



GENERALIZED MODEL FOR THE ENERGY SPECTRUM OF ELECTRONS IN TUNNEL-COUPLED SEMICONDUCTOR QUANTUM WELLS

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ABSTRACT

The electronic properties of both symmetric and asymmetric with respect to the geometric dimensions of the semiconductor structure layers have been studied. In this case, the Schrödinger equation is solved both for the general wave function and for quantum wells, taking into account the difference in effective masses in the layers of the structure.

The expression for the gap between the energy levels of the energy appearing in the quantum well is analyzed. It is shown that the energy gap is determined by a quantity that is a measure of the asymmetry of two quantum wells, and it is equal to zero for symmetric wells. In the case when the asymmetry of the wells is negligibly small, then the gap between the levels in the tunnel-coupled wells is determined by the value characterizing the tunneling splitting of the energy levels.

It is determined that in tunnel-coupled wells, the energy levels are shifted relative to the levels of isolated wells, and wave functions arise from the wave functions of isolated wells as a result of their "mixing".

KEYWORDS: energy levels, quantum well, tunneling, tunnel-coupled potential wells, size quantization, energy spectrum, potential well.

INTRODUCTION

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]. In [2–17], the kinetic properties of multilayer and nanosized semiconductor structures were studied. 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 δ shaped potential barrier. In the above-mentioned works, the problem was solved without taking into account the Bastard condition: the difference in the effective masses of current carriers in adjacent layers of the structure was not taken into account. And also, tunnel-bound electronic states in quantum wells, between which there is a narrow tunnel-transparent potential barrier, have not been studied. This work is devoted to this case.

General Ratios

In structures with two (or more) closely spaced potential wells, the wave functions of adjacent wells overlap with each other in the barrier region between the wells, so that the probability of detecting an electron in the barrier region is noticeably different from zero. Consequently, current carriers can pass from one well to another with a noticeable probability, despite the fact that their energies do not exceed the barrier value. Such a quantum phenomenon is called the tunneling effect [18]. Quantum wells, in which the probability of the tunneling effect is not small, are called tunnel-coupled.

The emergence of a tunnel coupling as the wells approach each other affects the position of the energy levels in them and the shape of the wave functions. To calculate the size quantization levels and the wave functions belonging to them, we must solve the Schrödinger equation for the chosen potential with Bastard boundary conditions, where $\psi(x)$ the wave function and

$\frac{1}{m} \frac{d\psi}{dx}$ magnitudes remain continuous at the interface of the potential well (A layer) and the barrier (B layer) [7], i.e. .

$$\psi|_A = \psi|_B, \quad \left. \frac{1}{m} \frac{d\psi(x)}{dx} \right|_A = \left. \frac{1}{m} \frac{d\psi(x)}{dx} \right|_B \quad (1)$$

Therefore, in further calculations it is necessary to take into account (1) at each heterointerface (and it is necessary to take into account the decrease in the wave functions for if the wave vector of the current carriers is real). In a nanostructure with two wells, there are two interfaces. Therefore, conditions (1) give a relatively cumbersome system of equations for eight unknowns.

Let $U_1(x)$ and $U_2(x)$ are single-well potentials (left and right wells) considered independently of each other. Here it is convenient to assume that the energy reference point is chosen at the level of the barrier, and each of the functions $U_1(x)$, $U_2(x)$ differs from zero only within its own layer. Then the potential $U(x)$ for the structure with two wells is written as the sum of $U_1(x)$ and $U_2(x)$, and the Schrödinger equation in the two-well problem with coordinate-independent effective mass m takes the form:

$$H\psi = E\psi, \quad (2)$$

where $H = H_1 + H_2 + U_1 + U_2$, $H_1(U_1)$, and $H_2(U_2)$ the operator of the Hamiltonian (potential) for the left and right potential wells. Then the general Schrödinger equation takes the form

$$\left(-\frac{\hbar^2}{2m_1} \nabla^2 - \frac{\hbar^2}{2m_2} \nabla^2 + U_1 + U_2 \right) \psi = E\psi$$

