SYNCHROINFO JOURNAL

www.media-publisher.eu/synchroinfo-journal

TUNNEL BROADENING OF RESONANT LEVELS IN LAYERED QUANTUM-SIZE STRUCTURES

Alexey P. Zhilinsky [1], **Vladimir F. Degtyarev** [1],

[1] Moscow technical University of communications and Informatics, Moscow, Russia; vfsteel2008@gmail.com

ABSTRACT

The microparticles interaction with potential barriers of various nature and form is the quantum physics and nanoelectronics basis. The nature of this interaction largely determines modern radio engineering devices and complexes operation, information transmission and processing systems. At present, semiconductor quantum-well structures, in particular hetero-structures with quantum wells (QWs) and barriers (QWs), occupy leading positions as materials for opto- and nanoelectronics. It has been found that chain consisting of a sequence formation of potential wells and barriers gives rise to resonant levels for which the structure transparency is equal to unity. With an increase in the number of chain links, these levels split into close sublevels, the energy and half-width of which depend on the barriers parameters and the number of chain cells. A technique is proposed to determine the characteristics of these levels, in particular, the half-width of sublevels. The wave function dependence on chain parameters is studied. Problems related to the propagation of waves in layered media also arise in many other branches of science and technology. In particular, such media as plasma, ionosphere, atmosphere, ocean contain layered structures. Solving the problems of wave propagation in these media, calculating the reflection and transmission coefficients during the propagation of electromagnetic waves are of great importance both for calculating radio paths with reflection from the ionosphere and for many problems of remote diagnostics of ionospheric plasma. The issues discussed in this paper may be of interest to specialists in these areas.

KEYWORDS: *Quantum mechanics, Quantum barrier, Wave function, Transparency, Nanoelectronics, tunneling.*

DOI: 10.36724/2664-066X-2023-9-1-30-37

Received: September 05, 2022
Accepted: October 20, 2022

Citation: Alexey P. Zhilinsky, Vladimir F. Degtyarev, "Tunnel broadening of resonant levels in layered quantum-size structures," *Synchroinfo Journal* **2023**, vol. 9, no. 1, pp. 30-37.

Licensee IRIS, Vienna, Austria.

1. Introduction

The main parameter of tunnel effect - transmittance (transparency) of a potential barrier or a chain of barriers. This parameter is usually calculated for single rectangular potential barriers with/or without QWs [1, 2]. The influence of the formation of a chain of barriers on the characteristics of levels has not been studied enough

Problems related to the propagation of waves (electromagnetic, electronic) in layered media also arise in many other branches of science and technology. In particular, such media as plasma, ionosphere, atmosphere, ocean contain layered structures. Solving the problems of wave propagation in these media, calculating the reflection and transmission coefficients during the propagation of electromagnetic waves are of great importance both for calculating radio paths with reflection from the ionosphere and for many problems of remote diagnostics of ionospheric plasma [3].

2. Technique modeling

In this paper, the wave functions and transparency coefficients of the barrier system were found by directly solving the stationary Schrödinger equation with the corresponding boundary conditions in the MAPLE computer algebra system.

This equation in this case has the form

$$\frac{d^2\Psi}{dx^2}+\frac{2m}{h^2}(E-U)\Psi=0 \qquad (1)$$

where E – Is the energy of a microparticle incident on the chain, Ψ – волновая функция.

A chain of wells and barriers with the following parameters was considered: the barrier width (a) is 10 angstroms, its height (U) is 2 eV, and the well width (b) is 10 angstroms. The amplitude of the incident wave was taken equal to unity ($\Psi_{in}(x)=e^{ikx}$). The T(E) dependence (T is the transparency coefficient of the chain) was used to determine the position of the peak maximum (E0), its energy width ΔE_{05} at half height and quality factor ($Q=\frac{E_0}{\Delta E_{05}}$). Since goodness is expressed in terms of E_0 and ΔE_{05}, the main attention was paid to these characteristics. We emphasize that the results obtained in this example, as well as the developed technique, also apply to chains with other parameters.

