Mathematical model of coherent the electron transfer for nanostructures with an applied magnetic field of constant strength

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Abstract

A mathematical model, which describes the processes of coherent electron transfer through a plane semiconductor nanosystem with a constant magnetic field applied longitudinally to it is proposed. A finite difference scheme has been constructed that provides software implementation of time-dependent solutions to the complete Schrödinger equation. The direct implementation of the mathematical model was carried out using the Wolfram Mathematica system. The mathematical model was verified for the parameters of an experimentally realized nanosystem with typical geometric and physical parameters.

Keywords

Nanostructure, electron transfer, finite difference method, quantum transitions

1. Introduction

The transport properties of the nanostructures that make up these devices play a decisive role in the practical functioning of nanoscale devices. Consequently, theoretical studies are usually carried out in mathematical models of two-three and multilayer open nanosystems without constant external fields, and mainly only taking into account the interaction of electrons with the electromagnetic field [1-3]. Later, the influence of constant electric and magnetic fields on electron tunneling through nanostructures was studied [4-8]. It turned out that a constant electric field directed along the electron flow through the nanostructures plays an important positive role in the operation of quantum cascade lasers, since it coordinates the operation of all cascades [4-6]. As for the constant magnetic field, its role in the operation of nanodevices turned out to be quite complex. As has been established experimentally and theoretically [9, 10], a magnetic field with a strength parallel to the current through the nanostructure does not affect the peak current value for a resonant tunnel diode. This is due to the fact that a longitudinal magnetic field does not affect the movement of charge carriers along the current, but only causes a change in the density of states.

It was also investigated that the inclusion of a longitudinal magnetic field causes the appearance of steps in the current-voltage characteristic, the number of which is related to the number of operating Landau levels. With the advent of optoelectronic nanodevices, experimental studies of the behavior of electrons in quantum superlattices in a constant magnetic field have intensified. Thus, in experimental papers [11, 12], quantum cascade nanodevices were first implemented, the operation of which is based on quantum transitions between Landau energy levels in a magnetic field with a strength parallel to the current through the nanosystem. Theoretical papers [11-13] were mainly concerned with the calculation of the quasi-stationary energy spectrum of an electron in such superlattices, and they also studied the dependence of the electron transparency coefficient of multilayer nanosystems on the magnitude of the applied magnetic field. Thus, we can conclude that the most complete correct

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model of the electronic states of a nanosystem with a constant magnetic field, which would correspond to most practical problems, is missing

Inn proposed paper, we consider the general case that corresponds to the mathematical model of electron tunnel transport with the presence of a constant longitudinal magnetic field and satisfies experimentally realized quantum cascade lasers and detectors.

2. Mathematical model of electronic ballistic transport in a longitudinal magnetic field of constant strength

The mathematical model of a ballistic electron flow through flat nanosystems in a magnetic field with a strength parallel to the direction of the current in the proposed paper will be developed in an approach as described below. We consider a plane semiconductor nanostructure geometric and the energy scheme of which, such as those shown in Fig. 1.

To begin with, we choose the vector potential of the magnetic field in the following form:

$$\vec{A} = \frac{1}{2}[\vec{B} \times \vec{r}]. \tag{1}$$

where the magnetic field is such that it is directed perpendicular to the planes of the nanosystem, i.e. along the direction of electron tunneling (Oz axis) (Fig. 1).

The electron Hamiltonian using a model of various effective masses in the wells and barriers of a multilayer nanosystem looks is obtained as follows:

$$\begin{aligned}\widehat{H} &= \frac{1}{2\mu(z)}\left[\left(\widehat{p}_x - eA_x\right)^2 + \left(\widehat{p}_y + eA_y\right)^2\right] + \frac{1}{2}\widehat{p}_z \frac{1}{\mu(z)}\widehat{p}_z + U(z) = \\ &= \frac{1}{2\mu(z)}\left[\left(\widehat{p}_x - \frac{eB}{2}y\right)^2 + \left(\widehat{p}_y + \frac{eB}{2}x\right)^2\right] + \frac{1}{2}\widehat{p}_z \frac{1}{\mu(z)}\widehat{p}_z + U(z).\end{aligned} \tag{2}$$

where $\widehat{p}_x, \widehat{p}_y$ are the components of the electron momentum in the direction perpendicular to the tunneling direction, $\widehat{p}_z$ is the component along the tunneling direction, $U(z)$ and $\mu(z)$ are the potential energy and effective mass of the electron in the layers of the nanosystem, respectively.