and for the one-dimensional case we have

$$\left(-\frac{\hbar^2}{2\mu_{12}^+} \frac{\partial^2}{\partial z^2} + U_1 + U_2 \right) \psi(x) = \left(E - \frac{\hbar^2 k_{\perp}^2}{2\mu_{12}^+} \right) \psi(x) \quad (3)$$

where $\frac{1}{\mu_{12}^+} = \left(\frac{1}{m_1} + \frac{1}{m_2} \right)$, $k_{\perp}^2 = k_x^2 + k_y^2$.

Then the Schrödinger equation for the left and right potential wells can be written as

$$\left(-\frac{\hbar^2}{2m_1} \frac{\partial^2}{\partial z^2} + U_1 \right) \psi_1 = \left(E_1 - \frac{\hbar^2 k_{\perp}^2}{2m_1} \right) \psi_1, \quad \left(-\frac{\hbar^2}{2m_2} \frac{\partial^2}{\partial z^2} + U_2 \right) \psi_2 = \left(E_2 - \frac{\hbar^2 k_{\perp}^2}{2m_2} \right) \psi_2. \quad (4)$$

If we take into account the principle of superposition, then we have

$$\psi(x) = C_1 \psi_1(x) + C_2 \psi_2(x) \quad (5)$$

Then substitution (5) into equation (3) and taking into account (4), we obtain:

$$\begin{aligned} & C_1 \left(\frac{m_1}{\mu_{12}^+} \left[-\frac{\hbar^2}{2m_1} \frac{\partial^2 \psi_1(x)}{\partial z^2} + U_1 \psi_1(x) \right] + \left(1 - \frac{m_1}{\mu_{12}^+} \right) U_1 \psi_1(x) + U_2 \psi_1(x) \right) + \\ & + C_2 \left(\frac{m_2}{\mu_{12}^+} \left[-\frac{\hbar^2}{2m_2} \frac{\partial^2 \psi_2(x)}{\partial z^2} + U_2 \psi_2(x) \right] + U_1 \psi_2(x) + \left(1 - \frac{m_2}{\mu_{12}^+} \right) U_2 \psi_2(x) \right) = \\ & = C_1 \left(E - \frac{\hbar^2 k_{\perp}^2}{2\mu_{12}^+} \right) \psi_1(x) + C_2 \left(E - \frac{\hbar^2 k_{\perp}^2}{2\mu_{12}^+} \right) \psi_2(x) \end{aligned} \quad (6)$$

Then multiplying (6) on the left side by $\psi_1^*(x)$ and $\psi_2^*(x)$ alternately, as well as integrating, we obtain

$$\begin{cases} C_1 \left[\tilde{E}_1 \sigma + \left(1 - \frac{m_1}{\mu_{12}^+}\right) U_1^{(21)} + U_2^{(21)} - \tilde{E} \sigma \right] + C_2 \left[\tilde{E}_2 + U_1^{(22)} + \left(1 - \frac{m_2}{\mu_{12}^+}\right) U_2^{(22)} - \tilde{E} \right] = 0, \\ C_1 \left[\tilde{E}_1 + \left(1 - \frac{m_1}{\mu_{12}^+}\right) U_1^{(11)} + U_2^{(11)} - \tilde{E} \right] + C_2 \left[\tilde{E}_2 \sigma + U_1^{(12)} + \left(1 - \frac{m_2}{\mu_{12}^+}\right) U_2^{(12)} - \tilde{E} \sigma \right] = 0. \end{cases} \quad (7)$$

Здесь $U_1^{(21)} = \int \psi_2^*(x) U_1 \psi_1(x) \cdot dx$, $U_2^{(21)} = \int \psi_2^*(x) U_2 \psi_1(x) \cdot dx$, $U_1^{(22)} = \int \psi_2^*(x) U_1 \psi_2(x) \cdot dx$,