Equations of type (1) also arise in problems of seismic, optics, and plasma physics, for example, when describing the incidence of a plane wave on a layered medium at different angles [4]. In this case, the results obtained can be used to describe the propagation of any plane waves, if their "stationary state" is described by an equation similar to (1). In addition, since the dependence U(x) describes plane inhomogeneities in space, then, at oblique incidence of the wave on such obstacles, all the features of the solutions presented below remain valid if we replace E to $E_{eff} = E(1-\sin^2\theta) = E\cos^2\theta$, where θ – angle of a plane wave incidence on the barrier. The resonant energy values will then depend on θ.

3. Simulation results and discussion

The simulation results show that resonant tunneling levels (RTL) are formed in the system of successive potential wells and barriers, for which the transparency of the structure is equal to unity. The appearance of these levels is due to the resonance of the forward and backward waves. The energy of these peaks depends on the width and depth of the well and is determined by the condition that an integer number of half-waves of the electron wave function fit within the well width [5, 6]. For the elementary link of the considered chain, these levels have the following energy values:

E_{01} = 0.228949 eV, E_{02} = 0.887201 eV and E_{03} = 1.818140 eV.

Since the transparency of the barriers is small, these values are close to the energy eigenvalues in a potential well of finite depth [5, 6].

A typical curve of the dependence of the transparency of one link on the energy of a microparticle for the lower energy level is shown in Figure 1. The characteristic parameters of such a curve are: the energy position of the maximum transparency is E_0, the width of the peak at half its height (half-width) – ΔE_{05}, and corresponding wave function. For the single link first level in the considered system E_{01} = 0.228949 eV, ΔE_{05} = 2.80 10^{-7} eV.

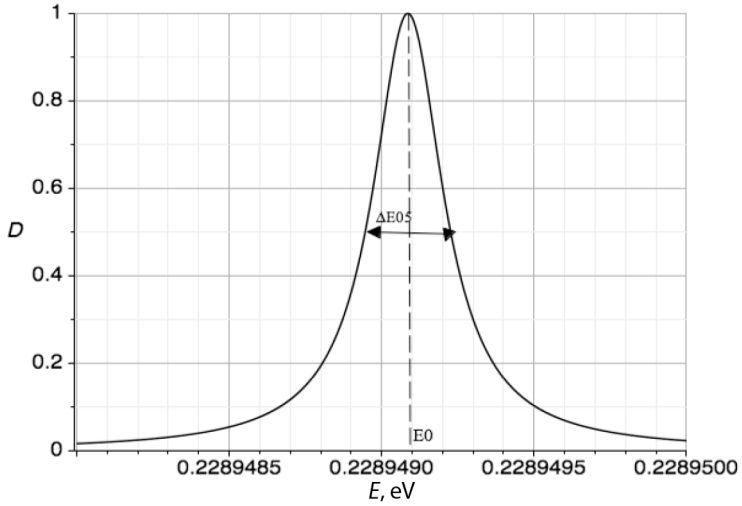

Fig. 1: Dependence of the transparency of a single link in the chain on the energy of the micropar-ticle for the resonance peak E_{01} = 0.228949 eV

It can be seen from the figure that the shape of the resonance transparency curve corresponds to the Lorentz one and is determined by the mechanism of passage of microparticles through a given structure. In a chain of barriers, the behavior of resonant peaks is much more complicated. In this regard, the following can be noted:

1. When a chain is formed, the resonant levels that arise in a single link are split into a system of sublevels, the number of which is equal to the number of cells in the system. The energy position of these sublevels is determined by the effectiveness of the interaction of links. The scheme of splitting of the initial level with energy E01 = 0.228949 eV in a chain of 11 links is shown in Figure 2. The parameters of the resulting sublevels are given in Table 1. It can be seen from the figure that the split sublevels are located symmetrically with respect to the initial level. This behavior of RTA is associated with the features of the vibrational spectrum of microparticles in a system of interacting cells, where each peak is associated with the excitation of a certain vibrational mode [7, 8]. So, for example, the first peak (Fig. 2) corresponds to the first oscillation mode, when oscillations in all cells occur in one phase and one half-wave fits along the length of the chain, for the second - two. For the third peak, three half-waves fit along the length of the chain, and so on. It should be noted that oscillations in neighboring half-waves occur in opposite phases [7, 8].

