THEORETICAL INVESTIGATION OF ENERGY STATES IN A MULTILAYER SEMICONDUCTOR STRUCTURE IN THE QUASICLASSICAL APPROXIMATION

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ABSTRACT

Electronic states in multilayer semiconductor structures are theoretically investigated in the semiclassical approximation, where one-electron wave functions of the stationary Schrödinger equation are calculated in the presence of various types of potential, which is a slowly varying function of the coordinate .

Wave functions and energy spectra of electrons are analyzed in linear, quadratic and other approximations. It is shown that to fulfill the condition of finiteness of wave functions at infinity, there are two types of energy spectrum, and both depend nonlinearly on the size quantization number, i.e. the dimensionally quantized energy spectrum is non-equidistant.

It is determined that the energy spectrum of electrons in the potential in the quadratic, cubic and biquadratic approximation takes discrete values and the steepness of the energy spectrum depends on the parameters of the expansion of the potential with respect to the coordinate.

Keywords : energy spectrum, multilayer structure, Schrödinger equation, size quantization, semiclassical approximation.

INTRODUCTION

The progress of modern microelectronics is largely determined by the study of the properties of systems with non-uniformly distributed parameters, the development of methods for effective theoretical analysis of such systems, the development and provision of objective methods for controlling technological processes that allow creating semiconductor layers with desired properties [1-4] . In this connection, below we consider the general problems of the propagation of electron waves in a medium whose properties change only along a certain direction. The approach is based on the use of the one-electron stationary Schrödinger equation to describe the processes of elastic scattering and tunneling of non-interacting spinless particles under the condition that their total energy is conserved .

The study of the electronic properties of both symmetric and asymmetric with respect to the geometric dimensions of the layers of a semiconductor structure is relevant in connection with the use of these structures in micro- or nanoelectronics and in other areas of solid state physics.

In the works, the dynamic conductivity σ (ω) or current j(ω) was calculated, i.e. system response to external action in a semiconductor multilayer structure. The theory was created in different models using different mathematical methods for solving the Schrödinger equation for a system of electrons interacting with an electromagnetic field in a structure with a $\delta-$shaped potential barrier. In these papers , the problem was solved without taking into account the Bastard condition, i.e., the difference between the effective masses of current carriers in neighboring layers of the structure is not taken into account .

At present, molecular beam epitaxy and other methods of modern technology make it possible to obtain semiconductor layers with an arbitrary profile of composition change (structure with a quantum well) to improve the characteristics of devices based on them. In this case, the problem of electronic states reduces to the problem of behavior of a particle in potential wells of an arbitrary shape. In particular, to create a new generation of resonant tunneling diodes and heterolasers with separated electronic and optical confinement, structures with rectangular size-quantized wells are used, in the center of which there is an additional energy dip.

The study of the electronic states in the above structures leads to the calculation of the one-electron wave functions of the stationary Schrödinger equation in the semiclassical approximation in the presence of the potential $U(x)$, which we will consider as a slowly varying function of the *x coordinate.*

Then the one-dimensional Schrödinger equation can be written as

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+U(x)\psi=E\psi, \qquad (1)$$

where, by substituting $\psi(x)=\exp\left(iS(x)/\hbar\right)$ and obtain the equation for the function $S(x)$ [19]

$$\frac{1}{2m}\left(\frac{dS(x)}{dx}\right)^2-\frac{i\hbar}{2m}\left(\frac{d^2S(x)}{dx^2}\right)=E-U(x). \qquad (2)$$

Assuming that the system under consideration is close to the classical one in its properties, we will look for a solution in the form of a series in powers of the Planck constant, i.e.

$$S(x)=S_0(x)+\frac{\hbar}{i}S_1(x)+\left(\frac{\hbar}{i}\right)^2S_2(x)+\dots \qquad (3)$$

Then the general solution of equation (1) has the form

$$\psi(x)=\frac{C_1}{\sqrt{p(x)}}\exp\left(\frac{i}{\hbar}\int p(x)dx\right)+\frac{C_2}{\sqrt{p(x)}}\exp\left(-\frac{i}{\hbar}\int p(x)dx\right), \qquad (4)$$

where $p(x)=\left[2m\left(E-U(x)\right)\right]^{1/2}$, m and are E the effective mass and energy of current carriers.