$U_2^{(22)} = \int \psi_2^*(x) U_2 \psi_2(x) \cdot dx$, $U_1^{(11)} = \int \psi_1^*(x) U_1 \psi_1(x) dx$, $U_2^{(11)} = \int \psi_1^*(x) U_2 \psi_1(x) dx$,

$U_1^{(12)} = \int \psi_1^*(x) U_1 \psi_2(x) dx$, $U_2^{(12)} = \int \psi_1^*(x) U_2 \psi_2(x) dx$, $\sigma = \int \psi_2^*(x) \psi_1(x) \cdot dx$, $\tilde{E} = E - \frac{\hbar^2 k_{\perp}^2}{2\mu_{12}^+}$

$$\tilde{E}_a = E_a - \frac{\hbar^2 k_{\perp}^2}{2m_a}, \tilde{E}_1 = \frac{m_1}{\mu_{12}^+} \left(E_1 - \frac{\hbar^2 k_{\perp}^2}{2m_1} \right), \tilde{E}_2 = \frac{m_2}{\mu_{12}^+} \left(E_2 - \frac{\hbar^2 k_{\perp}^2}{2m_2} \right).$$

In order for the system of homogeneous equations (7) to have a nonzero solution, it is necessary to equate its determinant to zero. Then

$$\begin{bmatrix} \tilde{E}_1 \sigma + \left(1 - \frac{m_1}{\mu_{12}^+}\right) U_1^{(21)} + U_2^{(21)} - \tilde{E} \sigma & \tilde{E}_2 + U_1^{(22)} + \left(1 - \frac{m_2}{\mu_{12}^+}\right) U_2^{(22)} - \tilde{E} \\ \tilde{E}_1 + \left(1 - \frac{m_1}{\mu_{12}^+}\right) U_1^{(11)} + U_2^{(11)} - \tilde{E} & \tilde{E}_2 \sigma + U_1^{(12)} + \left(1 - \frac{m_2}{\mu_{12}^+}\right) U_2^{(12)} - \tilde{E} \sigma \end{bmatrix} = 0. \quad (8)$$

Where do we get the algebraic equation of the second degree for the variable \tilde{E}

$$a\tilde{E}^2 - b \cdot \tilde{E} + c = 0, \quad (9)$$

which has two of its roots \tilde{E}_{\pm} , which are the desired energy levels of an electron in a double-well potential $U(x)$

$$\tilde{E}_+ = \frac{b}{2a} \left(-1 + \sqrt{1 - 4 \frac{ac}{b^2}} \right), \tilde{E}_- = \frac{b}{2a} \left(-1 - \sqrt{1 - 4 \frac{ac}{b^2}} \right) \quad (10)$$

где $a = (1 + \sigma^2)$, $b = (1 + \Xi_6 + \Xi_2 + \Xi_3)$, $c = \Xi_4 - \Xi_1$,

$$\Xi_1 = \left(\tilde{E}_1 \sigma + \left(1 - \frac{m_1}{\mu_{12}^+}\right) U_1^{(21)} + U_2^{(21)} \right) \left(\tilde{E}_2 \sigma + U_1^{(12)} + \left(1 - \frac{m_2}{\mu_{12}^+}\right) U_2^{(12)} \right),$$

$$\Xi_2 = \left(\tilde{E}_2 \sigma + U_1^{(12)} + \left(1 - \frac{m_2}{\mu_{12}^+}\right) U_2^{(12)} \right) \sigma, \Xi_3 = \left(\tilde{E}_1 \sigma + \left(1 - \frac{m_1}{\mu_{12}^+}\right) U_1^{(21)} + U_2^{(21)} \right) \sigma,$$

$$\Xi_4 = \left(\tilde{E}_1 + \left(1 - \frac{m_1}{\mu_{12}^+}\right) U_1^{(11)} + U_2^{(11)} \right) \cdot \left(\tilde{E}_2 + U_1^{(22)} + \left(1 - \frac{m_2}{\mu_{12}^+}\right) U_2^{(22)} \right),$$



$$\Xi_5 = \left(\tilde{E}_2 + U_1^{(22)} + \left(1 - \frac{m_2}{\mu_{12}^+} \right) U_2^{(22)} \right), \Xi_6 = \left(\tilde{E}_1 + \left(1 - \frac{m_1}{\mu_{12}^+} \right) U_1^{(11)} + U_2^{(11)} \right)$$

