Metallophysics and Advanced Technologies
Металофіз. новітні технол.
Metallofiz. Noveishie Tekhnol.
2022, vol. 44, No. 8, pp. 963–974
https://doi.org/10.15407/mfint.44.08.0963
Reprints available directly from the publisher

PACS numbers: 71.15.-m, 71.20.Nr, 71.30.+h, 73.20.-r, 73.43.-f

Calculation of the Energy Spectrum of Quantum Particle in Double Potential Pit

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The problem of quantum particle in infinitely deep potential pit with an internal potential barrier of finite height is solved. The solution is performed in a simple algorithmic approach, which allows you to use the result in the study of semiconductor nanostructures. The real heterostructure corresponding to this model should look like thin layer of wideband semiconductor placed between two slightly thicker layers of narrowband semiconductor. To ensure the 'infinite depth' of the potential pit, layers of conductor must be applied to the outer side surfaces of the triple semiconductor heterostructure and negative electric potential must be applied. Another option for the practical implementation of the model can be done by placing two electrons in one potential pit. In this case, the pit is a local space, at the boundary of which negative electric potential is applied. The internal potential barrier arises due to the Coulomb interaction of electrons. An example of such a structure is a nanopore on the surface, or in the volume of a metal sample.

Key words: quantum particle, potential pit, heterostructure, potential barrier.

Розв'язано задачу про квантову частинку в нескінченно глибокій потенціяльній ямі з внутрішнім потенціяльним бар'єром скінченої висоти. Розв'язок виконано в простому алгоритмічному підході, що дає змогу використовувати одержаний результат в дослідженнях напівпровідникових наноструктур. Реальна гетероструктура, яка відповідає цьому моделю,

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Citation: A. S. Lazarenko, K. M. Tikhovod, S. S. Kovachov, I. T. Bohdanov, and Y. O. Sychikova, Calculation of the Energy Spectrum of Quantum Particle in Double Potential Pit, *Metallofiz. Noveishie Tekhnol.*, **44**, No. 8: 963–974 (2022). DOI: 10.15407/mfint.44.08.0963

повинна виглядати як тонкий шар широкозонного напівпровідника, вміщений між двома дещо товщими шарами вузькозонного напівпровідника. Для забезпечення «нескінченної глибини» потенціяльної ями на зовнішні бокові поверхні потрійної напівпровідникової гетероструктури необхідно нанести шари провідника і подати від'ємний електричний потенціял. Інший варіянт практичної реалізації моделю можна здійснити розмістивши два електрони в одній потенціяльній ямі. В цьому випадку яма являє собою локальний простір, на межі якого подається від'ємний електричний потенціял. Внутрішній потенціяльний бар'єр виникає через Кулонову взаємодію електронів. Прикладом такої структури є нанопора на поверхні або в об'ємі металевого зразка.

Ключові слова: квантова частинка, потенціяльна яма, гетероструктура, потенціяльний бар'єр.

(Received June 12, 2022; in final version, July 11, 2022)

1. INTRODUCTION

Achievements and needs of modern technologies determine the leading topical direction of development of research in metal physics and semiconductor physics as the study of the properties of low-dimensional structures (nanostructures) and the development of scientifically sound means of their synthesis [1, 2]. Modern experimental methods provide the possibility of creating porous structures single-crystal layers [3, 4] and multilayer heterostructures [5, 6]. The thickness of the layers in such structures, or the characteristic pore size, is from one to ten nanometres, which corresponds to the de Broglie wavelength of the charge carriers [7, 8].