In classically inaccessible energy regions, i.e. at $E<U(x)$, the momentum of the current carriers becomes imaginary. Then in these regions (4) takes the form

$$\psi(x)=\frac{C_1}{\sqrt{|p(x)|}}\exp\left(\frac{1}{\hbar}\int|p(x)|dx\right)+\frac{C_2}{\sqrt{|p(x)|}}\exp\left(-\frac{1}{\hbar}\int|p(x)|dx\right) \qquad (5)$$

Note that the accuracy of the semiclassical approximation does not allow taking into account both terms simultaneously, and therefore, in some cases, we will not take into account the exponentially small term in (4) and (5).

Linear and quadratic approximation

Let us consider an isolated classical turning point at $x=a$, far from which the semiclassical approximation is applicable for calculating the transparency coefficient of a potential barrier [20]. Therefore, the solutions of the Schrödenger equation in the allowed and forbidden areas can be found by formulas (4) - (5).

The wave function near the turning point can be found by solving the Schrödinger equation, where the $(x=a)$ potential energy near the turning point can be $U(x)$ represented as

$$U(x) \approx U(x=a)+\left.\frac{dU}{dx}\right|_{x=a}(x-a)+\frac{1}{2}\left.\frac{\partial^2 U}{\partial x^2}\right|_{x=a}(x-a)^2 \qquad (6a)$$

or

$$U(x) \approx U(\varsigma=0)+U'_{\varsigma=0}\varsigma+U''_{\varsigma=0}\varsigma^2 . \qquad (6b)$$

Then the Schrödinger equation can be written as

$$\frac{d^2\psi}{d\varsigma^2}+\frac{1}{E_a}\left(E-U_0-U'_{\varsigma=0}\varsigma-U''_{\varsigma=0}\varsigma^2\right)\psi=0,$$

or

$$\frac{d^2\psi}{d\varsigma^2}+\left(k_0-k_0\varsigma-k_2\varsigma^2\right)\psi=0, \qquad (7)$$

whose general solution is an arbitrary linear combination of hypergeometric functions, i.e.

$$\psi(\varsigma)=C_1\cdot{}_1F_1\left[\left(\frac{1}{4}-\frac{k_1^2}{16k_2^{3/2}}-\frac{k_0}{4k_2^{1/2}}\right),\frac{1}{2},\frac{\left(2k_2\varsigma+k_1\right)^2}{4k_2^{3/2}}\right]\exp\left[-\frac{\varsigma\left(2k_2\varsigma+k_1\right)}{2\sqrt{k_2}}\right]+$$

$$+C_2\cdot{}_1F_1\left[\left(\frac{3}{4}-\frac{k_1^2}{16k_2^{3/2}}-\frac{k_0}{4k_2^{1/2}}\right),\frac{3}{2},\frac{\left(2k_2\varsigma+k_1\right)^2}{4k_2^{3/2}}\right]\left(2k_2\varsigma+k_1\right)\exp\left[-\frac{\varsigma\left(2k_2\varsigma+k_1\right)}{2\sqrt{k_2}}\right], \qquad (1.68)$$

where $\varsigma=\frac{x-a}{a}$, $E_a=\frac{\hbar^2}{2ma^2}$, $k_1=\frac{1}{E_a}U'_{\varsigma=0}=\frac{1}{E_a}\left.\frac{\partial U(\varsigma)}{\partial\varsigma}\right|_{\varsigma=0}$, $k_2=\frac{1}{E_a}U''_{x=a}=\frac{1}{E_a}\left.\frac{\partial^2 U(\varsigma)}{\partial\varsigma^2}\right|_{\varsigma=0}$,

$$k_0^2=\frac{2m}{\hbar^2a^2}\left(E-U(x=0)\right).$$

In the general case ${}_1F_1\left[\left(\frac{1}{4}-\frac{k_1^2}{16k_2^{3/2}}-\frac{k_0}{4k_2^{1/2}}\right),\frac{1}{2},\frac{\left(2k_2\varsigma+k_1\right)^2}{4k_2^{3/2}}\right]\propto\exp\left[\frac{\left(2k_2\varsigma+k_1\right)^2}{4k_2^{3/2}}\right]$, which corresponds to an exponentially growing wave function. Therefore, to choose a wave function that satisfies the conditions of finiteness of the wave functions at infinity, i.e. satisfying this quantum mechanical approach, there are two alternative cases:

