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THE THEORY OF QUASISTATIONARY ENERGY STATES IN A SPHERICAL POTENTIAL WELL

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ABSTARCT

Quasi-stationary electronic states in a spherically symmetric semiconductor potential well are determined in the semiclassical approximation based on the calculation of matrix elements of the transfer matrix. In this case, three regions of the potential well were taken into account, which differ from each other in geometric dimensions. The calculation was carried out by solving the Schrödenger equation in a spherical coordinate system.

KEYWORDS: ***quasistationary electronic states, spherically symmetric semiconductor potential well, semiclassical approximation, matrix elements of the transfer matrix***

INTRODUCTION

The progress of modern microelectronics is largely determined by the study of the properties of systems with nonuniformly 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 allow creating semiconductor layers with desired properties [1–4].

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 [1–6]. In works [7–17] were calculated the dynamic conductivity σ(ω) or the density of current j(ω) of the response of the system to an external action in a semiconductor multilayer structure. The theory was created in different models using different mathematical methods for solving the complete Schrödinger equation for a system of electrons interacting with an electromagnetic field in a structure with a $\delta-$shaped potential barrier. In the above-mentioned works, the problem was solved without taking into account the Bastard condition [5], i.e., the difference between the effective masses of current carriers in neighboring layers of the structure is not taken into account. Also, they did not study quasi-stationary electronic states in a spherically symmetric well in the semiclassical approximation. This work is devoted to this case.

$$U_N(r)=\begin{cases}U_1 & \text{at} \quad r<r_1\\ U_2 & \text{at} \quad r_1<r<r_2\\ U_3 & \text{at} \quad r>r_2\end{cases} \tag{1}$$

where $r=\sqrt{x^2+y^2+z^2}$ is the radial coordinate variable, R- is the quantum dot radius. We shall consider only spherically symmetric solutions and calculate the spectrum of states of a particle in a three-dimensional barrier $U_N(r)$. Then the solution of the stationary Schrödinger equation with a spherically symmetric potential

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$$\frac{\partial}{\partial r}\left(r^2\frac{\partial f_N(r,\theta,\varphi)}{\partial r}\right)+\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f_N(r,\theta,\varphi)}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 f_N(r,\theta,\varphi)}{\partial\varphi^2}\right]+$$

$$+\frac{2m}{\hbar^2}r^2\left(E-U_N(r)\right)f_N(r,\theta,\varphi)=0 \qquad (2)$$

looking for in the form

$$f_N(r,\theta,\varphi)=\frac{1}{r}\chi_N(r)Y_{LM}(\theta,\varphi) \qquad (3)$$

where $Y_{LM}(\theta,\varphi)$ are spherical functions [18], L- is the orbital angular momentum, M is the projection of the angular momentum onto the z axis. The radial function $\chi_N(r)$ is a solution to the Schrödinger equation with effective potential

$$\frac{d^2\chi_N(r)}{dr^2}+\left(\frac{2m_N}{\hbar^2}\left(E-U_N(r)\right)-\frac{L(L+1)}{r^2}\right)\chi(r)=0. \qquad (4)$$

Then, after notations $\xi_A=k_Ar$, $\xi_B=k_Br$, $k_A=\sqrt{\frac{2m_A}{\hbar^2}E}$, where $k_B=\sqrt{\frac{2m_B}{\hbar^2}(U-E)}$ we modify (4) as

$$\frac{\partial^2\chi(\xi_A)}{\partial\xi_A^2}+\left(1-\frac{L(L+1)}{\xi_A^2}\right)\chi(\xi_A)=0,\quad at\quad 0\le r\le r_1 \qquad (5)$$

$$\frac{\partial^2\chi(\xi_B)}{\partial\xi_B^2}+\left(1-\frac{L(L+1)}{\xi_B^2}\right)\chi(\xi_B)=0,\quad at\quad r\rangle r_1 \qquad (6)$$

If the solutions of equations (5) and (6) are represented as $\chi(x)=x^{1/2}F(x)$, then $F(\xi_A)$ and $F(\xi_B)$ are the solution of the following Bessel equations

$$\xi_A^2\frac{\partial^2F(\xi_A)}{\partial\xi_A^2}+\xi_A\frac{\partial F(\xi_A)}{\partial\xi_A}+\left(\xi_A^2-(L+1)^2\right)F(\xi_A)=0, \qquad (7)$$

$$\xi_B^2\frac{\partial^2F(\xi_B)}{\partial_B^2}+\xi_B\frac{\partial F(\xi_B)}{\partial\xi_B}+\left(-\xi_B^2-(L+1)^2\right)F(\xi_B)=0, \qquad (8)$$