By substituting alternately these roots in (7), we can find two solutions of the system, $(C_1/C_2)_+$ and $(C_1/C_2)_-$, which, according to (7), determine the wave functions $\tilde{\psi}_1(z), \tilde{\psi}_2(z)$ belonging to the energy levels \tilde{E}_+ and \tilde{E}_- .

RESULTS AND CONCLUSIONS

Thus, in tunnel-coupled wells, the energy levels shift relative to the levels of isolated wells, and the wave functions arise from the wave functions of isolated wells as a result of their "mixing" - the formation of linear combinations (7).

It is easy to see that the mixing of functions $\psi_1(z)$ and $\psi_2(z)$ is due to the presence of the following expressions

$$\tilde{E}_2 + U_1^{(22)} + \left(1 - \frac{m_2}{\mu_{12}^+} \right) U_2^{(22)} - \tilde{E} \quad \text{and} \quad \tilde{E}_1 + \left(1 - \frac{m_1}{\mu_{12}^+} \right) U_1^{(11)} + U_2^{(11)} - \tilde{E},$$

since in the absence of these expressions in the system of equations (7) it has only solutions for which one of the coefficients C_1, C_2 is equal to zero. Therefore, system (7) can be simplified, retaining the main features of its solutions, if we neglect the contributions from $U_{1,2}^{(m)}$, where $n = 1, 2$. Then (7) takes the form

$$\begin{cases} \Re_1 C_1 + C_2 (\tilde{E}_2 - \tilde{E}') = 0, \\ C_1 (\tilde{E}_1 - \tilde{E}') + \Re_2 C_2 = 0, \end{cases} \quad (11)$$

where $\Re_1 = \left(1 - \frac{m_1}{\mu_{12}^+} \right) U_1^{(21)} + U_2^{(21)}$, $\Re_2 = U_1^{(12)} + \left(1 - \frac{m_2}{\mu_{12}^+} \right) U_2^{(12)}$. Then, equating the determinant of the system of equations (11) to zero, we obtain instead of (8) a less cumbersome equation

$$\tilde{E}'^2 - (\tilde{E}_1 + \tilde{E}_2) \tilde{E}' + \tilde{E}_1 \tilde{E}_2 + \Re_1 \Re_2 = 0, \quad (12)$$

the roots of which are equal

$$\tilde{E}'_{\pm} = \frac{1}{2} \left[\tilde{E}_1 + \tilde{E}_2 \pm \sqrt{(\tilde{E}_1 - \tilde{E}_2)^2 + 4\Re_1 \Re_2} \right]. \quad (13)$$

Let us now analyze the expression for the gap between energy levels (13), i.e. the value $\Delta E = |\tilde{E}'_+ - \tilde{E}'_-|$. The value $\Delta E_{asym} = |\tilde{E}_1 - \tilde{E}_2|$ is a measure of the asymmetry of two quantum wells, and it is equal to zero for symmetric wells. If its square dominates under the root sign in (4), then $\Delta E \approx \Delta E_{asym}$. In this case, the solutions of system (11) correspond to wave functions $\tilde{\psi}_1(z), \tilde{\psi}_2(z)$ close to the original functions ψ_1, ψ_2 , i.e. there is almost no mixing of the wave functions. In the opposite case, when the asymmetry of the wells is negligibly small, then the gap between the levels (13) in the tunnel-coupled wells is $\Delta E \approx \sqrt{4\Re_1 \Re_2}$, where this value characterizes the tunneling splitting of the energy levels. In this case, the solutions of system (11) correspond to a strong mixing of the initial wave functions, where the coefficients C_1 and C_2 are comparable in absolute value to each other.