1. $C_1\neq0$, $C_2=0$ and $\frac{1}{4}-\frac{k_1^2}{16k_2^{3/2}}-\frac{k_0}{4k_2^{1/2}}=-4n$. In this case, the wave function takes the form

$$\psi_{2n}(\varsigma)={}_1F_1\left[-n,\frac{1}{2},\frac{\left(2k_2\varsigma+k_1\right)^2}{4k_2^{3/2}}\right]\exp\left[-\frac{\varsigma\left(2k_2\varsigma+k_1\right)}{2\sqrt{k_2}}\right], \qquad (9)$$

and the energy spectrum of current carriers is quantized and is defined as

$$k_0 = (1+16n)k_2^{1/2} - \frac{k_1^2}{4k_2^{1/2}} . \qquad \text{(ten)}$$

From (10) we obtain an expression for the size-quantized energy spectrum in the form

$$E = U(x=0) + \frac{\hbar^2}{2m}k_2\left[(1+16n) - \frac{k_1^2}{4k_2}\right]^2$$

or

$$E_1 - U(x=0) = U''_{\varsigma=0}\left[(1+16n) - \frac{1}{4E_a}\frac{(U'_{\varsigma=0})^2}{U''_{\varsigma=0}}\right]^2 . \qquad \text{(eleven)}$$

2. $C_2 \neq 0$, $C_1 = 0$ and $\frac{3}{4} - \frac{k_1^2}{16k_2^{3/2}} - \frac{k_0}{4k_2^{1/2}} = -2(2n+1)$. In this case, the wave function takes the form

$$\psi_{2n+1}(\varsigma) = {}_1F_1\left[-n, \frac{3}{2}, \frac{(2k_2\varsigma + k_1)^2}{4k_2^{3/2}}\right](2k_2\varsigma + k_1)\exp\left[-\frac{\varsigma(2k_2\varsigma + k_1)}{2\sqrt{k_2}}\right], \qquad (12)$$

and the energy spectrum of current carriers is quantized and is determined by the relation:

$$E_2 - U(x=0) = U''_{\varsigma=0}\left[(11+16n) - \frac{1}{4E_a}\frac{(U'_{\varsigma=0})^2}{U''_{\varsigma=0}}\right]^2 . \qquad (13)$$

For a quantitative analysis of the size-quantized energy spectrum, we assume that $U''_{\varsigma=0} = \xi_U \cdot U'_{\varsigma=0}$. Then we have an expression for the size-quantized energy spectrum in a form convenient for quantitative calculation

$$\frac{E_2 - U(x=0)}{\xi_U \cdot U''_{\varsigma=0}} = \left[(1+16n) - \frac{1}{4}x\right]^2 , \qquad (14)$$

where $x = \frac{U'_{\varsigma=0}}{E_a\xi_U}$, $\xi_U = U''_{\varsigma=0}/U'_{\varsigma=0}$.

Similarly, it is easy to obtain the following expression

$$\frac{E_2 - U(x=0)}{\xi_U \cdot U'_{\varsigma=0}} = \left[(11+16n) - \frac{1}{4}x\right]^2 . \qquad \text{(fifteen)}$$

From (11) and (13) formulas, it can be seen that to fulfill the condition of finiteness of the wave functions at infinity, there are two types of energy spectrum, and both depend nonlinearly on the size quantization number, i.e. the dimensionally quantized energy spectrum is not equidistant.