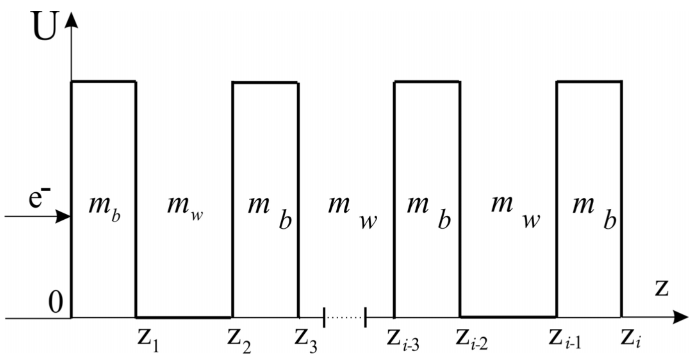

Figure 1: Schematic energy and geometric diagram of the studied multilayer nanosystem

By introducing the creation $\widehat{a}^+$ and annihilation $\widehat{a}$ operators by analogy with a harmonic oscillator, the electron Hamiltonian is presented in the following convenient form:

$$\widehat{H} = \left(\frac{1}{2} + \widehat{n}\right)\hbar\omega + \frac{1}{2}\widehat{p}_z \frac{1}{\mu(z)}\widehat{p}_z + U(z). \tag{3}$$

where ω is the cyclotron frequency; $\widehat{n} = \widehat{a}^+\widehat{a}$ – filling number operator. Next, we take into account the fact that $\Theta_n(x, y)$ these are the known eigenfunctions of the Hamiltonian of a two-dimensional harmonic oscillator:

$$\hat{n}\Theta_n(x,y) = n\Theta_n(x,y), \qquad n = 0, 1, 2, ... \tag{4}$$

then from the form of Hamiltonian (3) it immediately follows that the Landau quantum energy levels are now determined by the formula:

$$E_n = \left(\frac{1}{2} + n\right)\hbar\omega; \quad n = 0, 1, 2, ...\infty \tag{5}$$

Consequently, the energy of longitudinal motion of an electron in a nanosystem is determined as:

$$E_z(z) = E - E_n(z)., \tag{6}$$

The spatial wave function of electron motion is now found from the stationary Schrödinger equation (expressions (5) and (6) was used in the equation (3)):

$$\left[\left(\frac{1}{2} + \hat{n}\right)\hbar\omega_i + \frac{1}{2}\hat{p}_z \frac{1}{\mu(z)}\hat{p}_z + U(z)\right]\Psi(\vec{r}) = E\Psi(\vec{r}). \tag{7}$$

The wave function in equation (7) in order to separate the longitudinal motion of the electron from the transverse one is sought in the following form:

$$\Psi(\vec{r}) = \Theta_n(x,y)\Phi(z) \tag{8}$$

Now the Schrödinger equation (7) takes the following appearance:

$$-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{\mu(z)}\frac{d}{dz}\Phi(z) + U_{eff}(z)\Phi(z) = E_\perp\Phi(z). \tag{9}$$

where

$$E_z = E - \left(\frac{1}{2} + n\right)\hbar\omega. \tag{10}$$

is the energy of the longitudinal motion of the electron, and U_{eff} is the effective potential of the electron, which has the form:

$$U_{eff} = \begin{cases} 0, & (wells) \\ U_b(n,B) = U_0 - \left(1 - \dfrac{m_w}{m_b}\right)\left(\dfrac{1}{2} + n\right)\hbar\omega, & (barriers) \end{cases}. \tag{11}$$

m_w, m_b are the effective electron masses in the wells and barriers of the nanosystem, respectively. As can be seen, the effective potential in which the electron moves along the Oz axis depends on the quantum number n and on the magnetic field induction B.

Boundary conditions for solutions of the Schrödinger equation (9), describing their continuity and the continuity of probability flows at the boundaries of the sth layer of the nanosystem:

$$\left[\Phi^{(s)}(z)\Big|_{z\to z_{s-0}} = \Phi^{(s)}(z)\Big|_{z\to z_{s+0}}; \ \frac{1}{\mu_s}\frac{d\Phi^{(s)}(z)}{dz}\Bigg|_{z\to z_{s-0}} = \frac{1}{\mu_{s+1}}\frac{d\Phi^{(s+1)}(z)}{dz}\Bigg|_{z\to z_{s+0}} \right. . \tag{11}$$

Now solutions to the Schrödinger equation (9) taking into account are sought on a one-dimensional grid:

$$\Omega_m = \{(z) : z_m = m\Delta z_m, \ m = 0,1,2,3...M\}. \tag{13}$$

As a result, we obtain the following finite difference scheme:

$$\begin{cases} \Phi_0 - \Phi_1 = 0; \\ \Phi_{M-1} - \Phi_M = 0; \\ \Phi_{m-1} - \Phi_m\left(1 + \dfrac{\mu_m}{\mu_{m+1}}\right) + \dfrac{\mu_m}{\mu_{m+1}}\Phi_{m+1} = 0; \\ \Phi_{m-1} + \left\{\dfrac{2\mu_m E_\perp h^2}{\hbar^2} + h^2\left[U_0 - \left(1 - \dfrac{m_w}{m_b}\right)\left(\dfrac{1}{2} + n\right)\hbar\omega\right] - 2\right\}\Phi_m - \Phi_{m+1} = 0. \end{cases} \tag{14}$$

