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ENERGY STATES OF PARTICLES IN A QUANTUM SIZED STRUCTURE WITH A COMPLEX SHAPED BAND DIAGRAM

The **subject** of research in the article is the energy spectrum of a multilayer quantum sized structure with an energy profile of a complex shape. The **goal** of this work is to study the interaction of quantum-confined and quasi- continuum energy states of particles under the action of an external stationary electric field applied perpendicular to the planes of quantum confinement. The following **tasks** were solved in the article: The spectrum of eigenfunctions and eigenvalues of particle energy is determined, both in the area of the quantum confinement and in the area of the quasi-continuum. The definition of the eigenfunctions takes into account the fact that the phase of the eigenfunctions changes due to the motion of particles over the quantum well. The following **methods** were used to solve the set tasks: quantum mechanical modeling of stationary states in a structure with an energy profile of a complex shape; methods of the theory of small perturbations for describing the interaction of particles in such a structure. The following **results** were obtained: the basic calculation relations of the mathematical model of the energy states of particles and quasiparticles in quantum-limited and quasi-continuum states were obtained within the framework of the quantum-mechanical approach. The interaction of energy states of particles and quasiparticles in each of the bands between quantum-confined and quasi-continuum states is described depending on the external influence. The theory of small perturbations is applied in the paper to assess the degree of interaction. **Conclusions**: Analysis of the results of modeling the energy spectrum of a structure with two quantum wells, calculated for an unperturbed state and for the case of external action in the form of a stationary electric field, leads to the following conclusions: in the absence of an external field acting on the considered quantum well structure, electrons and holes located above the separation barrier are characterized by a non-monotonically increasing spectrum of energy states. In this case, the particles are predominantly localized above the quantum wells; the action of a constant external electric field on the structure under consideration leads to the manifestation of the quantum-limited Stark effect both for solitary and for multilayer periodic quantum well structures. In this case, the delocalization of the wave functions and the shift of the corresponding energy levels (the lowest energy levels in the structure under consideration) is expressed as strongly as in multilayer symmetric structures. At the same time, the effect is almost invisible for the higher levels. This is especially pronounced for the energy levels lying above the separation barrier. Thus, it can be expected that an equidistant energy spectrum can be realized at a certain external field strength, which in turn should simplify significantly the attainment of the second harmonic generation mode if the structure under consideration is used in the active region of a semiconductor laser.

Keywords: energy spectrum; quantum limitation; wave function; electron; heavy hole; easy hole; quasi-continuum.

Introduction

Optical nonlinearity in superlattices becomes pronounced when the so-called resonance condition is satisfied, when the energy levels of the spectrum of the system are located equidistantly and the difference in their energies is a multiple of the photon energy of the primary radiation. The problem of finding the limiting potential that ensures the equidistance of several energy levels is a complex variational problem, which, even with a fixed form of the potential, does not have an unambiguous solution. The potential parameters can be varied in such a way that when the positions of the levels change, the equidistance between them is preserved. In turn, the variation of the parameters, without violating the resonance conditions, strongly affects the values of the dipole matrix elements, which in turn can lead to a significant change in the values of the optical characteristics of the system. Thus, by changing the parameters of the structure, a large value of the second harmonic generation (SHG) coefficient can be achieved. At the same time, the maximum SHG coefficient does not mean at all that the observed intensity of the generated radiation at the doubled frequency will necessarily be maximum. Indeed, in the double resonance regime, both lasing and generated radiation can be strongly absorbed, i.e., resonant optical transitions can lead to strong lasing at the frequency 2ω, but at the same time to strong absorption at frequencies ω and 2ω [1-6].

From what has been said, in particular, it follows that the problem of finding the conditions for optimal generation for the second harmonic cannot be completely solved within the framework of microscopic theory, i.e. by revealing the parameters of a nanostructure with a maximum SHG coefficient or a minimum value of the absorption coefficient at a doubled frequency. The complete optimization theory, along with the determination of the optical characteristics of the system, should also consider the solutions of the equations of macroscopic fields that determine the intensities of the main and generated radiation at different values of the optical characteristics of the system.

In connection with the problem of SHG radiation in the infrared region of wavelengths due to both interband and intersubband optical transitions, there are numerous asymmetric low-dimensional structures with several equidistantly spaced energy levels. Such as quantum wells with a complex structure or simple wells located in a built-in or external electric field. Nonlinear optical properties of asymmetric quantum-well semiconductor structures are applicable to heterosystems GaAs/AlGaAs, Si/SiGe, AlInAs/GaInAs, GaN/AlGaN [5, 8-13].

Analysis of the problem and existing methods

With the development of nanoelectronics and its semiconductor element base, researchers are paying more and more attention to the creation of semiconductor nanoelectronic devices for both optoelectronic and non-optoelectronic applications. In the production of

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nanoelectronic devices, a number of technological problems arise: the integration of discrete nanoelectronic devices and their simplest assemblies into standard microelectronic circuits with a well-established technological implementation. The creation of purely nanoelectronic circuits is still a serious problem; creation of reliable electrical connections both between nano-sized circuit elements and between nano- and microelectronic components; temperature stability of nanoelectronic elements; bringing the parameters of the newly created nanoelectronic element base to existing standards for one or another type of equipment, or creating new standards; suppression of undesirable effects in the operation of a new element base, the occurrence of which is associated with the quantum nature of physical processes occurring in the active regions of nanoelectronic devices, etc.