From the point of view of the physical approach, it provides means of studying and using the fundamental phenomena caused by the manifestations of corpuscular-wave dualism of charge carriers. These include, in particular, such dimensional quantum effects as quantization of energy and momentum of charge carriers in thin layers of semiconductor heterostructures [9], resonant passage of charge carriers through them [10]. Quantization, which is due to the spatial localization in nanostructures, including nanopores formed on the surface and in the volume of metal conductors, qualitatively changes the energy spectrum of charge carriers and quasiparticles; forms specific properties of specific metal and semiconductor heterostructures [11, 12]. Thus, the controlled change of geometric dimensions and configuration of nanoobjects and nanostructures makes it possible to determine and shape the physical properties of semiconductor devices [13, 14]. The implementation of these capabilities requires both advanced experimental methods [15, 16] and effective theoretical approaches to the calculation and design of metal and semiconductor nanostructures with certain properties [17, 18].

Typical dimensions of metal and semiconductor objects and structures used in modern micro- and nanoelectronics are in the range from one hundred to one nanometre units [19, 20]. From the point of view of subatomic physics, such dimensions fall beyond the fundamental limit of linear scale, which determines the transition from the classical physical model of state description to quantum. This reduction in the size of physical objects and systems changes all their properties and characteristics at a qualitative level [21]. The description of the state at the level of averaging over a large number of individual parts of single macroscopic system is inferior to the quantum approach of the probabilistic description of the state of single nanoobject.

Quantum properties and effects determine the unique physical characteristics of the so-called heterostructures, *i.e.*, artificial periodic layered formations [22]. Usually, individual layers of heterostructures have the thickness of about nanometres [23]. Conscious and predicted by modelling the formation of layered heterostructures makes it possible to obtain the required energy spectrum of charge carriers. In addition, recent research in metal physics is aimed at developing technologies for the deposition of quantum metal nanoparticles (Ni, Pd, Cu, Ag, Au) on the surface of semiconductors, as well as establishing the functional properties of semiconductors and ceramics doped with metals to high concentrations (Zn, S, La, Eu) [24–26].

The description of nanoobjects and nanostructures by means of mathematics and theoretical physics is based entirely on the fundamental principles of quantum mechanics, using a wide range of modelling and computing apparatus of modern mathematics. In the most general approach, the calculation of the electronic states of nanostructures should be performed as a solution of the corresponding three-dimensional problem of the structure of energy zones. Such problems are usually not suitable for direct analytical solution, they have developed effective numerical methods for computer calculation of quantum states in nanostructures. At the fundamental physical level, these methods are based on microscopic models of strong bonds, or pseudopotentials [27].

For some specific cases, approximate methods are successfully used: effective mass (for the case of simple energy zones); effective Hamiltonian (for degenerate energy zones); smooth envelopes (for multi-zone model) [28, 29].

In approximate methods, for each layer of the heterostructure, the solution is found separately as a linear combination of independent solutions of the corresponding Schrцdinger problem. The complete solution for the heterostructure is written as the superposition of the solutions for the individual layers with cross-linking. To perform cross-linking, the boundary conditions for the wave functions of charge carriers and their first derivatives at the boundaries of the heterostruc-

ture layers are formulated.

The approximate effective mass method allows to calculate the energy spectrum and probabilities of quantum states of charge carriers using the stationary Schrödinger equation [30]. In this case, the motion of the charge carriers is considered one-dimensional and occurs in directions perpendicular to the planes of the heterostructure.

The article proposes to solve the problem of quantum particle in infinitely deep potential pit with internal potential barrier of finite height.

2. STATEMENT OF THE PROBLEM

The problems of metal quantum particle in infinitely deep rectangular potential pit, of tunnelling quantum particle through a potential barrier of finite height, are widely known, and their solutions are standard examples in textbooks and manuals [31].

The logical continuation of the problem of tunnelling metal quantum particle through a potential barrier of finite height is the problem of potential relief with two or three barriers. In fact, these are problems of a single or double potential pit of finite depth, separated from space with zero potential energy by barriers of finite thickness.

As original part of the study, we solve the model problem of quantum particle in infinitely deep potential pit with internal potential barrier of finite height (Fig. 1).

