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ENERGY STATES OF CURRENT CARRIERS IN MULTILAYER SEMICONDUCTOR STRUCTURES. WENTZEL-KRAMERS-BRILLOUIN APPROXIMATION

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Abstract. States of electrons 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.

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 in coordinates.

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 inhomogeneously distributed parameters, the development of methods for the effective theoretical analysis of such systems, the development and provision of objective methods for controlling technological processes that make it possible to create semiconductor layers with desired properties (Shchuka A.A., 2007; Usanov, D.A. 2013). In this regard, below we consider the general questions 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 noninteracting 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 (Dragunov, 2006; Ivchenko, 2005; Rasulov, 2018; Petrov, 1994; Rasulov, 2020; Golub, 1995; Rasulov, 2020).

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 (Usanov, D. A., 2013). In this case, the problem of electronic states is reduced to the problem of the 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 structures mentioned above 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.

Basic relationships

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, making the substitution $\psi(x)=$ $=\exp\left(iS(x)/\hbar\right)$, we obtain the equation for the function $S(x)$

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

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 rows indegrees of the Planck constant, i.e.

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

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 E are the effective mass and energy of current carriers.

In classically inaccessible energy regions, i.e. at, 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. 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 potential energy *U(x)* near the turning point $(x=a)$ can be represented as

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

or

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

Then the Schrödinger equation can be written as

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

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

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

$$+C_2\cdot{}_1F_1\left[\left(\frac{3}{4}-\frac{k_1^2}{16k_2^{3/2}}-\frac{k_0}{4k_2^{1/2}}\right),\frac{3}{2},\frac{\left(2k_2\varsigma+k_1\right)^2}{4k_2^{3/2}}\right]\left(2k_2\varsigma+k_1\right)\exp\left[-\frac{\varsigma\left(2k_2\varsigma+k_1\right)}{2\sqrt{k_2}}\right], \qquad (8)$$

where $\varsigma=\frac{x-a}{a}$, $E_a=\frac{\hbar^2}{2ma^2}$,

$$k_1=\frac{1}{E_a}U'_{\varsigma=0}=\frac{1}{E_a}\frac{\partial U(\varsigma)}{\partial\varsigma}\bigg|_{\varsigma=0},$$

$$k_2=\frac{1}{E_a}U''_{x=a}=\frac{1}{E_a}\frac{\partial^2U(\varsigma)}{\partial\varsigma^2}\bigg|_{\varsigma=0},$$

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

In the general case,

$${}_1F_1\left[\left(\frac{1}{4}-\frac{k_1^2}{16k_2^{3/2}}-\frac{k_0}{4k_2^{1/2}}\right),\frac{1}{2},\frac{\left(2k_2\varsigma+k_1\right)^2}{4k_2^{3/2}}\right]\propto$$

$$\propto\exp\left[\frac{\left(2k_2\varsigma+k_1\right)^2}{4k_2^{3/2}}\right],$$ 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

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

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

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

$$k_0=(1+16n)k_2^{1/2}-\frac{k_1^2}{4k_2^{1/2}}. \qquad (10)$$

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

$$E_1-U(x=0)=$$

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

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

$$\psi_{2n+1}(\varsigma)=k_1F_1\left[-n,\frac{3}{2},\frac{\left(2k_2\varsigma+k_1\right)^2}{4k_2^{3/2}}\right]\times$$

$$\times\left(2k_2\varsigma+k_1\right)^{-\frac{\varsigma\left(2k_2\varsigma+k_1\right)}{2\sqrt{k_2}}}, \qquad (12)$$

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

$$E_2-U(x=0)=$$

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

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

$$\frac{E_2-U(x=0)}{\xi_U\cdot U'_{\varsigma=0}}=\left[\left(11+16n\right)-\frac{1}{4}x\right]^2 \quad .(15)$$

It can be seen from formulas (11) and (13) 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.

Figure 1 *a* and *b* shows the dependences of the size-quantized energy spectra, characterized by the values of $\frac{E_1(n)-U(x=0)}{\xi_U\cdot U'_{\varsigma=0}}$ and $\frac{E_2(n)-U(x=0)}{\xi_U\cdot U'_{\varsigma=0}}$, on the parameter $x=\frac{U'_{\varsigma=0}}{E_a\xi_U}$.