The study of mechanical and electromagnetic oscillations in systems consisting of N identical links was carried out in a number of works [7, 8, 12-17].

A system of two connected links can be considered as two independent oscillators with resonant frequencies equal to

$$\omega_1 = \frac{\omega_0}{\sqrt{1+K}} \quad \text{and} \quad \omega_2 = \frac{\omega_0}{\sqrt{1-K}}$$

In this case, oscillators with frequency ω1 oscillate in one phase, and c ω_2 in anti-phase (the wave functions in cells 1 and 2 have opposite signs).

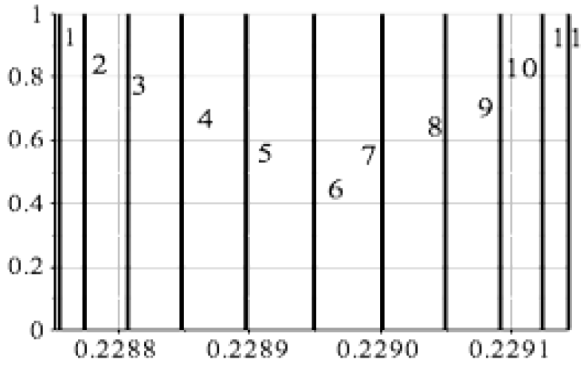

Fig. 2: Scheme of splitting a single level E_{01}=0.228949 eV in a chain consisting of 11 links

Table 1. Characteristics of resonant tunneling levels in a chain (N is the number of links)

Links number	Mode number	Energy, eV	Peak half-width ΔE_{05}, eV. Complex modeling results	Peak half-width ΔE_{05}, эВ. Calculation by ratio (5)
1	1	0.228949	$2.800\ 10^{-7}$	$2.800\ 10^{-7}$
3	1	0.228806	$7.00\ 10^{-8}$	$7.00\ 10^{-8}$
	2	0.228949	$1.400\ 10^{-7}$	$1.400\ 10^{-7}$
	3	0.229091	$7.00\ 10^{-8}$ 2.810^{-7}	$7.00\ 10^{-8}$ $2.8\ 10^{-7}$
5	1	0.228774	$2.67*10^{-8}$	$2.33\ 10^{-8}$ $7.03\ 10^{-8}$ $9.38\ 10^{-8}$
	2	0,228848	$6.67*10^{-8}$	$7.00\ 10^{-8}$ $2.33\ 10^{-8}$ $2.807\ 10^{-7}$
	3	0.228949	$1.00*10^{-7}$	
	4	0.229049	$6.67*10^{-8}$	
	5	0,229123	$2.33*10^{-8}$ $2.834\ 10^{-7}$	
11	1	0.228755	$3.20\ 10^{-9}$	$3.15\ 10^{-9}$
	2	0.228775	$1.11\ 10^{-8}$	$1.17\ 10^{-8}$
	3	0.228807	$2.30\ 10^{-8}$	$2.33\ 10^{-8}$
	4	0.228849	$3.49\ 10^{-8}$	$3.50\ 10^{-8}$
	5	0.228897	$4.38\ 10^{-8}$	$4.40\ 10^{-8}$
	6	0.228949	$4.67\ 10^{-8}$	$4.67\ 10^{-8}$
	7	0.229001	$4.38\ 10^{-8}$	$4.38\ 10^{-8}$
	8	0.229049	$3.52\ 10^{-8}$	$3.50\ 10^{-8}$
	9	0.229091	$2.34\ 10^{-8}$	$2.34\ 10^{-8}$
	10	0.229124	$1.2\ 10^{-8}$	$1.17\ 10^{-8}$
	11	0.229144	$3.2\ 10^{-9}$ $2.78\ 10^{-7}$	$3.2\ 10^{-9}$ $2.803\ 10^{-7}$

A system consisting of three oscillators has three resonant frequencies

$$\omega_1 = \frac{\omega_0}{\sqrt{1+K^*}}, \omega_2 = \omega_0, \omega_3 = \frac{\omega_0}{\sqrt{1-K^*}}.$$

Here K and K^* are the coefficients of mutual connection for chains consisting of 2 and 3 links, respectively, ω_0 is the natural frequency of a separate link. The amount of splitting essentially depends on the binding energy of the links, which in turn is determined by the width of the potential barrier between them.