3. THEORETICAL SOLUTION OF THE PROBLEM

The dependence of the potential energy $U(x)$ of quantum particle on the coordinate is represented as a system:

$$U(x) = \begin{cases} +\infty, \; x \le -a/2, \\ 0, \; -a/2 < x < a/2, \\ U_0, \; -\delta/2 \le x \le \delta/2, \\ +\infty, \; x \ge a/2, \end{cases} \tag{1}$$

where U_0 is the height of the potential barrier, a is the width of the potential well, δ is the width of the potential barrier.

Let's solve the Schrödinger problem for the left part of the potential pit.

The stationary Schrödinger equation has the form:

$$\frac{d^2\psi_1(x)}{dx^2} + \frac{2mE_1}{\hbar^2} = 0, \tag{2}$$

where $\psi_1(x)$ is the wave function of the particle in the left part of the

$\hbar$ is Planck's table has been modified. We can use one boundary condition:

$$\psi_1(-a/2) = 0. \tag{3}$$

In order to demonstrate the possibilities of the general approach, we solve the problem by the method of characteristic equation. In this case, the general solution is:

$$\psi_1(x) = A_1 \exp\left(\frac{i}{\hbar}\sqrt{2mE_1}x\right) + B_1 \exp\left(\frac{i}{\hbar}\sqrt{2mE_1}x\right), \tag{4}$$

where A_1, B_1 are integration constants. After substitution in the boundary condition (3) we can relate the values of the integration constants:

$$B_1 = -A_1 \exp\left(-\frac{ia}{\hbar}\sqrt{2mE_1}\right).$$

The wave function of the particle in the left part of the pit can now be written as follows:

$$\psi_1(x) = A_1\left[\exp\left(\frac{i}{\hbar}\sqrt{2mE_1}x\right) - \exp\left(-\frac{i}{\hbar}\sqrt{2mE_1}(x+a)\right)\right]. \tag{5}$$

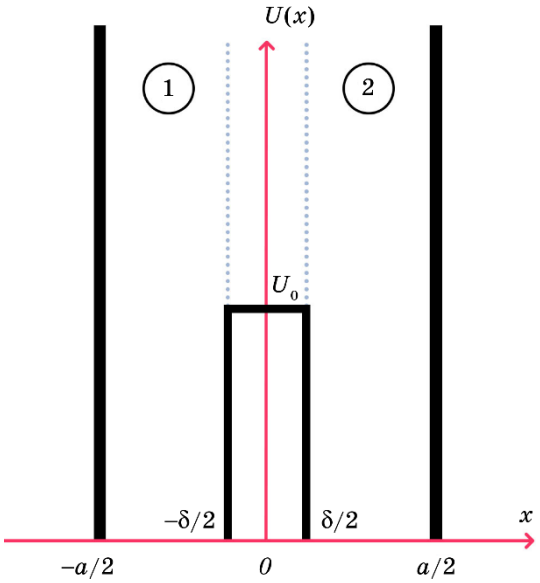

Fig. 1. Potential energy profile: a combination of an infinitely deep potential well and a potential barrier of finite height.

The wave function of quantum particle for the right part of potential pit is obtained in a similar way. It will look like:

$$\psi_2(x) = A_2\left[\exp\left(\frac{i}{\hbar}\sqrt{2mE_2}x\right) - \exp\left(-\frac{i}{\hbar}\sqrt{2mE_2}(x+a)\right)\right], \tag{6}$$

where A_2 is the integration constant, E_2 is particle energy.

Solve the Schrödinger problem for quantum particle in the central part of a potential pit.

For the case when the energy of the particle E is less than the height of the potential barrier U_0, the Schrödinger equation has the form:

$$\frac{d^2\psi(x)}{dx^2} - \frac{2m(U_0 - E)}{\hbar^2}\psi(x) = 0, \tag{7}$$

where $\psi(x)$ is the wave function of the quantum particle for:

$$-\delta / 2 \le x \le \delta / 2.$$

Solving by the method of characteristic equation we obtain:

$$\psi(x) = A\exp\left(\frac{\sqrt{2m(U_0 - E)}}{\hbar}x\right) + B\exp\left(-\frac{\sqrt{2m(U_0 - E)}}{\hbar}x\right), \tag{8}$$

where A, B are integration constants.