Fig . 1 *a* and *b* show the dependences of the size-quantized energy spectra, characterized by the values $\frac{E_1(n) - U(x=0)}{\xi_U \cdot U'_{\varsigma=0}}$ and $\frac{E_2(n) - U(x=0)}{\xi_U \cdot U'_{\varsigma=0}}$ from parameter $x = \frac{U'_{\varsigma=0}}{E_a\xi_U}$. It can be seen from these figures that with increasing $x = \frac{U'_{\varsigma=0}}{E_a\xi_U}$ values $\frac{E_1(n) - U(x=0)}{\xi_U \cdot U'_{\varsigma=0}}$ and $\frac{E_2(n) - U(x=0)}{\xi_U \cdot U'_{\varsigma=0}}$ s $n = 2,3,...$

decreases. These energy quantities with $n=1$ growth $x=\frac{U'_{\varsigma=0}}{E_a\xi_U}$ first decreases and is reached to a minimum, and then increases.

We note here that in quantitative calculations it is convenient to use the connection of the above hypergeometric functions with Hermite polynomials:

$$H_{2n}\left(\zeta^2\right)=(-1)^n\frac{(2n)!}{n!}\cdot {}_1F_1\left(-n,\frac{1}{2},\zeta^2\right),\quad H_{2n+1}\left(\zeta^2\right)=(-1)^n\frac{(2n+1)!}{n!}2\cdot\zeta\cdot {}_1F_1\left(-n,\frac{3}{2},\zeta^2\right).$$

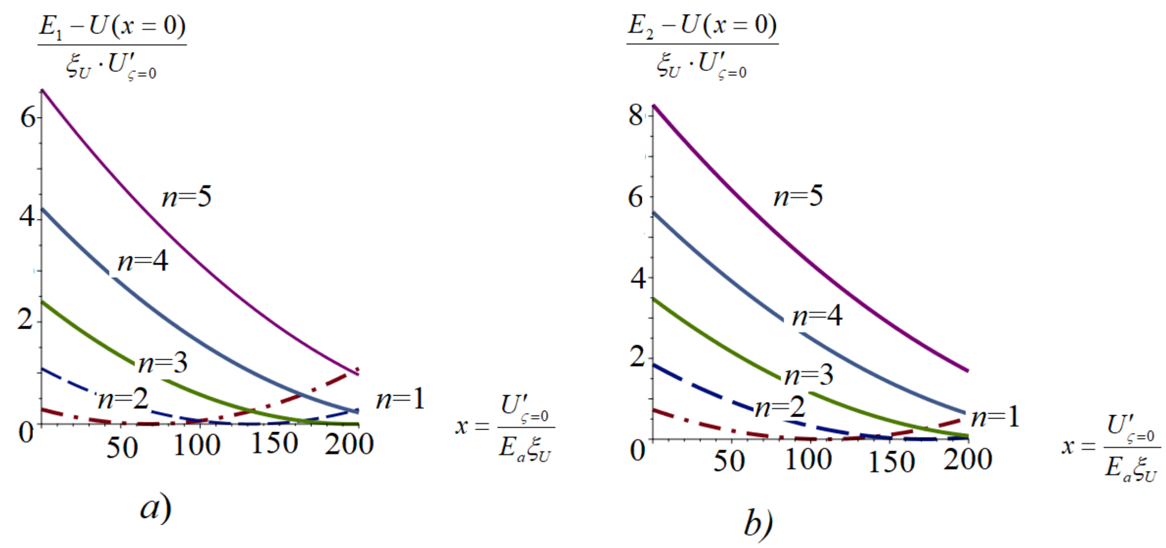


Fig.1 Dependences of energy quantities $\frac{E_1(n)-U(x=0)}{\xi_U\cdot U'_{\varsigma=0}}$ and $\frac{E_2(n)-U(x=0)}{\xi_U\cdot U'_{\varsigma=0}}$ from $x=\frac{U'_{\varsigma=0}}{E_a\xi_U}$ for different values of the size quantization number, where $\xi_U=U''_{\varsigma=0}/U'_{\varsigma=0}$.