2. The wave functions in the considered layered structures are complex. Their form depends on the number of links and the vibration mode. So for the first mode of oscillations of a chain of 11 links, the form of the wave function is shown in Figure 3. Let us pay attention to the symmetrical form of the wave function relative to the middle of the chain. It is this configuration that ensures the equality of particle fluxes from left to right and from right to left, which gives the greatest transparency of the barrier. Note also that the value of Ψ^2 characterizes the probability of finding a microparticle in a given cell [5, 6].

Therefore, as the value of Ψ^2 increases, the velocity of the particle decreases and the number of transitions from one link to another decreases. A more detailed consideration of wave functions will be carried out in the next publications.

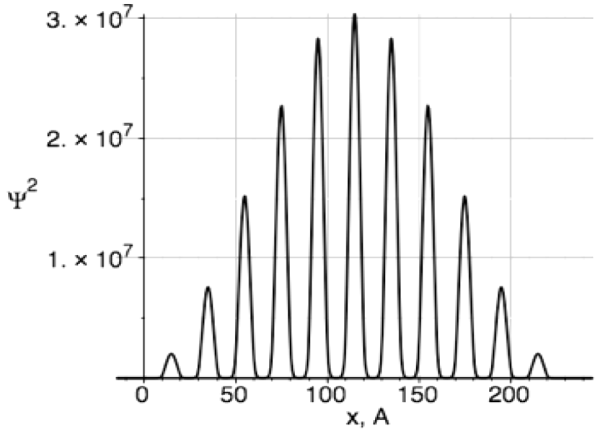

Fig. 3: Wave function of the 1st oscillation mode for a chain of 11 links

3. Let us now consider the question of the width of resonance peaks [9–11]. Assuming that the peaks have a Lorentzian shape, we come to the conclusion that the linewidth is determined primarily by the time the particle stays in the chain. The longer this time, the narrower the line. In our case, the main role is played by the following factors: the number of collisions per unit time with a potential barrier, the transparency of this barrier, and the probability of finding a particle in a cell. Figure 4 shows the dependence of the RTU width on the thickness of the potential barrier separating the cells.

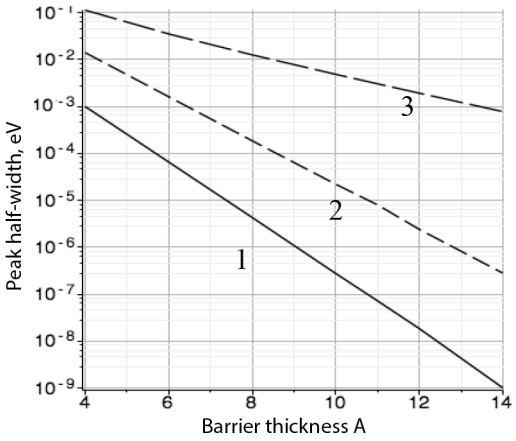

Fig. 4: Dependence of the half-width of the resonance peaks on the thickness of the barrier separating the cells:
1 – one half-wave is laid on the width of the pit; 2 – two half-waves; 3 – three half-waves

It can be seen from the figure that in all three cases this dependence is of an exponential nature. This character of the curve testifies in favor of the tunneling mechanism of particle motion, since the transparency of the barrier decreases exponentially with an increase in its thickness. Consider first a chain consisting of only one link. The width of the RTD peak (ΔE_1) in this case can be estimated using the uncertainty relation:

$$\Delta E_1 = \frac{h}{\tau_1} \tag{2}$$

where $\tau 1$ is the residence time of the particle in the link; h is Planck's constant. Knowing the value of ΔE_1 (at least from the simulation results), from relation (2) it is possible to determine $\tau 1$.