The greatest interest in the creation and modernization of the element base of nanoelectronics is the production of discrete elements for optoelectronic and non-optoelectronic applications, such as injection semiconductor lasers and highly directional high-power LEDs, amplifiers and modulators of optical radiation, as well as field-effect transistors with a nanochannel, resonant tunneling diodes, resonant-tunnel transistors, bipolar transistors with nanoscale base. With the development of technological methods of nanoelectronics, special attention is paid to the creation of semiconductor devices with superlattices [7-10].

As the main materials for the creation of semiconductor nanoelectronic devices, double AIIIBV compounds and their ternary and quaternary solid solutions were most often used. The choice of this group of materials is based on their wide use in microwave semiconductor electronics. In the last five to six years, the attention of researchers has been attracted by AIIBVI semiconductor compounds and their ternary and quaternary compounds. This group of materials was also used to create devices for semiconductor microwave electronics and optoelectronics, however, since this group of materials contains a large number of volatile compounds, the temperature instability of which manifests itself in technologically used temperature ranges, it was difficult to create high-quality and sharp p-n junctions based on materials of this group. For this reason, devices based on AIIIBV compounds, and especially AIIBVI compounds, have not become widespread, except for individual samples and series of devices.

With the development of epitaxial technologies, a previously inaccessible opportunity has appeared to vary the energy diagram of semiconductor structures both in the width of the regions and the height of potential barriers, and in the directions of crystal growth. It became possible to create structures with alternating materials in a given order with different electrophysical and crystallographic properties. The concept of "zone engineering" appeared, which implies the artificial production of materials with electrophysical properties that do not exist in nature.

This work is devoted to the study of quasicontinuous states that arise in multilayer quantum-dimensional structures in the case when the internal potential barriers are lower than the external ones, between which the energy states of particles arise, much higher than the ground states in individual quantum-limited regions and also experiencing quantum confinement.

Highlighting previously unsolved parts of a common problem. Purpose of the work

The possibility of obtaining layers with an arbitrary profile of changing the composition made it possible to use structures with quantum wells (QWs) of complex shapes to improve the characteristics of devices. Thus, to create a new generation of resonant tunneling diodes and heterolasers with separate electronic and optical confinement, structures with rectangular QWs are used, in the center of which there is an additional dip (fig. 1).

Varying the structural parameters of the double quantum well makes it possible, at the design stage of the structure, to "tune" the semiconductor laser or optical amplifier to a given frequency (wavelength) of an external source.

A change in the width of the separating barrier for a given thickness of the entire structure and the position of the barrier in the structure can maintain a given energy distance between the levels within a fairly wide range.

Changing the height of the limiting barriers of the structure allows you to plan frequency doubling in the direction of increasing the frequency of the external signal.

The growth of semiconductor nanostructures with almost arbitrary, predetermined, structural and compositional characteristics using modern technologies does not pose significant difficulties. Thanks to this, at present, it has become possible to implement low-dimensional systems with the required properties of the energy spectrum, as well as the degree of overlap of the wave functions of various energy levels of dimensional quantization. This capability, in turn, makes it possible not only to design and create various highly efficient optical devices with active elements based on quantum objects, but also on the basis of appropriate calculations of the parameters of these objects to optimize their performance. [1, 2, 17].

The problem of finding the conditions for optimal generation for the second harmonic cannot be completely solved within the framework of microscopic theory, i.e. revealing the parameters of the nanostructure with the maximum SHG coefficient or the minimum value of the absorption coefficient at the doubled frequency. The complete optimization theory, along with the determination of the optical characteristics of the system, should also consider the solutions of the equations of macroscopic fields that determine the intensities of the main and generated radiation at various values of the optical characteristics of the system.

In connection with the problem of SHG radiation in the infrared region of wavelengths caused by both interband and intersubband optical transitions, numerous asymmetric low-dimensional structures with several equidistantly spaced energy levels were considered. Thus, quantum wells with a complex structure or simple wells

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located in a built-in or external electric field were considered [7, 8, 10, 13, 16].

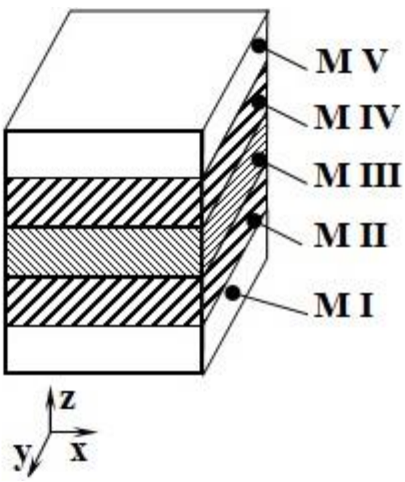
The **aim** of this work is to study the interaction of quantum-confined and quasicontinuum energy states of particles under the action of an external stationary electric field applied perpendicular to the planes of quantum confinement.

Materials and methods

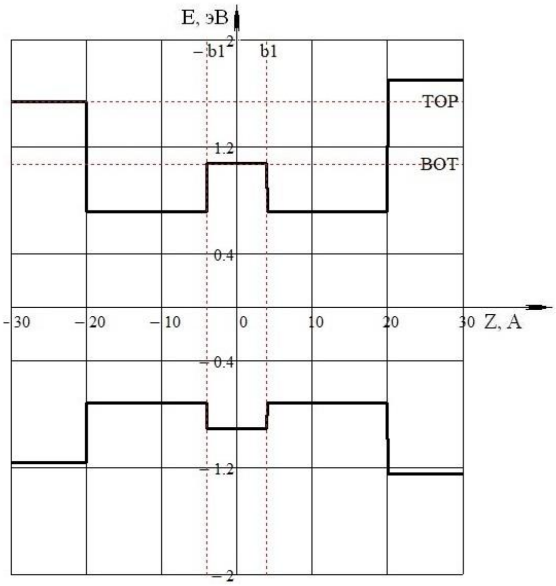
One of the most common quantum dimensional structures with a complex energy profile is shown in fig. 1, general view - fig. 1a, and the energy diagram is shown in fig. 1b. Moreover, the shown structure can be used both by itself and as part of a repeating construct - as an element of a complex superlattice.