Given the symmetry of the problem, which is that the left and right parts of the pit are equal with respect to the location of the quantum particle, we can obtain a relationship between the integration constants:

$$\psi(-\delta / 2) = \psi(\delta / 2),\ A = B.$$

With this result in mind, the wave function will look like:

$$\psi(x) = A\left[\exp\left(\frac{\sqrt{2m(U_0 - E)}}{\hbar}x\right) + \exp\left(-\frac{\sqrt{2m(E - U_0)}}{\hbar}x\right)\right]. \tag{9}$$

Similarly, for the case when the energy of the particle E is greater than the height of the potential barrier U_0, we obtain the result:

$$\psi(x) = A\left[\exp\left(\frac{i}{\hbar}\sqrt{2m(U_0 - E)}x\right) + \exp\left(-\frac{i}{\hbar}\sqrt{2m(E - U_0)}x\right)\right] \tag{10}$$

We obtained wave functions that determine the state of quantum particle in three parts of the pit. The functions contain three integra-

tion constants and the parameter E (quantum particle energy). The number of independent integration constants can be reduced due to the obvious symmetry of the problem. Since the left and right parts of the potential well are equal with respect to the random placement of the particle, the condition must be met:

$$\int_{-a/2}^{-\delta/2} \left|\psi_1(x)\right|^2 dx = \int_{\delta/2}^{a/2} \left|\psi_2(x)\right|^2 dx. \tag{11}$$

As a result of rather cumbersome integration we receive:

$$\int_{-a/2}^{-\delta/2} \left|\psi_1(x)\right|^2 dx = \left|A_1\right|^2 \left[(a-\delta) - \frac{\hbar}{\sqrt{2mE_1}} \sin\left(\frac{\sqrt{2mE_1}}{\hbar}(a-\delta)\right)\right],$$

$$\int_{\delta/2}^{a/2} \left|\psi_2(x)\right|^2 dx = \left|A_2\right|^2 \left[(a-\delta) - \frac{\hbar}{\sqrt{2mE_1}} \sin\left(\frac{\sqrt{2mE_1}}{\hbar}(a-\delta)\right)\right].$$

Due to the symmetry of the problem and the fundamental law of conservation of energy $E_1 = E_2 = E$. Accordingly, we obtain $A_1 = A_2 = A_0$. Thus, the number of independent integration constants is reduced to two.

To determine the integration constants A_0, A and the energy values E, we use the conditions of crosslinking of wave functions at the potential barrier:

$$\begin{aligned} &\psi_1(-\delta/2) = \psi(-\delta/2), \\ &\left.\frac{d\psi_1}{dx}\right|_{-\delta/2} = \left.\frac{d\psi}{dx}\right|_{-\delta/2}, \\ &\psi_2(\delta/2) = \psi(\delta/2), \\ &\left.\frac{d\psi_2}{dx}\right|_{\delta/2} = \left.\frac{d\psi}{dx}\right|_{\delta/2}. \end{aligned} \tag{12}$$

Additionally, if necessary, you can use the rationing condition:

$$\int_{-a/2}^{-\delta/2} \left|\psi_2(x)\right|^2 dx + \int_{-\delta/2}^{\delta/2} \left|\psi(x)\right|^2 dx + \int_{\delta/2}^{a/2} \left|\psi_2(x)\right|^2 dx = 1. \tag{13}$$