Under condition $F(\xi_{A,B}\to 0)\to 0$, solution (7) is a Bessel function with a half-integer index, i.e. : $F(\xi_A)=C_A\cdot J_{l+1/2}(\xi_A)$. When the function $F(\xi_B)$ is bounded at $\xi_B\to\infty$, solution (8) is the MacDonald function [19] with a half-integer index, i.e., : $F(\xi_B)=C_B\cdot K_{l+1/2}(\xi_B)$

Thus, the radial part $f_N(r)=\frac{1}{r}\chi_N(r)$ of the wave function (2) is represented in the form

$$f_N(r)=\begin{cases}C_1j_l(k_Ar), & npu \quad 0\le r\le r_1\\ C_2\kappa_l(k_Br), & npu \quad r>r_1\end{cases} \qquad (9)$$

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$$f_N(r)=\begin{cases} C_1 j_l\left(k_A r\right), & at \quad 0\le r\le r_1 \\ C_2\kappa_l\left(k_B r\right), & at \quad r>r_1 \end{cases} \tag{9}$$

Here

$$j_l\left(\xi_A\right)=\frac{1}{\sqrt{\xi_A}}J_{l+1/2}\left(\xi_A\right)\ ,\ \kappa_l\left(\xi_B\right)=\frac{1}{\sqrt{\xi_B}}K_{l+1/2}\left(\xi_B\right). \tag{10}$$

To simplify the solution of this problem, we further assume that $L=0$, i.e., consider s-states. Then we rewrite (4) as

$$\frac{d^2\chi_N(r)}{dr^2}+k_N^2\chi_N(r)=0. \tag{11}$$

whose solution we represent in the form

$$\chi_N(r)=A_N e^{ik_N r}+B_N e^{-ik_N r}, \tag{12}$$

where $N=1$ corresponds to region $r<r_1$, $N=2$ corresponds to region $r_1<r<r_2$, $N=3$ corresponds to region $r>r_2$ $r<r_1$, $k_N^2=\frac{2m_N}{\hbar^2}\left(E-U_N\right)$, m_N - is the effective mass of current carriers in the region (if these regions are the same in terms of physical and chemical properties, then the effective masses will take the same values). The unknown quantities A_N and B_N, as usual, are determined from the Bastard condition [5] at the points $r=r_1$ and $r=r_2$.

Note that the difference between the solution of the Schrödenger equation in the Cartesian and spherical coordinate systems is that the existence of an additional boundary at $r=0$ must be replaced by the condition $\chi_N\left(r=0\right)=0$. As indicated in [20], to determine the energy spectrum of localized states, we will use the criterion for the existence of such states, which is determined by the equality of the diagonal matrix element of the transfer matrix to zero (see, for example, [20]). In this case, we take into account that the localized state of the particle in the potential well corresponds to such a distribution of the wave function, in which the solutions of the Schrödinger equation for this case are increasing. Therefore, in solutions (for a certain case) it is necessary to exclude terms of the form $B_N e^{ik_N r}$. Then the criterion for the existence of localized states is determined by the relation

$$\begin{pmatrix} -A_1 \\ A_1 \end{pmatrix}=\hat{T}\begin{pmatrix} A_3 \\ 0 \end{pmatrix}, \tag{14}$$

where the matrix elements of matrix $\hat{T}$ are defined as

$$T_{11}^{(N,N+1)}=\frac{1}{2}\left(1+\frac{\tilde{k}_{N+1}}{\tilde{k}_N}\right)e^{i(k_{N+1}-k_N)r},T_{12}^{(N,N+1)}=\frac{1}{2}\left(1-\frac{\tilde{k}_{N+1}}{\tilde{k}_N}\right)e^{-i(k_{N+1}+k_N)r},$$
$$T_{21}^{(N,N+1)}=T_{12}^{(n,N+1)*},T_{22}^{(N,N+1)}=T_{11}^{(N,N+1)*}, \tag{15}$$

$\tilde{k}_N=k_N/m_N \quad N=1,2,3,\ldots,$ the sign * means complex conjugation.

Following [20], in cases $U_1=U_3$ and $E<U_2$, we have expressions for matrix elements, i.e., for sub-barrier $\left(E\langle U_j\right)$ passage of electrons. In the latter case, it is convenient to use transformations like $\tilde{k}_{m+n}=i\tilde{\kappa}_{m+n}$, $\tilde{k}_m\pm\tilde{k}_{m+n}=\sqrt{\left(\tilde{k}_m\right)^2\pm\left(\tilde{\kappa}_{m+n}\right)^2}e^{\pm i\varphi_{m,m+n}}$ when $\tilde{k}_m$ is real and $\tilde{k}_{m+n}$ is imaginary, where $arctg\left(\varphi_{m,m+n}\right)=\frac{\tilde{\kappa}_{m+n}}{\tilde{k}_m}$. Then, it should