The structure considered in this work is based on GaAs/AlXGa1-XAs materials and is five-layer. The materials of the first and fifth layers MI, MV, consist of the AlXGa1-XAs solid solution with the maximum aluminum content, which provides the largest band gap in these layers, and, as a consequence, the highest potential barriers for carriers of both types throughout the structure.

The materials of the second and fourth layers - M II, M IV, on the contrary, have a minimum aluminum content or completely consist of gallium arsenide. This ensures the formation of rectangular quantum wells in the second and fourth layers for carriers of both types. In the material of the third layer - M III, the aluminum content is higher than in the materials of the second and fourth layers, but less than in the materials of the first and fifth layers of the structure. Thus, in the second, third, and fourth layers above the potential barrier of the third layer and between the potential barriers of the first and fifth layers, a quasi-continuum zone is formed, since the carriers in the second and fourth layers experience quantum confinement, their thickness does not exceed the de Broglie wavelength, the thickness of the separation barrier is also small since the barrier is considered to be permeable; however, the total distance between the barriers of the first and fifth layers, in the general case, can approach the values of a bulk sample [5–7].



a)



b)

M I - M V - designations of materials of layers of a quantum dimensional structure; Ec and Ev are the boundaries of the conduction and valence bands, respectively; -b, b - boundaries of the central part of the structure - the barrier above which the state of the quasi-continuum is formed; markers "TOP" and "BOT" - the upper and lower boundaries of the quasi-continuum region for electrons in the conduction band

Fig. 1. Five-layer structure of an asymmetric superlattice

In fig. 1b: (-b), (b) are shown boundaries of the central part of the five-layer nanostructure, a similar region exists for heavy and light holes in the valence band (not shown in the figure).

The energy diagram of the structure shown in fig. 1b was calculated based on the electrophysical parameters of the ternary substitutional solid solution GaAs/AlXGa1-XAs given in table 1.

Table 1. *Physical parameters of ternary substitutional solid solution GaAs/AlXGa1-XAs*

Parameter	GaAs	AlAs	$Al_XGa_{1-X}As$
Eg, eV	1,424	3,018	1,424+1,247·X, 0 < X < 0,45 1,424+1,247·X+1,147·(X - 0,45), 0,45 < X < 1,0
m_C^*/m_0	0,067	0,124	0,067+0,057·X
γ_1	6,85	3,45	6,85 – 3,4·X
γ_2	2,1	0,68	2,1 – 1,42·X

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The effective masses of heavy and easy holes are calculated according to the formulas:

$$m_{hh}^{*}=\frac{m_0}{\gamma_1-2\cdot\gamma_2}\ , \qquad (1)$$

$$m_{lh}^{*}=\frac{m_0}{\gamma_1+2\cdot\gamma_2}\ , \qquad (2)$$

where m_{hh}^{*} is an effective mass of a heavy hole; m_{lh}^{*} is an effective mass of an easy hole; m_0 - free electron mass; γ_1 i γ_2 - Luttinger's material constants.

The law of dispersion of the valence band of double semiconductor compounds is approximated using Luttinger constants. Luttinger constants uniquely characterize the effective masses of heavy and light holes near the extremes of the band diagrams of homogeneous semiconductor materials and semiconductor compounds constructed in the space of wave vectors (inverse lattice) [23-25]. This approach is also applicable for triple and quadruple solid solutions of substitution. Formulas (1) and (2) allow us to determine the effective masses of light and heavy holes of a triple solid solution of AlxGa1-XAs substitution. For this solid solution, the main electrophysical parameters are given in table 1 and are semi-empirical. The convenience of this approach allows to consider the change of electrophysical constant throughout the range of variation of the chemical composition of a ternary solid solution. I.e. to take into account the influence of the material at the transition from layer to layer in the nanostructure. Thus, formulas (1) and (2), as well as those given in table 1, can serve as an acceptable basis for determining the input parameters of the model of the nanostructure under consideration.

The determination of the energy eigenvalues and the eigenfunctions of the carriers is carried out within the framework of the quantum mechanical approach based on the solution of the stationary Schrödinger equation:

$$\hat{H}\Psi=E\cdot\Psi\ . \qquad (3)$$

In this paper, to solve equation (3), we used the standard procedure for determining the eigenvalues of the Hamilton operator using the conditions of continuity and smoothness of the eigenfunction. The solution to equation (3) for the energy eigenvalues in the region below the quasi-continuum - in the region of separation of quantum wells (quantum confinement), is written as:

$$\frac{1}{2}\cdot\left(arctg\left(\frac{k_1\cdot m_2^{*}}{k_2\cdot m_1^{*}}\right)+arctg\left(\frac{k_5\cdot m_2^{*}}{k_2\cdot m_5^{*}}\right)\right)-$$
$$-arctg\left(-\frac{k_3\cdot m_2^{*}}{k_2\cdot m_3^{*}}\cdot th\left(k_3\cdot b\right)\right)-k_2\cdot\left(a-b\right)+n\cdot\pi=0 \quad ;\ (4)$$

- for even solutions,

$$\frac{1}{2}\cdot\left(arctg\left(-\frac{k_2\cdot m_1^{*}}{k_1\cdot m_2^{*}}\right)+arctg\left(-\frac{k_2\cdot m_5^{*}}{k_5\cdot m_2^{*}}\right)\right)-$$
$$-arctg\left(\frac{k_2\cdot m_3^{*}}{k_3\cdot m_2^{*}}\cdot th\left(k_3\cdot b\right)\right)-k_2\cdot\left(a-b\right)+n\cdot\pi=0 \quad ;\ (5)$$

- for odd solutions.