Cubic and biquadratic approximation

Next, consider the following cubic and biquadratic terms in (6), i.e.

$$U(x)=\frac{1}{2}m\omega^2x^2+\varepsilon_3\left(\frac{x}{l}\right)^3+\varepsilon_4\left(\frac{x}{l}\right)^4, \qquad (16)$$

where $l=\sqrt{\frac{\hbar}{m\omega}}$. ε_3 and ε_4 are expansion coefficients $U(x)$ in a series in x/l. The solution of the Schrödinger equation can be done in a similar way. In this case, it passes into the Schrödinger equation for a harmonic oscillator at $\varepsilon_3=0$ and $\varepsilon_4=0$. Then it can be solved using perturbation theory [19]. In this case, the energy of particles in potential (16) in the zeroth approximation is equal to the energy of a harmonic oscillator:

$$E_n^0=\hbar\omega\left(n+\frac{1}{2}\right), \qquad (17)$$

and the wave function in the zero approximation has the form [19]

$$u_n^0(x)=\left(2^n n! l\sqrt{\pi}\right)^{-1/2} e^{-1/2\xi^2} H_n(\xi),\ \xi=\frac{x}{l}. \qquad \text{(eighteen)}$$

Then the calculation of the energy spectrum of electrons according to the perturbation theory gives the following result

$$E(k_\alpha,n)=E(k_\alpha)+\frac{1}{8}\hbar\omega\left\{\left(n+\frac{1}{2}\right)-30\left(\frac{\varepsilon_1}{\hbar\omega}\right)^2\left(n^2+n+\frac{11}{30}\right)+6g\frac{\varepsilon_1}{\hbar\omega}\left(2n^2+2n+1\right)-\right.$$

$$\left.-g^2\left(\frac{\varepsilon_1}{\hbar\omega}\right)^2\left(34n^3+51n^2+59n+21\right)\right\}, \qquad (19)$$

where m is the effective mass of electrons, oc b Ox is chosen as the size quantization axis, $g=\frac{\varepsilon_2}{\varepsilon_1}$, in the spherical approximation in the energy spectrum $E(k_\alpha)=\frac{\hbar^2}{2\cdot m}\left(k_y^2+k_z^2\right)$. $k_\alpha=0\ (y,z)$.

Figure 2 shows the dependence $E\left[k_\alpha=0,n,\left(\varepsilon_1/\hbar\omega\right)\right]$ on the parameter $\varepsilon_1/\hbar\omega$ for various n. It can be seen from Fig. 2 that the energy spectrum of electrons in potential (16) takes discrete values and the steepness of the energy spectrum is the more noticeable, the larger $g=\frac{\varepsilon_2}{\varepsilon_1}$, and it also decreases with increasing $\varepsilon_1/\hbar\omega$ for arbitrary values of n.

Linear approximation

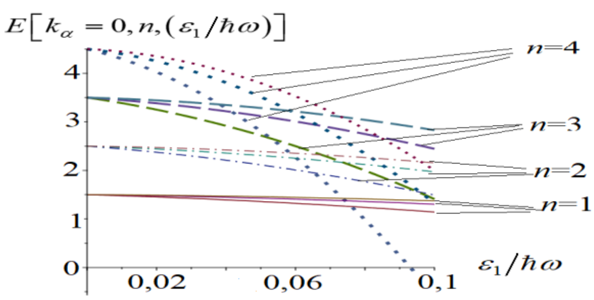
If we consider that $U''_{x=a}=0$ then the Schrödenger equation takes the form

$$\frac{d^2\psi}{d\xi^2}-\xi\psi=0, \qquad \text{(twenty)}$$

whose solution can be represented as a linear combination of the Airy functions of the first and second kind

$$\psi(\xi)=A_1 Ai(\xi)+B_1 Bi(\xi), \qquad (21)$$

where $\xi=(x-a)[2m(dU/dx)_a/\hbar^2]^{1/3}$. Unknown quantities A_1 and B_1,



Rice. 2. Dependence $E\left[k_\alpha=0,n,\left(\varepsilon_1/\hbar\omega\right)\right]$ on the parameter $\varepsilon_1/\hbar\omega$ for different n. From above, the first line corresponds to the value $g=0,1$, the second - $g=0,25$ and the third $g=0,5$ - for a different value n.

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determined from the boundary conditions of the problem under consideration, $Ai(\xi)$, $Bi(\xi)$ are the Airy functions, which oscillate for negative values of ξ both $Ai(\xi)$, $Bi(\xi)$ and for positive values ξ, the function $Ai(\xi)$

decays $Bi(\xi)$ exponentially and grows exponentially. Therefore, in the future, for example, to calculate the bound states of electrons, we consider that the coefficient $B_1 = 0$, since the wave function must decay at infinity (see Fig. 3) .