LITERATURE

1. A. A. Shchuka. *Nanoelectronics*. -M., Fizmatkniga. 2007. -465 p. [in Russian]
2. R.Ya.Rasulov, I.M.Eshboltaev, Zh.Rozikov, M.A.Mamatova. *theory of current transfer in multilayer semiconductor structures. Materials of the Republican Conference (with the participation of scientists from the CIS countries) "Modern problems of semiconductor physics" MPSP-2019. November 20, 2019 Nukus. pp.149-152.*
3. V.R. Rasulov, R.Ya.Rasulov, M.A. Mamatova, X.X. Raxmatullaev, I. Muminov. *Dimensionally quantization of electrons in a semiconductor with a composite conduction band. 8th Conference "Applied Sciences and technologies in the United States and Europe: common challenges and scientific findings". New York, USA. August 30, 2014. P.93-97.*
4. V.R.Rasulov, R. Ya. Rasulov, M.A.Mamatova, J.Arabboyev // EPRA IJMR. 2022. Vol. 8. no. 6. -Pp. 228-232.
5. G. Bastard, *Wave Mechanics Applied to Semiconductor Heterostructure, Editions de Physique. -Les Ulis, France. 1988. -317 p.*
6. E.L. Ivchenko, G.E. Pikus. *Superlattices and Other Heterostructures: Symmetry and Optical Phenomena, Springer Series in Solid-State Sciences. -Springer-Verlag, Berlin, Heidelberg. 1995; second edition 1997. -657 p.*
7. Rasulov, R. Y., Rasulov, V. R., Eshboltaev, I., & Mamadalieva, N. Z. (2019). *Photon-drag effect in p-type tellurium. Russian Physics Journal, 62(6), 1082-1090.*
8. R.Ya.Rasulov, V.R.Rasulov, U.M.Isomaddinova, F.Kasimov // *Electronic states in a multilayer semiconductor structure in the Wentzel-Kramers-Brillouin approximation. Part 1. The 1st International scientific and practical conference "Progressive research in the modern world" (October 5-7, 2022) BoScience Publisher, Boston, USA. 2022. 210-213 p.*
9. R.Ya.Rasulov, V.R.Rasulov, U.M.Isomaddinova, F.Kasimov // *Electronic states in a multilayer semiconductor structure in the Wentzel-Kramers-Brillouin approximation. Part 1. The 1st International scientific and practical conference "Progressive research in the modern world" (October 5-7, 2022) BoScience Publisher, Boston, USA. 2022. 214-217 p.*
10. E.I. Golant, A.B. Pashkovsky // -FTP. -2002. -T.36. -Number 3. -S.330-337. [in Russian]
11. Pashkovskii, A. B. (2005). *Parity and abrupt broadening of resonance levels in triple-barrier structures. Journal of Experimental and Theoretical Physics Letters, 82(4), 210-214.*
12. Elesin, V. F. (2002). *High-frequency response of double-barrier nanostructures. Journal of Experimental and Theoretical Physics (JETP)(in russian), 121(4), 925-932.*
13. Elesin, V. F. (2003). *Resonant tunneling of electrons interacting with phonons. Journal of Experimental and Theoretical Physics, 96(5), 966-974.*
14. Elesin, V. F. (2003). *Resonant tunneling and a nonlinear response in RF fields. Journal of Experimental and Theoretical Physics, 97(2), 343-357.*
15. V.F. Yelesin, I.Yu. Kateev // -FTP. -2008.-T. 42. -S. 586. [in Russian]
16. V.F. Yelesin // ZhETF. -2014. -T.145. -No. 6. -p.1078-1086. [in Russian]
17. V.I. Galiyev, A.N. Kruglov, A.F. Polupanov, Ye.M. Goldis, T.L. Tansli // -FTP. -2002. T. 36. -S. 576-581.18. Landau, L. D., & Lifshitz, E. M. (2013). *Quantum mechanics: non-relativistic theory (Vol. 3). Elsevier.*