The solution to equation (3) for the energy eigenvalues in the quasi-continuum region can be written as:

$$\frac{1}{2}\cdot\left(arctg\left(\frac{k_1\cdot m_2^{*}}{k_2'\cdot m_1^{*}}\right)+arctg\left(\frac{k_5\cdot m_2^{*}}{k_2'\cdot m_5^{*}}\right)\right)-$$
$$-arctg\left(-\frac{k_3'\cdot m_2^{*}}{k_2'\cdot m_3^{*}}\cdot tg\left(k_3'\cdot b\right)\right)-k_2'\cdot\left(a-b\right)+n\cdot\pi=0 \quad ;\ (6)$$

- for even solutions,

$$\frac{1}{2}\cdot\left(arctg\left(-\frac{k_2'\cdot m_1^{*}}{k_1\cdot m_2^{*}}\right)+arctg\left(-\frac{k_2'\cdot m_5^{*}}{k_5\cdot m_2^{*}}\right)\right)-$$
$$-arctg\left(\frac{k_2'\cdot m_3^{*}}{k_3'\cdot m_2^{*}}\cdot tg\left(k_3'\cdot b\right)\right)-k_2'\cdot\left(a-b\right)+n\cdot\pi=0 \quad ;\ (7)$$

- for odd solutions.

Equations (4) - (7) are transcendental equations for the eigenvalues of the carrier energy. The eigenfunctions of the Hamilton operator from relation (3), the wave functions of particles corresponding to the eigenvalues determined by expressions (4) - (7), are given by the relations:

$$\Psi_{1e}\left(z\right)=A_3\cdot\frac{ch\left(k_3\cdot b\right)\cdot\cos\left(k_2\cdot a+\varphi_e\right)}{\cos\left(k_2\cdot b+\varphi_e\right)}\cdot\exp\left(k_1\cdot\left(z+a\right)\right),\ -\infty<z<-a\ , \qquad (8\ a)$$

$$\Psi_{2e}\left(z\right)=A_3\cdot\frac{ch\left(k_3\cdot b\right)}{\cos\left(k_2\cdot b+\varphi_e\right)}\cdot\cos\left(k_2\cdot z-\varphi_e\right),\ -a\le z\le -b\ , \qquad (8\ b)$$

$$\Psi_{3e}\left(z\right)=A_3\cdot ch\left(k_3\cdot z\right),\ -a\le z\le -b\ , \qquad (8\ c)$$

$$\Psi_{4e}\left(z\right)=A_3\cdot\frac{ch\left(k_3\cdot b\right)}{\cos\left(k_2\cdot b+\varphi_e\right)}\cdot\cos\left(k_2\cdot z+\varphi_e\right),\ b\le z\le a\ , \qquad (8\ d)$$

$$\Psi_{5e}\left(z\right)=A_3\cdot\frac{ch\left(k_3\cdot b\right)\cdot\cos\left(k_2\cdot a+\varphi_e\right)}{\cos\left(k_2\cdot b+\varphi_e\right)}\cdot\exp\left(k_1\cdot\left(z-a\right)\right),\ a<z<+\infty \qquad (8\ e)$$

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- for even solutions in the area below the separation barrier;

$$\Psi_{1o}(z) = -B_3 \cdot \frac{sh(k_3 \cdot b) \cdot \sin(k_2 \cdot a + \varphi_o)}{\sin(k_2 \cdot b + \varphi_o)} \cdot \exp(k_1 \cdot (z + a)), \ -\infty < z < -a, \quad (9\ a)$$

$$\Psi_{2o}(z) = B_3 \cdot \frac{sh(k_3 \cdot b)}{\sin(k_2 \cdot b + \varphi_o)} \cdot \sin(k_2 \cdot z - \varphi_o), \ -a \le z \le -b, \quad (9\ b)$$

$$\Psi_{3o}(z) = B_3 \cdot sh(k_3 \cdot z), \ -a \le z \le -b, \quad (9\ c)$$

$$\Psi_{4o}(z) = B_3 \cdot \frac{sh(k_3 \cdot b)}{\sin(k_2 \cdot b + \varphi_o)} \cdot \sin(k_2 \cdot z + \varphi_o), \ b \le z \le a, \quad (9\ d)$$

$$\Psi_{5o}(z) = B_3 \cdot \frac{sh(k_3 \cdot b) \cdot \sin(k_2 \cdot a + \varphi_o)}{\sin(k_2 \cdot b + \varphi_o)} \cdot \exp(k_1 \cdot (z - a)), \ a < z < +\infty \quad (9\ e)$$

- for odd solutions in the region below the separation barrier.