The crosslinking conditions give the following system of equations:

$$\begin{cases} A_0[\exp(-\Upsilon) - \exp(-\Xi)] = A[\exp(-\Omega) + \exp(\Omega)], \\ A_0 iE^{1/2}[\exp(-\Upsilon) + \exp(-\Xi)] = A(U_0 - E)^{1/2}[\exp(-\Omega) - \exp(\Omega)], \\ A_0[\exp(\Upsilon) - \exp(\Xi)] = A[\exp(\Omega) + \exp(-\Omega)], \\ A_0 iE^{1/2}[\exp(\Upsilon) + \exp(\Xi)] = A(U_0 - E)^{1/2}[\exp(\Omega) - \exp(-\Omega)], \end{cases} \quad (14)$$

where:

$$\Upsilon = (i\delta / 2\hbar)(2mE)^{1/2},$$
$$\Xi = (i / \hbar)(2mE)^{1/2}(a - \delta / 2),$$
$$\Omega = \frac{(2m(U_0 - E))^{1/2}\delta}{2\hbar}.$$

The right-hand sides of all equations of system (14) are real numbers. Accordingly, in the left parts of the equations of the system the sum of imaginary components should be equal to zero. Using Euler's formula, we obtain a condition that agrees with all equations of system (14):

$$\sin\left(\frac{\sqrt{2mE}a}{\hbar}\right)\cos\left(\frac{\sqrt{2mE}\delta}{2\hbar}\right) - \left(1 + \cos\frac{\sqrt{2mE}a}{\hbar}\right)\sin\left(\frac{\sqrt{2mE}\delta}{2\hbar}\right) = 0. \quad (15)$$

Since the cosine and sine of the same argument cannot be zero together, condition (15) holds if:

$$\begin{cases} \sin((2mE)^{1/2}a / \hbar) = 0, \\ 1 + \cos((2mE)^{1/2}a / \hbar) = 0. \end{cases} \quad (16)$$

The solution of the system of equations allows to calculate the energy levels of the quantum system:

$$E_{\text{p}} = \frac{\Pi^2\hbar^2}{2ma^2}(2n - 1)^2,\ n = 1, 2, 3, \ldots. \quad (17)$$

As we can see, the expression for energy levels is similar to the expression of energy levels of an ordinary rectangular, infinitely deep potential pit:

$$E_k = \frac{\Pi^2\hbar^2}{2ma^2}k^2,\ k = 1, 2, 3, \ldots.$$

But there is an important difference: the calculation of expression (17) is performed only for odd values of $k = (2n - 1)$. That is, the distance between energy levels increases significantly.

Taking into account expression (17), the wave functions (4), (5), (9)

take the following form:

$$\psi_n^{(1)}(x) = 2A_0 \cos\left[\frac{(2n-1)\Pi}{a}x\right],\ n = 1,2,3,\ldots, \tag{18a}$$

$$\psi_n^{(2)}(x) = 2A_0 \cos\left[\frac{(2n-1)\Pi}{a}x\right],\ n = 1,2,3,\ldots, \tag{18b}$$

$$\psi_n(x) = A\left[\exp\sqrt{\frac{2mU_0}{\hbar^2} - \frac{\Pi^2}{a^2}(2n-1)^2}x\right] + \\ + \exp\left(-\sqrt{\frac{2mU_0^2}{\hbar^2} - \frac{\Pi^2}{a^2}(2n-1)^2}x\right),\ n = 1,2,3,\ldots. \tag{18c}$$

Further definition of integration constants contains the usual mathematical transformations, although quite cumbersome. As a result, we obtain the following expressions:

$$A_0 = \sqrt{\frac{\xi}{2\xi\left(a - \delta - \frac{a\sin\tau}{(2n-1)\Pi}\right) + 4\cos^2\left(\frac{\tau}{2}\right)\frac{2\delta\xi + \exp(\xi\delta) - \exp(-\xi\delta)}{2 + \exp(\xi\delta) + \exp(-\xi\delta)}}}, \tag{19}$$

where:

$$\tau = \frac{(2n-1)\Pi}{a}\delta,$$

$$A = A_0\frac{2\cos(\tau/2)}{\exp(\xi\delta/2) + \exp(-\xi\delta/2)}. \tag{20}$$

To reduce the record in expressions (19), (20) introduced the symbol:

$$\xi = \sqrt{\frac{2mU_0}{\hbar^2} - \frac{\Pi^2}{a^2}(2n-1)^2}.$$

Thus, the problem is solved analytically by using additional internal connections due to the symmetry of the quantum system.

