable becomes  $q$ , time -  $\tau$ ,  $t_a = ma^2/\hbar$ ,  $l_j$  and  $l_0$  are the localization poles and center of wave packet respectively, and  $\rho_j$  is the width of  $j$ -th resonance level. These variables give us a sufficient number of parameters to describe the wave packet tunneling through a quantum system with resonance levels. Now we make use of a modified saddle-point method to obtain a transmitted solution [1]. Time interval  $\tau$  after which we observe the outgoing wave packet should be larger than  $t_a$ . This is the necessary condition for the existence of the resonance. A saddle point position is defined by the stationarity conditions:

$$\begin{aligned}
\frac{dg(z)}{dz} &= 0, \quad \Im g(z) = \text{const}, \\
\Re g(z) &< \Re g(z_k),
\end{aligned} \quad (5)$$

where  $z_k$  is the  $k$ -th saddle point. The resulting part of the resonance wave function amplitude near the stationarity point is

$$\begin{aligned}
\Psi(q > 0, \tau) &\sim \frac{1}{a} e^{il_0(q - \frac{1}{2}l_0\tau)} \times \\
&\times \sum_{jk} e^{g_j^{res}(x_k^s)} \sqrt{-\frac{1}{e^{g_j^{res}{}'(x_k^s)} f_j^{res}(x_k^s)}}. \quad (6)
\end{aligned}$$

This formula gives the asymptotic representation for the wave packet passed through a resonance quantum system.

### 3. TUNNELING OF PACKETS THROUGH A QUANTUM DOT

Let us apply the developed method to investigate the tunneling of the squared-form wave packet through the quantum dot with one resonance level. The packet is described as the difference of two step-functions:

$$\Psi(x) = \Theta(x) - \Theta(x - a), \quad (7)$$

where  $a$  is the packet width. We use the known Fourier-transform for  $\Theta$ -function, obtained in Appendix (Eq. (14)). Applying the matching conditions (5) we find two saddle points. For outgoing wave packet, considering the two saddle points, we get superposition of each result (Fig. 4). For the Gaussian-form incident wave packet tunneling through this quantum system, like in the case with square-form packet, we obtain (Fig. 3):

$$\Psi(z) = \Psi_0 \exp(-z^2/2), \quad (8)$$

where  $\Psi_0$  is the amplitude,  $\Psi(z)$  is the form of the incident wave packet. In this way the exponential argument becomes:

$$g(z) = izq' - \beta z^2 - \ln(z - q_0). \quad (9)$$

Hence we find the saddle point:

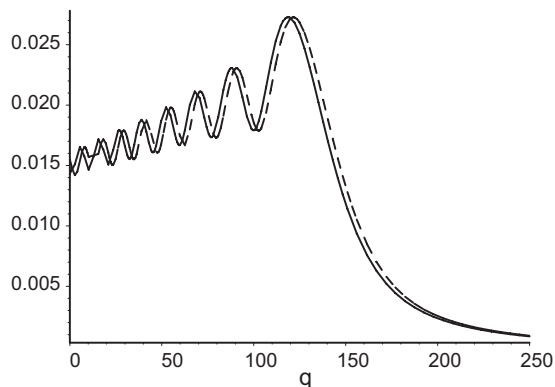
$$z_1 = \frac{1}{2} \left( q_0 + \frac{iq'}{2\beta} \left[ \left( q_0 - \frac{iq'}{2\beta} \right)^2 - \frac{1}{2} \right]^{1/2} \right). \quad (10)$$

For  $\tau \rightarrow \infty$  with the accuracy up-to-the-second order we obtain:

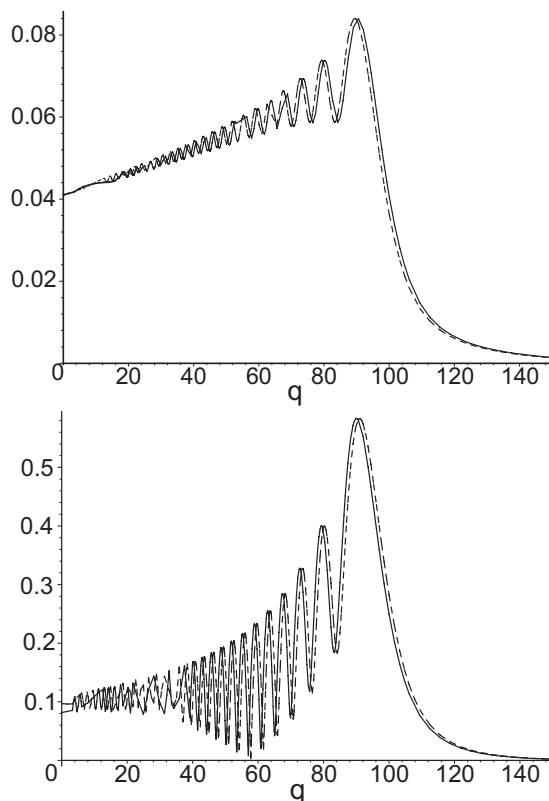
$$\Psi^{res}(q, \tau) = \frac{i\rho_j a_j}{\sqrt{2\pi}} e^{-\frac{(q-l_0\tau)^2}{2+2\tau^2} + i \arg(\Psi)} \times \frac{(1+\tau^2)^{1/4}}{[(q+\rho_i-l_i\tau)^2 + (\rho_i\tau+l_i-l_0)^2]^{1/2}}, \quad (11)$$

where the argument is

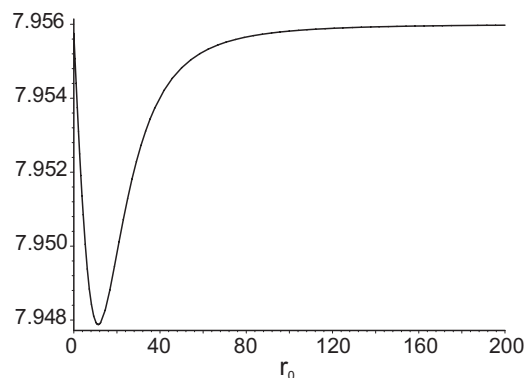
$$\arg(\Psi) = \frac{1}{2} \arctg(\tau) + \frac{(q-l_0\tau)^2\tau}{2+2\tau^2} - \arctg \left[ \frac{\rho_i\tau+l_i-l_0}{q+\rho_i-l_i\tau} \right]. \quad (12)$$



**Fig. 3.** Wave-function amplitude for the Gaussian pulse tunneling through the quantum dot, for the saddle point method (dashed line) and an exact integration (continues line) for  $\tau = 100$ ,  $a_1 = 1$ ,  $l_0 = l_1 = 1$ ,  $\rho = 0.09$



**Fig. 4.** Amplitude for the step-form pulse tunneling through the QD, for the saddle point method (dashed line) and an exact integration (continues line) for  $\tau = 100$ ,  $a_1 = 1$ ,  $l_0 = l_1 = 1$ ,  $\rho = 0.04$  (top) and  $\rho = 0.007$  (bottom)

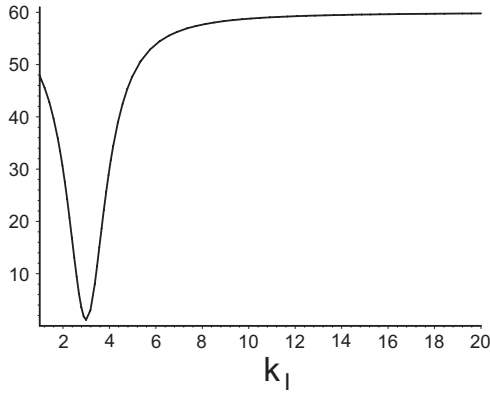


**Fig. 5.** Time-delay for the Gaussian pulse transmission (dependency from energy level width) with  $a = 1$ ,  $t_a = 1$ ,  $t = 100$ ,  $x = 300$ ,  $k_0 = 1$ ,  $k_i = 1$

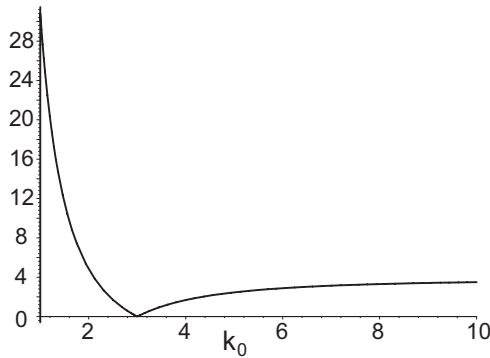
The wave function of the outgoing pulse differs from the incident wave packet by some phase factor. This factor depends on the kinetic energy of the incident pulse, the potential energy of a barrier and time-delay. The delay can be calculated (Figs. 5-7) following Ref. [2]:

$$\Delta t = \frac{d \arg(\Psi)}{dE}. \quad (13)$$

Hence the advantage of analytic (asymptotic) methods is obvious. The time-delay depends on the pulse and system parameters (the dependencies are shown in Figs. 5-7).