Taking into account the occurrence of a quasi-standing wave in the cell

$$\tau_1=\tau_0*\Psi_1^2, \quad (3)$$

Here Ψ_1^2 is the squared modulus of the wave function of a particle in a single link, $\tau_0 = \frac{1}{\nu_0}$ where ν_0 is the frequency of particle transition from a given link to a neighboring one. Unfortunately, the value of ν_0 is not known with sufficient accuracy and, therefore, it can only be used for order-of-magnitude estimates. An empirical approach that uses data on the wave function and the width of the RTD in a single link seems to be more effective.

In a chain consisting of N links, the half-width of the RTD corresponding to the nth mode can be determined as follows:

$$\Delta E_n = \frac{h}{\tau_n} = \frac{h}{\tau_0 \sum_{k=1}^{N} \Psi_{nk}^2} \quad (4)$$

Here Ψ_{nk}^2 – the wave function of an electron in the k link of a chain consisting of N links (takes into account the probability of finding an electron in a given cell in the n vibration mode);

$\tau_n=\tau_0 \Sigma\Psi_{nk}^2$ – the total residence time of an electron in the chain (for the n oscillation mode);

The value of τ_0 can be determined from (2) and (3). As a result of simple transformations, we obtain $\tau_0 = \frac{h}{\Delta E_1 \Psi_1^2}$

Then

$$\Delta E_n = \Delta E_1 \cdot \frac{\Psi_1^2}{\sum_{k=1}^{N} \Psi_{nk}^2} \quad (5)$$

Here ΔE_n is the half-width of the split peak corresponding to the nth vibration mode in a chain of N links;

ΔE_1 is the width of the resonant level in a single link (determined by the results of computer simulation);

$\sum_{k=1}^{N} \Psi_{nk}^2$ – wave function of an electron corresponding to the n oscillation mode in a chain of N links (for example, Fig. 3). The results obtained using relation (5) are shown in Figure 5. Comparison of these data (circles) with the results of computer simulation (solid line) shows a good match, which indicates the adequacy of the model used. Relation (5) was used to calculate the half-width of the peak corresponding to the first oscillation mode of a system consisting of 11 units. But it can also be applied to other modes, as well as to chains with an arbitrary number of links.

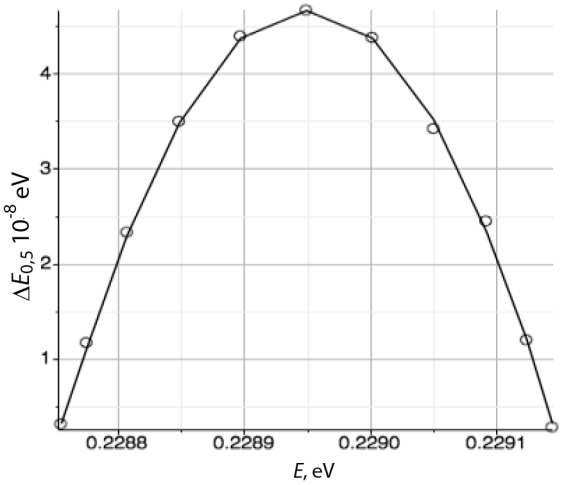

Fig. 5: Energy dependence of the half-width of the peaks split off from the first resonance level. The solid line is the simulation results; circles - calculation by relation (5)

Table 1 shows that the sum of the half-widths of the individual split sub-levels is a constant value for different chains and equal to the half-width of the initial single peak (approximately 2.8 10^{-7} eV). This, in our opinion, is caused by the fact that the excitation of different modes occurs independently of each other [10, 11]. Then, for the transition of the system from the initial state to the final state, there are N independent channels and $\frac{1}{\tau_1} = \sum_{n=1}^{N} \frac{1}{\tau_n}$. The summation is carried out here over all vibration modes. Eventually

$$\sum_{n=1}^{N} \Delta E_n = \sum_{n=1}^{N} \frac{h}{\tau_n} = h \sum_{n=1}^{N} \frac{1}{\tau_n} = \frac{h}{\tau_1} = \Delta E_1$$

Thus, the sum of all split peaks half-widths in the chain turns out to be equal to original peak half-width before splitting.

6. Conclusion

The paper considers some properties of resonant-tunneling levels that arise during the formation of a chain of potential wells and barriers.