4. SEARCH FOR REAL RELEVANCE AND PROSPECTS FOR RESEARCH DEVELOPMENT

At first glance, the chosen model of infinitely deep potential pit with potential barrier of finite height in the middle seems rather artificial. But, in fact, it is easy to imagine a real heterostructure that corresponds to this model.

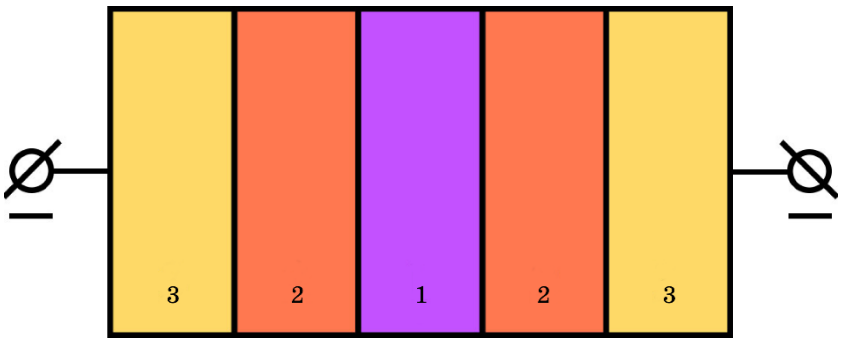

Fig. 2. Heterostructure corresponding to the theoretical model: 1—wide-band semiconductor layer, 2—narrow-band semiconductor layers, 3—conductive layers (metals).

Such heterostructure should look like the thin layer of wideband semiconductor placed between two slightly thicker layers of narrow-band semiconductor. To ensure the 'infinite depth' of the potential pit on the outer side surfaces of the triple semiconductor heterostructure, it is necessary to apply layers of conductor (metal) and apply negative electric potential (Fig. 2).

Another option for the practical implementation of the model can be done by placing two electrons in one potential pit. In this case, the pit is a local space—a nanopore on the surface, or in the volume of a metal sample, at the boundary of which negative electric potential is applied. The internal potential barrier arises due to the Coulomb interaction of electrons.

Thus, further perspectives and directions of research will be connected with practical approbation and improvement of the model.

5. CONCLUSION

1. The quantum-mechanical problem on particle in potential pit of infinite depth with a potential barrier of finite height in the centre of the pit was formulated and solved.
2. The defining difference of the energy levels of quantum particle in a potential pit of infinite depth with a potential barrier of finite height in the centre of the well is revealed. The energy gaps between successive levels increase significantly compared to a normal rectangular, infinitely deep potential well. The value of the energy levels is a multiple of the squares of odd natural numbers.
3. Variants of the semiconductor heterostructure and Coulomb potential well on the surface or in the volume of the metal sample are proposed, which in practice may correspond to the theoretical model con-

sidered in the study.

The study was supported by the Ministry of Education and Science of Ukraine, namely: the state budget research project No. 0122U000129 'The search for optimal conditions for nanostructures synthesis on the surface of A3B5, A2B6 semiconductors and silicon for photonics and solar energy', project No. 0121U10942 'Theoretical and methodological bases of the system fundamentalization of the future nanomaterials experts training for productive professional activity'.

Y. Sychikova thanks Goethe-Institut for supporting the House of Europe graduate emergency scholarship programme.

We also thank the Armed Forces of Ukraine for the safety to carry out this work. This work was only possible thanks to the resilience and courage of the Ukrainian Army.

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