It can be seen from these figures that as $x=\frac{U'_{\varsigma=0}}{E_a\xi_U}$ increases, the values of $\frac{E_1(n)-U(x=0)}{\xi_U\cdot U'_{\varsigma=0}}$ and $\frac{E_2(n)-U(x=0)}{\xi_U\cdot U'_{\varsigma=0}}$ decrease from $n=2,3,....$ These energy values from $n=1$ with the growth of $x=\frac{U'_{\varsigma=0}}{E_a\xi_U}$ 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:

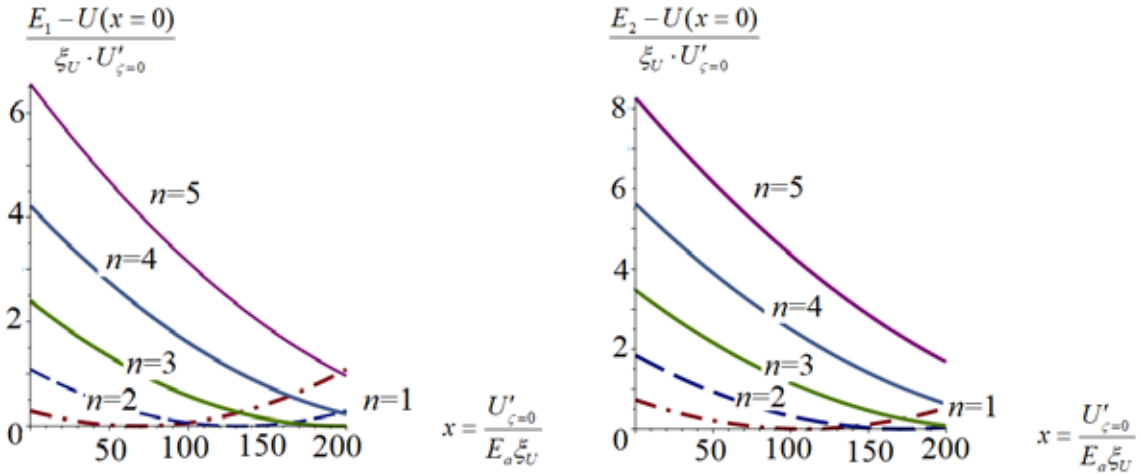
$$H_{2n}\left(\zeta^2\right)=(-1)^n\frac{(2n)!}{n!}\cdot{}_1F_1\left(-n,\frac{1}{2},\zeta^2\right),$$

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

$$\cdot\zeta\cdot{}_1F_1\left(-n,\frac{3}{2},\zeta^2\right).$$

Figure 1. *Dependences of the energy quantities*

a) b)



$\frac{E_1(n)-U(x=0)}{\xi_U\cdot U'_{\varsigma=0}}$ and $\frac{E_2(n)-U(x=0)}{\xi_U\cdot U'_{\varsigma=0}}$

on $x=\frac{U'_{\varsigma=0}}{E_a\xi_U}$ for different values of the size quantization number, where $\xi_U=U''_{\varsigma=0}/U'_{\varsigma=0}$

Conclusion

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

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

where $l=\sqrt{\hbar/(m\omega)}$. ε_3 and ε_4 are the expansion coefficients of $U(x)$ in a series of x/l. The solution of the Schrödinger equation can be done in a similar way. In this case, it passes into the Schrödenger equation for a harmonic oscillator at $\varepsilon_3=0$ and $\varepsilon_4=0$. Then it can be solved using perturbation theory (Landau, 1981). In this case, the energy of particles in

potential (16) in the zeroth approximation is equal to the energy of a harmonic oscillator:

$$E_n^0 = \hbar\omega\left(n+1/2\right), \quad (17)$$

and the wave function in the zero approximation has the form

$$u_n^0(x) = \left(2^n n! l\sqrt{\pi}\right)^{-1/2} e^{-1/2\xi^2} H_n(\xi), \quad (18)$$

$\xi = x/l$.

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

$$E(k_\alpha, n) = E(k_\alpha) + \\ + \frac{1}{8}\hbar\omega\left\{\left(n+1/2\right) - 30\kappa^2\left(n^2+n+11/30\right) + \right. \\ + 6g\kappa\left(2n^2+2n+1\right) - \\ \left. - g^2\kappa^2\left(34n^3+51n^2+59n+21\right)\right\}, \quad (19)$$

where $\kappa = \varepsilon_1/(\hbar\omega)$, m is the effective electron mass, the Ox axis is chosen as the size quantization axis, $g = \varepsilon_2/\varepsilon_1$, in the spherical approximation in the $E(k_\alpha) = \hbar^2\left(k_y^2+k_z^2\right)/\left/\left(2\cdot m\right)\right.$energy spectrum. Calculations show that the energy spectrum of electrons in potential (16) takes discrete values and the steepness of the energy spectrum is more noticeable, the greater $g = \varepsilon_2/\varepsilon_1$, and it also decreases with increasing $\varepsilon_1/(\hbar\omega)$ for arbitrary values of n.

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