$$\Psi'_{1e}(z) = A'_3 \cdot \frac{\cos(k'_3 \cdot b) \cdot \cos(k'_2 \cdot a + \varphi'_e)}{\cos(k'_2 \cdot b + \varphi'_e)} \cdot \exp(k_1 \cdot (z + a)), \ -\infty < z < -a, \quad (10\ a)$$

$$\Psi'_{2e}(z) = A'_3 \cdot \frac{\cos(k'_3 \cdot b)}{\cos(k'_2 \cdot b + \varphi'_e)} \cdot \cos(k'_2 \cdot z - \varphi'_e), \ -a \le z \le -b, \quad (10\ b)$$

$$\Psi'_{3e}(z) = A'_3 \cdot \cos(k'_3 \cdot z), \ -a \le z \le -b, \quad (10\ c)$$

$$\Psi'_{4e}(z) = A'_3 \cdot \frac{\cos(k'_3 \cdot b)}{\cos(k'_2 \cdot b + \varphi'_e)} \cdot \cos(k'_2 \cdot z + \varphi'_e), \ b \le z \le a, \quad (10\ d)$$

$$\Psi'_{5e}(z) = A_3 \cdot \frac{\cos(k'_3 \cdot b) \cdot \cos(k'_2 \cdot a + \varphi'_e)}{\cos(k'_2 \cdot b + \varphi'_e)} \cdot \exp(k_1 \cdot (z - a)), \ a < z < +\infty \quad (10\ e)$$

- for even solutions in the field of the separation barrier;

$$\Psi'_{1o}(z) = -B'_3 \cdot \frac{\sin(k'_3 \cdot b) \cdot \sin(k'_2 \cdot a + \varphi'_o)}{\sin(k'_2 \cdot b + \varphi'_o)} \cdot \exp(k_1 \cdot (z + a)), \ -\infty < z < -a, \quad (11\ a)$$

$$\Psi'_{2o}(z) = B'_3 \cdot \frac{\sin(k'_3 \cdot b)}{\sin(k'_2 \cdot b + \varphi'_o)} \cdot \sin(k'_2 \cdot z - \varphi'_o), \ -a \le z \le -b, \quad (11\ b)$$

$$\Psi'_{3o}(z) = B'_3 \cdot \sin(k'_3 \cdot z), \ -a \le z \le -b, \quad (11\ c)$$

$$\Psi'_{4o}(z) = B'_3 \cdot \frac{\sin(k'_3 \cdot b)}{\sin(k'_2 \cdot b + \varphi'_o)} \cdot \sin(k'_2 \cdot z + \varphi'_o), \ b \le z \le a, \quad (11\ d)$$

$$\Psi'_{5o}(z) = B'_3 \cdot \frac{\sin(k'_3 \cdot b) \cdot \sin(k'_2 \cdot a + \varphi'_o)}{\sin(k'_2 \cdot b + \varphi'_o)} \cdot \exp(k_1 \cdot (z - a)), \ a < z < +\infty \quad (11\ e)$$

- for odd solutions in the field of the separation barrier.
Here

$$\varphi_e = \frac{1}{4} \cdot \left(arctg\left(\frac{k_1 \cdot m_2^*}{k_2 \cdot m_1^*} \right) + arctg\left(\frac{k_5 \cdot m_2^*}{k_2 \cdot m_5^*} \right) \right) + \\ + \frac{1}{2} \cdot \left(arctg\left(-\frac{k_3 \cdot m_2^*}{k_2 \cdot m_3^*} \cdot th(k_3 \cdot b) \right) - k_2 \cdot (a + b) \right) + n \cdot \pi \quad (12)$$

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- phase of the wave function for even solutions in the region below the separation barrier,

$$\varphi_o = \frac{1}{4}\cdot\left(arctg\left(-\frac{k_2\cdot m_1^*}{k_1\cdot m_2^*}\right)+arctg\left(-\frac{k_2\cdot m_5^*}{k_5\cdot m_2^*}\right)\right)+ \\ +\frac{1}{2}\cdot\left(arctg\left(\frac{k_2\cdot m_3^*}{k_3\cdot m_2^*}\cdot th\left(k_3\cdot b\right)\right)-k_2\cdot\left(a-b\right)\right)+n\cdot\pi \tag{13}$$

- phase of the wave function for odd solutions in the region below the separation barrier,

$$\varphi_e' = \frac{1}{4}\cdot\left(arctg\left(\frac{k_1\cdot m_2^*}{k_2'\cdot m_1^*}\right)+arctg\left(\frac{k_5\cdot m_2^*}{k_2'\cdot m_5^*}\right)\right)+ \\ +\frac{1}{2}\cdot\left(arctg\left(-\frac{k_3'\cdot m_2^*}{k_2'\cdot m_3^*}\cdot tg\left(k_3'\cdot b\right)\right)-k_2'\cdot\left(a+b\right)\right)+n\cdot\pi \tag{14}$$

- phase of the wave function for even solutions in the region of the separation barrier,

$$\varphi_o' = \frac{1}{4}\cdot\left(arctg\left(-\frac{k_2'\cdot m_1^*}{k_1\cdot m_2^*}\right)+arctg\left(-\frac{k_2'\cdot m_5^*}{k_5\cdot m_2^*}\right)\right)+ \\ +\frac{1}{2}\cdot\left(arctg\left(\frac{k_2'\cdot m_3^*}{k_3'\cdot m_2^*}\cdot tg\left(k_3'\cdot b\right)\right)-k_2'\cdot\left(a-b\right)\right)+n\cdot\pi \tag{15}$$

- phase of the wave function for odd solutions in the region of the separation barrier.

Expressions (12) - (15) were obtained taking into account relations (4) - (7). The dash in expressions (6), (7), (10), (11), (14) and (15) denotes that the expression belongs to the description of the solution in the region of the separation barrier.

