Nuclear Instruments and Methods in Physics Research B xxx (2014) xxx–xxx

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

Some peculiarities in an electron conductivity in a system of quantum dots

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ARTICLE INFO

Article history:
Received 30 July 2014
Received in revised form 6 November 2014
Accepted 7 November 2014
Available online xxxx

Keywords:
Quantum tunneling
Quantum dots
Numerical calculations
Virtual levels

ABSTRACT

Based on the laws of quantum mechanics with the usage of numerical methods the peculiarities in a tunnel transition of a particle in a system of quantum wells and barriers are considered.

1. Introduction

Methods of the one-particle quantum theory allow us to understand the sufficiently complex phenomena in physics, which actually to be realized in the modern microelectronic devices which size is comparable with the length of De-Broglie wave of electron on the Fermi surface (see e.g., [1–3]). Among other important notions which have been arisen in physics with the creation of quantum mechanics the significant position belongs to the tunneling. In his Nobel Prize lecture [4] the creator of the tunnel diode L. Esaki mentioned some significant achievements in which the key role belongs to the tunneling effect. Oppenheimer explained the autoionization of the excited state of atomic hydrogen as a tunnel effect. On the basis of the submission of the electronic tunneling Fowler and Nordheim explained the main features of the phenomenon of cold emission of metals exposed to a strong external electric field. These ideas were used by Gamow and Gurney & Condon to describe the α-decay as a tunneling process. Subsequently, with this theory, Rice gave a description of molecular dissociation. There is a considerable number of other applications of the tunnel effect. We would like to mention here of a series of papers devoted to the so-called cascade lasers (see e.g., [5,6]), where the resonance tunneling in heterostructures defined the mostly important properties of the device. This kind of tunneling is more complicated because it performs at the presence of external high frequency electromagnetic field.

Previously [7,8] we have investigated those peculiarities of conductivity as the oscillating processes during the tunneling from one quantum dot to another. These movements sometime occur on a background of a continuous trend. In particular, such a reciprocating oscillatory tunneling of the electron in a hydrogen atom scattering by a proton at rest. As another example, one can specify the phenomenon of quasi-tunneling in multidimensional problems, when the passage of an electron from one quantum dot to another through a barrier in the presence of a peculiar gap in it occurs due to the partial overlap of the potential fields of neighboring quantum dots. Influence of an external electric field on these processes is an important issue that needs to be studied adequately in detail, since it has considerable practical importance. In particular, results of such investigations are important in the problem of interaction of a projectile with a crystal surface, at a proper description of the surface peak in experiments on Rutherford back scattering and its relation to the channeling phenomena in a crystal. Moreover, in the latest time the great interest was attracted by the problem of scattering of particles on porous targets [9]. The 3-dimensional tunnel transitions of the electron between the Coulomb potential wells allow us to estimate the time of tunnel transition of the hole in a silicon crystal. This time could help us to estimate such an important parameter as the effective mass of the hole in Si. In all of the problems we are mostly dealing with the real particles and therefore we consider the real mass of the electron in all our tasks. In our work we are restricting ourselves with the mentioned set of tasks.

The plan of the article is follows. In the second subsection we consider a free motion of the particle in one-dimensional

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http://dx.doi.org/10.1016/j.nimb.2014.11.027
0168-583X/

Kronig–Penney type periodic structure. We apply the matrix form of calculations. In the third subsection we solve the same problems but at the presence of the external electric field. In the fourth subsection we consider more complex one-dimensional structure with the sequence of parabolic wells, assuming the propagation of the wave packet instead of the individual state. In subsection 5 we consider the demolition of the zone structure at the presence of external field. Subsection 6 is devoted to the 3-dimensional cases. In subsection 7 we present the main results of the work.

In the paper, unless explicitly stated, atomic units are used.

2. Motion of particles in one-dimensional and layered structures of barrier type

In this section the consideration of motion of electrons is performed for one-dimensional Kronig–Penney structure. These structures could be obtained and really performed artificially, for example, in heterostructures (see e.g., in [3]). The other example presents the projectile which is falling on the one-dimensional structure (alternatively, on the layered structure) being not the plane wave. First we consider the periodic structure. The barriers assume to be rectangular with the width a and the inter barrier distance b. The period of the structure is $d = a + b$ (Fig. 1). The analysis of dependence the reflection and transmission coefficients on the parameters represents important theoretical and technological information. It is known, for example, that at the penetration of a particle through a barrier system the sharp maxima of the transmittance will occur in consequence of the resonant tunneling (see e.g., in [10]). The example of solution of the problem is presented below (Fig. 2). In a case of two barriers we have:

$$\psi = \begin{cases} A_1 e^{ikx} + B_1 e^{-ikx}, & x < 0 \\ C_1 e^{-\gamma x} + D_1 e^{\gamma x}, & 0 < x < a \\ A_2 e^{ik(x-a)} + B_2 e^{-ik(x-a)}, & a < x < a+b \\ C_2 e^{-\gamma(x-d)} + D_2 e^{\gamma(x-d)}, & d < x < d+a \\ A_3 e^{ik(x-a-d)} + B_3 e^{-ik(x-a-d)}, & d+a < x \end{cases}$$