**Fig. 6.** Time-delay for the Gaussian pulse transmission (dependency from  $s$ -matrix poles position) with  $t_a = 1, t = 100, a = 1, x = 300, k_0 = 1, \Gamma = 1$



**Fig. 7.** Time-delay for transmission Gaussian pulse (dependency from incident pulse momentum) with  $t_a = 1, t = 100, a = 1, x = 300, k_i = 1, \Gamma = 1$

#### 4. CONCLUSIONS

Tunneling of the wave-packets having the Gaussian and the rectangular form is investigated. The results obtained show that the usage of the  $S$ -matrix formalism and the saddle point method gives enough pa-

rameters to describe the dynamics of the scattering processes. This approach gives a possibility to calculate a time-delay of the wave packet transmitting through quantum systems like quantum dots, double-well diodes, transistors. It was shown, in particular, that for some specific values of the system and the pulse parameters a full internal scattering is realized. This means that an outgoing pulse is absent, tunneling does not happen.

#### 5. APPENDIX

For completeness, let us present the outgoing wavefunction for the step-form pulse tunneling through the quantum dot:

$$\Psi(q, \tau) = \frac{1}{a\sqrt{2\pi}} e^{il_0(q - \frac{1}{2}l_0\tau)} \int_{-\infty}^{\infty} dz \left\{ \frac{a}{iz} + \pi\delta\left(\frac{z}{a}\right) - e^{-iz} \left[ \frac{a}{iz} + \pi\delta\left(\frac{z}{a}\right) \right] \right\} e^{izq' - (\beta - \frac{1}{2})z^2}. \quad (14)$$

#### References

1. U. Wulf, V.V. Skalozub, and A. Zaharov. Multi-saddle-point approximation for pulse propagation in resonant tunneling // *Phys. Rev.* 2008, v. B77, p. 045318-045325.
2. M. Razavy. *Quantum Theory of Tunneling*. "World Scientific", 2003, p. 351-375.
3. N.A. Ivanov, V.V. Skalozub. Propagation of wave packets through resonant quantum systems // *Theoretical and Mathematical Physics*. 2010, v. 168 (2), p. 1096-1104.
4. L. Brillouin. *Wave Propagation and Group Velocity*. New York: "Academic Press", 1960.
5. P.N. Racec. *Ph. D. Thesis*. Cottbus: University of Technology, 2002.

### ПРОХОЖДЕНИЕ ВОЛНОВЫХ ПАКЕТОВ ЧЕРЕЗ ОТКРЫТЫЕ МЕЗОСКОПИЧЕСКИЕ СИСТЕМЫ

*Н.А. Иванов, В.В. Скалозуб*

На основе решения уравнения Липпманна-Швингера для возмущенного потенциала рассчитывается матрица рассеяния туннельного диода. Используя формализм  $S$ -матрицы и модифицированный метод седловой точки, аналитически рассчитывается форма волнового пакета, выходящего из квантовой точки при подаче на нее пакетов гауссовой и прямоугольной форм. Найдена и проиллюстрирована зависимость времени задержки сигнала гауссовой формы при туннелировании для случая квантовой точки.

### ПРОХОДЖЕННЯ ХВИЛЬОВИХ ПАКЕТІВ КРІЗЬ ВІДКРИТІ МЕЗОСКОПІЧНІ СИСТЕМИ

*М.А. Іванов, В.В. Скалозуб*

На основі розв'язку рівняння Липпманна-Швінгера для збуреного потенціалу розраховано матрицю розсіювання тунельного діоду. Користуючись формалізмом  $S$ -матриці та модифікованого методу сідлової точки, аналітично розраховується форма хвильового пакету, що виходить з квантової точки при подаванні на неї пакетів гауссової та прямокутної форм. Знайдено та проілюстровано залежність часу затримки сигналу гауссової форми при тунелюванні для випадку квантової точки.