The amplitude coefficients of the wave function in expressions (8) - (11) are determined by the relations:

$$A_3 = \frac{1}{\sqrt{IA_1+IA_2+IA_3+IA_4+IA_5}}, \tag{16 a}$$

where

$$IA_1 = \frac{ch^2\left(k_3\cdot b\right)\cdot\cos^2\left(k_2\cdot a+\varphi_e\right)}{2\cdot k_1\cdot\cos^2\left(k_2\cdot b+\varphi_e\right)}, \tag{16 b}$$

$$IA_2 = \frac{ch^2\left(k_3\cdot b\right)}{\cos^2\left(k_2\cdot b+\varphi_e\right)}\cdot\left(\frac{a-b}{2}+\frac{1}{2\cdot k_2}\cdot\sin\left(k_2\cdot\left(a-b\right)\right)\cdot\cos\left(k_2\cdot\left(a+b\right)+2\cdot\varphi_e\right)\right), \tag{16 c}$$

$$IA_3 = \frac{sh^2\left(2\cdot k_3\cdot b\right)}{2\cdot k_3}+b, \tag{16 d}$$

$$IA_4 = \frac{ch^2\left(k_3\cdot b\right)}{\cos^2\left(k_2\cdot b+\varphi_e\right)}\cdot\left(\frac{a-b}{2}+\frac{1}{2\cdot k_2}\cdot\sin\left(k_2\cdot\left(a-b\right)\right)\cdot\cos\left(k_2\cdot\left(a+b\right)+2\cdot\varphi_e\right)\right), \tag{16 e}$$

$$IA_5 = \frac{ch^2\left(k_3\cdot b\right)\cdot\cos^2\left(k_2\cdot a+\varphi_e\right)}{2\cdot k_1\cdot\cos^2\left(k_2\cdot b+\varphi_e\right)}, \tag{16 f}$$

- for even solutions in the area below the separation barrier;

$$B_3 = \frac{1}{\sqrt{IB_1+IB_2+IB_3+IB_4+IB_5}}, \tag{17 a}$$

where

$$IB_1 = \frac{sh^2(k_3 \cdot b) \cdot \sin^2(k_2 \cdot a + \varphi_e)}{2 \cdot k_1 \cdot \sin^2(k_2 \cdot b + \varphi_e)}, \quad (17\text{ b})$$

$$IB_2 = \frac{sh^2(k_3 \cdot b)}{\sin^2(k_2 \cdot b + \varphi_e)} \cdot \left(\frac{a-b}{2} - \frac{1}{2 \cdot k_2} \cdot \sin(k_2 \cdot (a-b)) \cdot \cos(k_2 \cdot (a+b) + 2 \cdot \varphi_e) \right), \quad (17\text{ c})$$

$$IB_3 = \frac{sh^2(2 \cdot k_3 \cdot b)}{2 \cdot k_3} - b, \quad (17\text{ d})$$

$$IB_4 = \frac{sh^2(k_3 \cdot b)}{\sin^2(k_2 \cdot b + \varphi_e)} \cdot \left(\frac{a-b}{2} - \frac{1}{2 \cdot k_2} \cdot \sin(k_2 \cdot (a-b)) \cdot \cos(k_2 \cdot (a+b) + 2 \cdot \varphi_e) \right), \quad (17\text{ e})$$

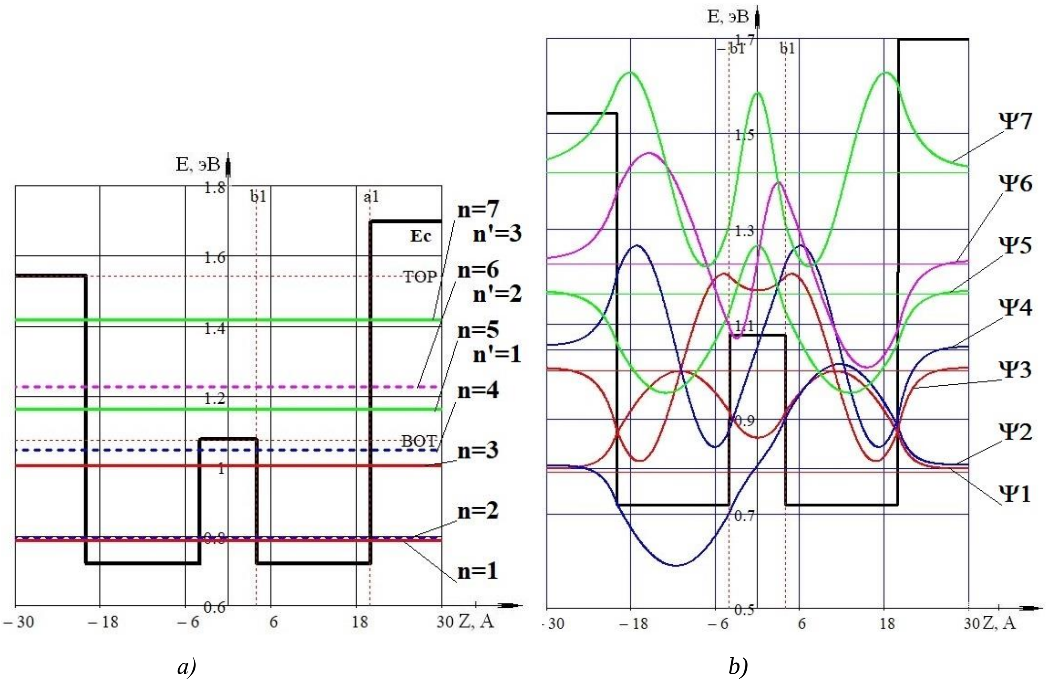
$$IB_5 = \frac{sh^2(k_3 \cdot b) \cdot \sin^2(k_2 \cdot a + \varphi_e)}{2 \cdot k_1 \cdot \sin^2(k_2 \cdot b + \varphi_e)}, \quad (17\text{ f})$$

- for odd solutions in the region below the separation barrier.