For definiteness, consider the case when the allowed area is to the left of the turning point $(\xi = 0)$, and the forbidden area is on the right. Then we will be interested in a solution that decays exponentially at $\xi \to +\infty$ and oscillates at $\xi \to -\infty$. Such a solution to the Schrödenger equation is described by the Airy function of the first kind, which has the following asymptotics, i.e. etc $\xi \to +\infty$

$$\psi(\xi \to \infty) = A_1 (1/2)\xi^{-1/4} \times \exp\{-(2/3)\xi^{3/2}\},$$

$$\psi(\xi \to -\infty) = A_1 (-\xi)^{-1/4} \sin\left[(2/3)|(-\xi)^{3/2} + \pi/4\right] \quad (22)$$

Note that the relationship between damped and oscillating solutions (4) – (5) in the allowed and forbidden energy regions can be obtained without matching the wave functions in a certain coordinate. Let's illustrate this as follows. If we assume that the particle hits the triangular potential barrier) from the left, then from the right

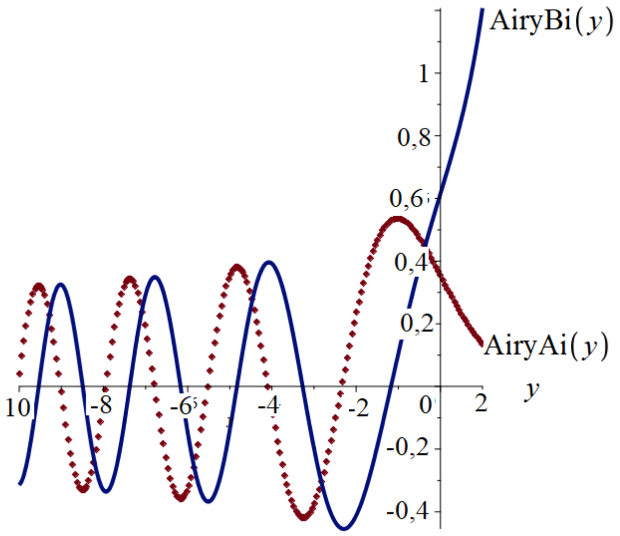

Fig.3. Airy function plot: Ai(y) (diamonds) and Bi(y) (solid line).

from the barrier (in the region $\xi > 0$) there will be only the following exponentially decreasing function:

$$\psi_{II}(x) = \frac{C}{\xi^{1/4}} \exp\left(-\frac{2}{3}\xi^{3/2}\right), \quad (23)$$

which coincides with the asymptotic expansion for the Airy function at $x \to +\infty$, where C *is a* constant determined from the boundary condition of the problem.

In the classically allowed region I ($x < a$), the wave function can be represented as two traveling waves

$$\psi_I(\xi) = \frac{C_1}{|\xi|^{1/4}} \exp(-\frac{2}{3}i|\xi|^{3/2}) + \frac{C_2}{|\xi|^{1/4}} \exp(+\frac{2}{3}i|\xi|^{3/2}) \quad (25)$$

In order for this expression to have the form of a standing wave and, thus, to coincide with the asymptotic expression for the Airy function at $\xi \to -\infty$, it is necessary to require, for example, $C_1 = -Ce^{-i\pi/4}/(2i)$ and $C_2 = Ce^{+i\pi/4}/(2i)$. In this case, formula (10) takes the following form

$$\psi_I(\xi) = \frac{C}{|\xi|^{1/4}} \sin\left(\frac{\pi}{4} - \frac{2}{3}\xi^{3/2}\right) \quad (26)$$

Thus, we have established that the exponentially decaying solution transforms into an oscillating solution.

In conclusion, we note that the complete and rigorous solution of the problem in the semiclassical approximation, which will allow one to describe the wave function for arbitrary values of *x,* now reduces to the problem of matching the exact solution of equation (6) near the point $\xi = 0$ *with* approximate solutions (4) - (5) in the region the applicability of the ratios. This case requires a separate consideration.

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