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be noted that during the transition from one region to another, a phase shift must occur in electron waves, associated with a mismatch in the phases of the waves propagating in different, but in neighboring, regions. To simplify further calculations, we assume that $k_1 = k_3 = k$, $k_2 = i\kappa$. Then the matrix elements of the transfer matrix for this case can be written as

$$T_{11} = \frac{e^{-ikr_1 + ik_2 r_1}}{4i\tilde{k}\tilde{\kappa}} \times \{(\tilde{k} + i\tilde{\kappa})^2 e^{\kappa d} - (\tilde{k} - i\tilde{\kappa})^2 e^{-\kappa d}\}, \quad (16)$$

$$T_{21} = \frac{e^{ikr_1 + ik_2 r_1}}{4i\tilde{k}\tilde{\kappa}} \times \left\{\left(\tilde{k} + i\tilde{\kappa}\right)\left(\tilde{k} - i\tilde{\kappa}\right)e^{\kappa d} - \left(\tilde{k} + i\tilde{\kappa}\right)\left(\tilde{k} - i\tilde{\kappa}\right)e^{-\kappa d}\right\}. \quad (17)$$

Having carried out the appropriate transformations, we obtain the condition for the existence of localized states as

$$e^{-ikr_1} \times \{(k + i\kappa)^2 e^{\kappa d} - (k - i\kappa)^2 e^{-\kappa d}\} =$$

$$= -e^{+ikr_1} \times \left\{\left(k + i\kappa\right)\left(k - i\kappa\right)e^{\kappa d} - \left(k + i\kappa\right)\left(k - i\kappa\right)e^{-\kappa d}\right\}, \quad (18)$$

or

$$\left(\frac{\kappa}{k}\tan kr_1 + 1\right) = -e^{-2\kappa d}\left(\frac{k - i\kappa}{k + i\kappa}\right) \times \left(\frac{\kappa}{k}\tan kr_1 - 1\right). \quad (19)$$

From the last relation at $\kappa d \gg 1$ it is easy to obtain the energy spectrum of stationary states in a spherical potential well with finite height as

$$\frac{\kappa_0}{k_0}\tan k_0 r_1 + 1 = 0, \quad (20)$$

where $k_0(\kappa_0)$ is the wave vector of electrons corresponding to their sub-barrier (above-barrier) passage through the potential barrier.

CONCLUSION

Taking into account the Bastard condition [5], from (10) it is easy to obtain the following equations

$$\begin{cases} j_l(k_A r_1) C_1 = \kappa_l(k_B r_1) C_2, \\ \dfrac{\partial j_l(k_A r_1)}{\partial(k_A r_1)} C_1 = \dfrac{m_A}{m_B}\dfrac{k_B}{k_A} C_2 \dfrac{\partial \kappa_l(k_B r_1)}{\partial(k_B r_1)} \end{cases} \quad (21)$$

откуда немедленно получаем соотношение для энергетического спектра
whence we immediately obtain the relation for the energy spectrum of electrons in a spherical quantum dot:

$$\frac{\partial \ln\left[j_l(k_A r_1)\right]}{\partial(k_A r_1)} = \beta \frac{\partial \ln\left[\kappa_l(k_B r_1)\right]}{\partial(k_B r_1)}, \quad (22)$$

where

$$\beta = \sqrt{\frac{m_B(U - E)}{m_A E}}.$$

Корни $E_{n,l}$ уравнения (22) при заданном l можно пронумеровать числом n = 0 ,1 ,2 ,... , равным числу узлов радиальной функции $f_N(r)$.Число l определяет поведение радиальной функции вблизи начала координат:

The roots $E_{n,l}$ of equation (22) for a given l can be numbered by the number n = 0,1,2,... , equal to the number of nodes of the radial function $f_N(r)$. The number l determines the behavior of the radial function near the origin: $f_N(r) = f_N^{(l)}(r) \propto r^l$.

In conclusion, we only note that as the radius of a size-quantized filament with a finite potential barrier height U_0 increases, the number of size-quantized levels in it increases. However, it should be noted that the level with the minimum energy corresponding to n=0, l=0, does not disappear even in the limit c $r \to 0$. Then for $x \gg 1$ using the following relations of the Bessel

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and MacDonald functions $J_0(x) \approx 1,\ K_0(x) \approx 0.116 - \ln x,\ \frac{\partial J_0(x)}{\partial x} \approx -0.5x,\ \frac{\partial K_0(x)}{\partial x} \approx x^{-1}$ [21] it is easy to obtain an expression for the minimum value of the energy spectrum of a semiconductors filament with a finite potential barrier height U_0

$$E_{0,0} \approx U_0 - 0.63\frac{\hbar^2}{m_B r_1^2}\exp\left(-\frac{2\hbar^2}{m_B r_1^2 U_0}\right). \qquad (23)$$

It can be seen from the latter, that in the semiconductor filament, where condition $k_A r_1, k_B r_1 \langle\langle 1$ is satisfied, there is at least one size-quantized level, the value of which is exponentially small relative to the height of the potential barrier.

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