A feature of the presented solution is the presence of a phase term that takes into account the effect of multiple reflection processes of the wave function at the "barrier - well" and "well - barrier" boundaries in the region above the separation barrier.

Research results and discussion

Mathematical modeling of the energy states of carriers and the corresponding wave functions, both in stationary and in perturbed states, are shown in figs. 2 and 3 respectively. The energy eigenvalues for electrons in the conduction band are shown in fig. 2(a). In fig. 2(b), the eigenfunctions of electrons in a stationary state are shown.



a) b)

Fig. 2. Energy eigenvalues and eigenfunctions of the Hamilton operator for electrons in the conduction band

Energy states of carriers under the action of an external constant electric field. When a quantum-dimensional structure with an energy profile of a complex external electric field is exposed, the state of particles in the region above the separation barrier undergoes significant changes caused, on the one hand, by the action of the external field strength, and on the other, by the presence of additional potential energy in particles in this region. In addition, particles located above the separation barrier interact with particles located in quantum wells under the action of an external field. The changes caused in the structure by an external electric field can be relatively easily traced using the second approximation of perturbation theory. Figs. 3(a) and 3(b), respectively, show the eigenvalues of the energy and distribution density of the probability of finding electrons in the conduction band, calculated for the case of the action of an external stationary electric field. Fig. 3(a), for comparison, shows the unperturbed energy states of electrons by dashed lines.

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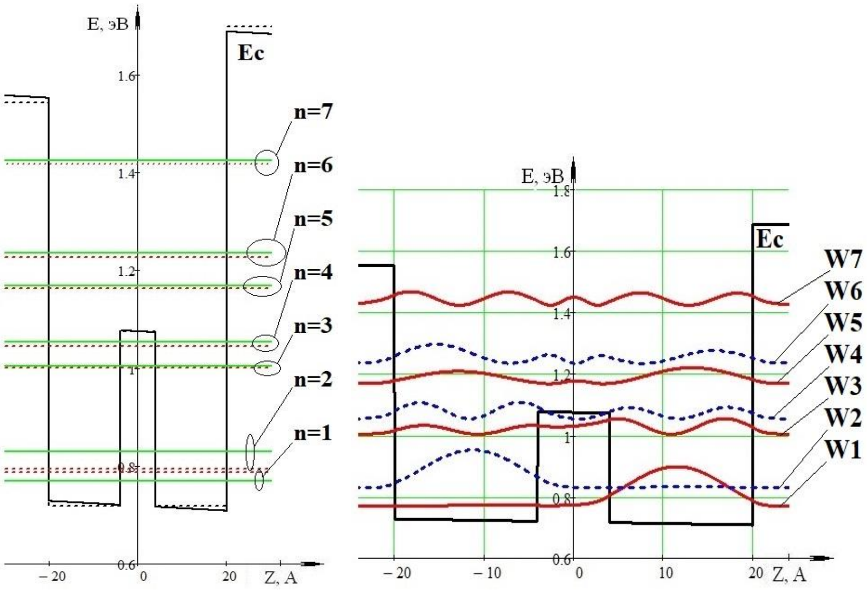

a) *b)*

Fig. 3. Effect of an external electric field on the states of carriers

Conclusions and prospects for further development

Modeling the spectrum of energy eigenvalues and carrier eigenfunctions in a quantum dimensional structure with an energy profile of a complex shape reveals a number of essential regularities. A quantum dimensional structure consisting of two quantum wells separated by a barrier, nevertheless, is a single structure. Since the external barriers are energetically higher than the separation one, the space above the separation barrier and adjacent quantum wells is a separate quantum-limited region.

Analysis of the results of modeling the energy spectrum of a structure with two quantum wells, calculated for the unperturbed state (fig. 2), and for the case of an external action in the form of a stationary electric field (fig. 3), leads to the following conclusions:

- in the absence of an external field acting on the considered quantum dimensional structure, the electrons and holes located above the separation barrier are characterized by a nonmonotonically increasing spectrum of energy states. In this case, the particles are predominantly localized above the quantum wells;

- as well as for solitary and for multilayer periodic quantum dimensional structures, the action of a constant external electric field on the structure under consideration leads to the manifestation of the quantum-limited Stark effect. In this case, the delocalization of the wave functions and the shift of the corresponding energy levels - the lowest energy levels in the structure under consideration, are expressed as strongly as in multilayer symmetric structures. At the same time, the effect is almost invisible for the higher levels. This is especially pronounced for energy levels lying above the separation barrier.

Thus, it can be expected that an equidistant energy spectrum can be realized at a certain external field strength, which in turn should significantly simplify the attainment of the second harmonic generation mode if the considered structure is used in the active region of a semiconductor laser.