Here we used well-known approximations for the first and second derivatives:

$$\frac{d\Phi}{dz} \to \frac{\Phi_{m+1} - \Phi_m}{h}; \ \frac{d^2\Phi}{dz^2} \to \frac{\Phi_{m-1} - 2\Phi_m - \Phi_{m+1}}{h^2}; \ h \approx \Delta z_m.$$

Outside the nanostructure, it is advisable to present solutions to the Schrödinger equation in the following simple analytical form:

$$\Phi(z)\big|_{z\to-\infty} = e^{ikz} + Be^{-ikz}; \qquad \Phi(z)\big|_{z\to+\infty} = Ae^{ikz}; \ k = \sqrt{2m_0 E}/\hbar. \quad (15)$$

The difference scheme, presented in the form (14), can already be directly implemented using applied software. As a result, the eigenvalues of the difference scheme (14) determine the electronic spectrum E_n. This allows us to directly determine the wave function inside the nanostructure, satisfying the normalization condition:

$$\int_{-\infty}^{+\infty} |\Phi(E_n, z)|^2 dz = 1. \quad (16)$$

As a result, this makes it possible to calculate the transparency coefficient of the nanosystem based on the following expression:

$$D(E) = |A(E)|^2. \quad (17)$$

3. Results and discussion

Direct calculations using a developed mathematical model of resonant electron transport were performed for an experimentally studied nanosystem [5], containing ten AlAs potential barriers, each 2 nm thick, and nine GaAs potential wells, each 3 nm thick. The height of the potential barrier was taken to be 520 meV, the effective mass of the electron in the potential barriers and wells was $0.72m_e$ and $0.67m_e$, respectively (me is the mass of a free electron).

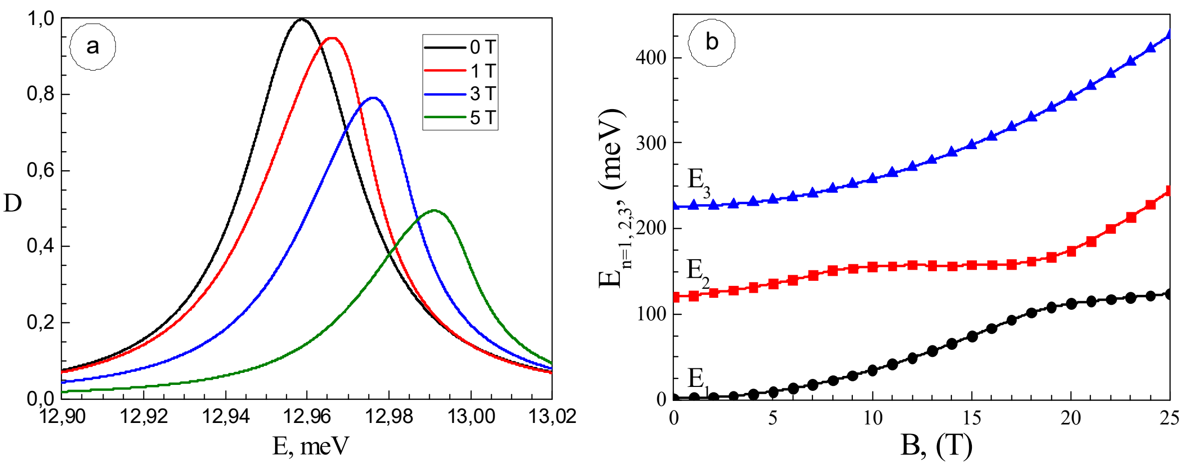

Figure 2: Dependence of the nanosystem transparency coefficient on electronic energy at different values of magnetic field induction (B) (a) and dependence of electron energy levels on the induction value (b).

In Fig. 2a are shown the dependence of the transparency coefficient of the nanosystem on the electronic energy scale. Calculations were performed depending on the magnitude of the applied magnetic field induction B. As can be seen from the figure, the magnetic field leads to a decrease in the maximum value of the transparency coefficient, while the levels of the electron energy spectrum also shift to the high-energy region. This can also be seen more clearly from Fig. 2b, which shows the dependences of the first three electronic levels on the magnetic field induction values. It should also be noted that as the magnetic field induction increases, the electronic levels form a “bottleneck” effect, which usually occurs when the geometric parameters of the nanosystems under study are varied.

The directly established effects will have a significant impact on the electron tunneling process. In particular, a decrease in the maximum value of the transparency coefficient will lead to a significant decrease in the intensity of quantum transitions between electronic levels. In turn, a shift in energy levels leads to a change in the working part of the devices due to the fact that electromagnetic waves will be generated with different frequencies different from the operating frequency.

4. Conclusions

A mathematical model of electron transport in nanosystems is proposed, taking into account the influence of an applied constant longitudinal magnetic field. Calculations based on the developed model using the parameters of an experimentally created nanosystem were used to study the influence of the magnetic field on the transparency coefficient of the nanosystem and the electronic spectrum. It has been established that the magnetic field reduces the transparency coefficient of the nanosystem and shifts the electron energy levels to a high-energy region.

The presented mathematical model can be the immediate basis for further research into problems associated with electron transfer in nanosystems.

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