Introduce the matrices:

$$P_1 = \begin{pmatrix} 1 & 1 \\ -\gamma & \gamma \end{pmatrix} \quad S_1 = \begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix},$$

$$P_2 = \begin{pmatrix} e^{-\gamma a} & e^{\gamma a} \\ -\gamma e^{-\gamma a} & \gamma e^{\gamma a} \end{pmatrix} \quad S_2 = \begin{pmatrix} e^{ikb} & e^{-ikb} \\ ike^{ikb} & -ike^{-ikb} \end{pmatrix},$$

matrices $M = S_1^{-1} P_2 P_1^{-1} S_1$ and $N = S_1^{-1} P_2 P_1^{-1} S_2$. Then, for example, for three barriers one gets

$$\begin{pmatrix} A_4 \\ B_4 \end{pmatrix} = N^2 M \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \quad A_1 = 1,\ B_4 = 0;\ E = N^2 M$$

$$\begin{pmatrix} 1 \\ B_1 \end{pmatrix} = E^{-1} \begin{pmatrix} A_4 \\ 0 \end{pmatrix} \rightarrow A_4 = \frac{1}{(E^{-1})_{11}},\ B_1 = \frac{(E^{-1})_{21}}{(E^{-1})_{11}}.$$

The virtual levels may be found from the condition, that the reflected wave must be equal to zero, or $(E^{-1})_{21} = 0$.

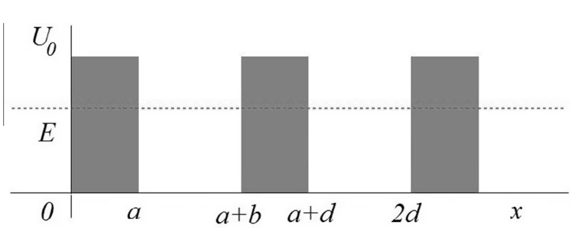

Fig. 1. The system of three barriers.

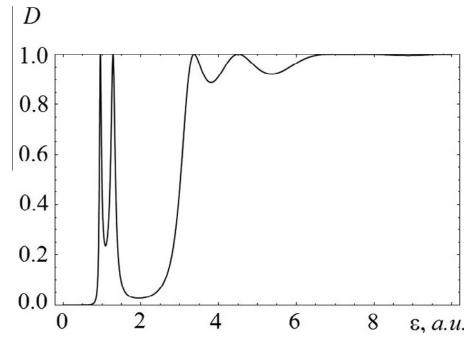

Fig. 2. The dependence of the transmission coefficient through the barriers shown in Fig. 1 ($a = 1$, $b = 1$). Two peaks in the energy region below the barrier height determined the zone of virtual levels. The first peak corresponds to the energy 0.957 a.u. The corresponding wave function is shown in Fig. 3.

The numerical analysis for the spatially bounded structures reveals a series of peculiarities of the phenomenon. For the ordered structure the number of maxima is turned to be equal to the number of barriers minus one. Additionally, at the energies which exceed the barrier height some energy zones also exist, in which the number of maxima is the same as in the tunneling process.

This fact can be understood as a manifestation of existence of some set of so-called virtual energy levels both below and above the barriers. Calculation of the wave functions of the electron experiencing resonant tunneling show its increased amplitude in the region between the barriers compared to area occupied by the barriers (see Fig. 3). There is an idea that the probability of the electron in resonance being between the barriers increases and therefore it penetrates through the entire barrier system with a certain time delay. This time should be determined according to Wigner from the phase of corresponding element of the scattering matrix by performing the derivation on the energy (see e.g., [11]). In our case, the answer can be obtained by dividing the average excess of the probability density inside the barrier system by the probability flux density in the incident wave. Evaluations show that the time delay significantly exceeds the time of the passage of the distance equal to the barrier structure size by a free particle.

For example, in Fig. 2 the virtual levels have two components located on a small energy distance from each other. There are the maxima placed over the height of barriers which should be considered as corresponding to the additional virtual levels (see Fig. 2). As we see, the energy distance between these upper virtual levels increases significantly compared to the bottom virtual levels and

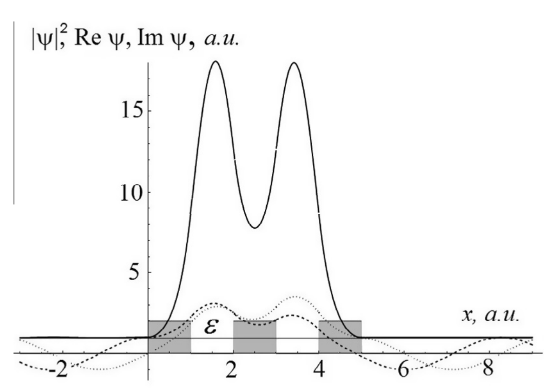

Fig. 3. The electron wave function corresponding to the resonance energy value (Fig. 2, left peak in the energy region below the barrier). The real part (dash line), the imaginary part (dot line) and the square of the modulus (solid line) are shown. The shaded boxes show the barriers; the energy level is indicated by the thin solid line ($a = 1$, $b = 1$).