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ЕНЕРГЕТИЧНІ СТАНИ ЧАСТИНОК У КВАНТОВІЙ РОЗМІРНІЙ СТРУКТУРІ ІЗ ЗОННОЮ ДІАГРАМОЮ СКЛАДНОЇ ФОРМИ

Предметом дослідження в статті є енергетичний спектр багатошарової квантової розмірної структури з енергетичним профілем складної форми. **Мета** роботи - дослідження взаємодії квантово-обмежених і квазіконтінуумних енергетичних станів частинок під дією зовнішнього стаціонарного електричного поля, прикладеного перпендикулярно до площин квантового обмеження. У статті вирішуються наступні **завдання:** Визначено спектр власних функцій і власних значень енергії частинок, як в області квантового обмеження, так і в області, яка знаходиться вище розділювального бар'єру. У визначенні власних функцій враховується факт зміни фази власних функцій внаслідок руху частинок над квантової ямою. Для вирішення поставлених завдань, в статті, використані наступні **методи**: квантово-механічне моделювання стаціонарних станів в структурі з енергетичним профілем складної форми; методи теорії малих збурень для опису взаємодії частинок в такій структурі. Отримані наступні **результати:** в рамках квантово-механічного підходу отримані основні розрахункові співвідношення математичної моделі енергетичних станів частинок і квазічастинок в квантово-обмежених і квазіконтінуумних станах. Взаємодія енергетичних станів частинок і квазічастинок в кожній із зон між квантово-обмеженими і квазіконтінуумними станами описується в залежності від зовнішнього впливу. Для оцінки ступеня взаємодії в статті застосована теорія малих збурень. **Висновки:** Аналіз результатів моделювання енергетичного спектру структури з двома квантовими ямами, розрахованого, для незбуреного стану, і для випадку зовнішнього впливу у вигляді стаціонарного електричного поля, призводить до наступних висновків: за відсутності зовнішнього поля, що діє на розглянуту квантову розмірну структуру, електрони і дірки, що знаходяться над розділювальним бар'єром, характеризуються немонотонно зростаючим спектром енергетичних станів. При цьому частинки переважно локалізуються над квантовими ямами; так само, як і для відокремлених, так і для багатошарових періодичних квантових розмірних структур, вплив постійного зовнішнього електричного поля на розглянуту структуру призводить до прояву квантово-обмеженого ефекту Штарка. При цьому делокалізація хвильових функцій і зміщення відповідних енергетичних рівнів - нижчих енергетичних рівнів в даній структурі, виражена також сильно, як в багатошарових симетричних структурах. У той же час для вищих рівнів ефект майже непомітний. Особливо це виражено для енергетичних рівнів, що лежать вище розділювального бар'єру; Таким чином, можна очікувати, що при певній напруженості зовнішнього поля може бути реалізований еквідистантний енергетичний спектр, що в свою чергу має суттєво спростити досягнення режиму генерації другої гармоніки, якщо використовувати розглянуту структуру в активній області напівпровідникового лазера.

Ключові слова: енергетичний спектр; квантове обмеження; хвильова функція; електрон; важка дірка; легка дірка; квазіконтінуум.

ЭНЕРГЕТИЧЕСКИЕ СОСТОЯНИЯ ЧАСТИЦ В КВАНТОВОЙ РАЗМЕРНОЙ СТРУКТУРЕ С ЗОННОЙ ДИАГРАММОЙ СЛОЖНОЙ ФОРМЫ

Предметом исследования в статье является энергетический спектр многослойной квантовой размерной структуры с энергетическим профилем сложной формы. **Цель** работы – исследование взаимодействия квантово-ограниченных и квазиконтинуумных энергетических состояний частиц под действием внешнего стационарного электрического поля, приложенного перпендикулярно плоскостям квантового ограничения. В статье решаются следующие **задачи:** Определен спектр собственных функций и собственных значений энергии частиц, как в области квантового ограничения, так и в области квазиконтинуума. В определении собственных функций учитывается факт изменения фазы собственных функций вследствие движения частиц над квантовой ямой. Для решения поставленных задач в статье использованы следующие методы: квантово-механическое моделирование стационарных состояний в структуре с энергетическим профилем сложной формы; методы теории малых возмущений для описания взаимодействия частиц в такой структуре. Получены следующие **результаты:** в рамках квантово-механического подхода получены основные расчетные соотношения математической модели энергетических состояний частиц и квазичастиц в квантово-ограниченных и квазиконтинуумных состояниях. Взаимодействие энергетических состояний частиц и квазичастиц в каждой из зон между квантово-ограниченными и квазиконтинуумными состояниями описывается в зависимости от внешнего воздействия. Для оценки степени взаимодействия в статье применена теория малых возмущений. **Выводы:** Анализ результатов моделирования энергетического спектра структуры с двумя квантовыми ямами, рассчитанного, для невозмущенного состояния, и для случая внешнего воздействия в виде стационарного электрического поля, приводит к следующим выводам: в отсутствии внешнего поля, действующего на рассматриваемую квантовую размерную структуру, электроны и дырки, находящиеся над разделительным барьером, характеризуются немонотонно возрастающим спектром энергетических состояний. При этом частицы преимущественно локализуются над квантовыми ямами; так же, как и для уединенных, так и для многослойных периодических квантовых размерных структур, воздействие постоянного внешнего электрического поля на рассматриваемую структуру приводит к проявлению квантово-ограниченного эффекта Штарка. При этом делокализация волновых функций и смещение соответствующих энергетических уровней – низших энергетических уровней в рассматриваемой структуре, выражена также сильно, как в многослойных симметричных структурах. В то же время для вышележащих уровней эффект почти незаметен. Особенно это выражено для энергетических уровней, лежащих выше разделительного барьера. Таким образом, можно ожидать, что при определенной напряженности внешнего поля может быть реализован эквидистантный энергетический спектр, что в свою очередь должно существенно упростить достижения режима генерации второй гармоники, если использовать рассмотренную структуру в активной области полупроводникового лазера.

Ключевые слова: энергетический спектр; квантовое ограничение; волновая функция; электрон; тяжелая дырка; легкая дырка; квазиконтинуум.

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