1. It has been established that during the formation of a chain, RTUs are split into a system of sublevels, the number of which is equal to the number of links in the chain.

2. The energy values of these sublevels are determined depending on the number of links. The transparency of the chain for these energy values is equal to unity.

3. The question of the RTD half-width and the mechanism of its dependence on the chain parameters is considered.

4. A method for calculating the RTU half-width is proposed. A good agreement was obtained between the values obtained as a result of computer simulation and calculation by the proposed method.

The paper presents mainly the results of computer experiments. These results naturally require further development and comprehension. In subsequent works, it is planned to consider longer chains and conduct a more detailed theoretical study of their properties.

REFERENCES

[1] V. P. Dragunov, I. G. Neizvestny, and V. A. Gridchin, “Fundamentals of Nanoelectronics,” Novosibirsk: NSTU, 2000. 331 p.

[2] A. Yu. Aladyshkin, “Tunneling phenomena in nanophysics,” Nizhny Novgorod: state un-t. N. Novgorod, 2011. 32 p.

[3] A. D. Stefanchuk, “Calculation of fields of electromagnetic waves in the layered ionosphere with allowance for nonlinear effects,” Moscow: Abstract, 2000, 24 p.

[4] V. E. Golant, A. P. Zhilinsky, and I. E. Sakharov, “Fundamentals of Plasma Physics,” Wiley &. Sons, New York, 1980.

[5] A. S. Davydov, “Quantum mechanics,” Moscow: Nauka, 1973, 702 p.

[6] V. G. Levich, Yu. A. Vdovin, V. A. Myamlin, “Course of Theoretical Physics,” vol. 2, Moscow: Nauka, 1971, 936 p.

[7] F. Crawford, “Berkeley course of physics,” vol. 3, Moscow: Nauka, 1984, 521 p.

[8] S. P. Strelkov, “Introduction to the theory of oscillations,” St. Petersburg: Lan, 2005, 440 p.

[9] G. I. Epifanov, “Solid State Physics,” Moscow: Higher school, 1965, 275 p.

[10] L. N. Kurbatov, “Optoelectronics of the visible and infrared ranges of the spectrum,” Moscow: MIPT, 1999. 320 p.

[11] A. N. Pikhtin, “Physical foundations of quantum electronics and optoelectronics,” Moscow: Higher school, 1983, 304 p.

[12] T. K. Popov, M. Dimitrova, R. Dejarnac, J. Stöckel, P. Ivanova, J. Kovačič, T. Gyergyek, M. A. Pedrosa, D. López-Bruna, C. Hidalgo, "Advances in Langmuir probe diagnostics of the plasma potential and electron-energy distribution function in magnetized plasma," *Plasma Sources Science and Technology*, 2016, vol. 25, no. 3, p. 033001.

[13] S. Mori, S. Okuzumi, "Electron heating in magnetorotational instability: implications for turbulence strength in the outer regions of protoplanetary disks," *The Astrophysical Journal*, 2016, vol. 817, no.1, p. 52.

[14] M. M. Mandour, S. A. Astashkevich, A. A. Kudryavtsev, "Electron vortexes in two-dimensional steady photoplasma," *Chinese Journal of Physics*, 2022, vol. 75, pp. 69-75.

[15] S. I. Lashkul, A. B. Altukhov, A. D. Gurchenko, E. Z. Gusakov, V. V. Dyachenko, L. A. Esipov, A. N. Konovalov, D. V. Kuprienko, S. V. Shatalin, A. Yu. Stepanov, "Distinctive features of lower hybrid current drive in plasma of the FT-2 TOKAMAK," *Plasma Physics Reports*, 2022, vol. 48, no. 5, pp. 453-461.

[16] B. N. Chetverushkin, O. G. Olkhovskaya, I. P. Tsigvintsev, "Numerical solution of high-temperature gas dynamics problems on high-performance computing systems," *Journal of Computational and Applied Mathematics*, 2021, vol. 390v, p. 113374.

[17] M. A. Rydalevskaya, "Simplified method for calculation of equilibrium plasma composition," *Physica A: Statistical Mechanics and its Applications*, 2017, vol. 476, pp. 49-57.