The use of asymptotic methods for modelling of the carriers wave functions in the Si/SiGe heterostructures with quantum-confined layers

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Abstract. The mathematical model that allows obtaining wave functions of electrons and holes and Coulomb potential in dependence on the parameters of the layer is proposed. In contrast to the common approach widely used in considerable literature, the proposed method allows to find the wave functions for all layers of the structure, both inside and outside the barrier layer. It was shown that increase of tunnel barrier transparency entails a transition from the dipolar electron-hole system (EHS) with a double-peak wave function of electrons to the spatially direct EHS. The proposed model takes into account the effect of the correlation interaction on the wave functions and the density of distribution of the carriers crosswise the layers. These calculations are useful for the analysis of many-particle nonequilibrium states occurring in low-dimensional structures.

1. Introduction

The pioneer works [1, 2] have laid the foundation of the wide investigations in physics of many-particle interaction concerning low-dimensional exciton and electron-hole systems (EHS) of high density. The research was mainly held in the type-I heterostructures GaAs/AlGaAs with quantum wells (QW) both for electrons and holes. In case of high density of nonequilibrium charge carriers there were detected different phases of the condensed matter – the dipolar electron-hole liquid, the Bose-Einstein matter with challenging coherent, superconductive, and superfluid properties. In the present work we investigated the type-II $Si/Si_{1-x}Ge_x/Si$ heterostructures with a strained layer $Si_{1-x}Ge_x$ forming a rather deep potential well for holes and not a high barrier for electrons in the zone diagram. The height of the barrier grows with increasing content of germanium x [3, 4]. In such structures the EHS must have not less interesting properties [5]. In the work the behavior of the wave functions of charge carriers when changing the barrier parameters is modelled. Consider the Bohr radius of the exciton in bulk Si to be about 5 nm; the calculations were held for heterostructures with the thickness of solid solution L varying from 1 to 70 nm. The distribution of the carrier density crosswise the layer is obtained by solving the system of three equations: the two one-particle Schrödinger equations both for holes and electrons and the Poisson equation for the Coulomb energy of their interaction. Commonly in considerable literature the solution of such a system is obtained separately outside and inside the layer and then is joined smoothly at the quantum barrier borders. The correlative interaction of the carriers influential in the case of high density is then neglected. In the present work the

correlative interaction was counted according to the method offered in [6], then the asymptotic analysis was held and the numerical solution was obtained using the "hard" one-staged complex-valued Rosenbrock scheme. We didn't employ any additional technique of smooth joining. The numerical calculations showed that with decreasing height and/or width of the barrier the transition from the spatially indirect (dipolar) EHS to the spatially direct one occurs. Also it was revealed that there are some characteristics of the barrier in the case of high carrier density when the combined formation of both spatially direct and dipolar states is possible.

2. The model

To describe the form of the charge carriers wave functions in quantum-confined layers in the type-II heterostructure ($Si/Si_{1-x}Ge_x/Si$) a one-dimensional boundary value problem for a system of three equations is set: two one-particle Schrödinger equations and the Poisson equation for the Coulomb energy:

$$\begin{cases} \dfrac{\hbar^2}{2m^*}\dfrac{d^2\Psi e}{dz^2} = \left(V_e(z) - \varphi(z) - E_e\right)\Psi e + E_{Ce}\Psi e \\ \dfrac{\hbar^2}{2m^*}\dfrac{d^2\Psi h}{dz^2} = \left(V_h(z) + \varphi(z) - E_h\right)\Psi h + E_{Ch}\Psi h \\ \dfrac{d^2\varphi}{dz^2} = \dfrac{e^2 n_0}{\varepsilon\varepsilon_0}\left(|\Psi e|^2 - |\Psi h|^2\right) \end{cases} \tag{1}$$

Here $\hbar$ is the Planck constant, ε – the dielectric constant, ε_0 – the electric constant, m^* is the effective mass of the carrier; it is intended that the effective mass of the electron, m_e^* and the effective mass of the hole, m_h^* are equal: $m^* = m_e^* = m_h^*$; e is the electron charge; n_0 is the sheet carrier density appearing in the system due to external radiation; Ψe, Ψh are normalized to unity wave functions of electrons and holes respectively: $\int_{-\infty}^{+\infty}(\Psi e)^2\,dz = 1$; . $\int_{-\infty}^{+\infty}(\Psi h)^2\,dz = 1$; φ is the Coulomb potential energy. The potential barrier for electrons $V_e(z)$ and the potential well for holes $V_h(z)$ are defined as following:

$$V_e(z) = \begin{cases} 0, & |z| > \dfrac{L}{2}, \\ V_e, & |z| < \dfrac{L}{2}; \end{cases} \qquad V_h(z) = \begin{cases} 0, & |z| > \dfrac{L}{2}, \\ -V_h, & |z| < \dfrac{L}{2}. \end{cases} \tag{2}$$

Here L is the width of the layer in nm.

In the model the correlative interaction was counted according to the method of density functional theory [6]. For this purpose, the components $E_{Ce}\Psi e$ and $E_{Ch}\Psi h$ were introduced in the Schrödinger equations in the system (1). As it was shown in [8] the correlation energy of the carriers is related to their wave functions $\Psi_{carrier}$ in the following way: $E_C \sim (n_0)^{1/4} \sim (\Psi_{carrier})^{1/2}$. The system (1) is considered on the segment $-A \le z \le A$, where A is a value greater than the strained layer width. On the borders the homogeneous Neumann conditions are adjusted. We rewrite the system in dimensionless form. We choose the exciton energy $E_x = \dfrac{me^4}{(4\pi\varepsilon_0)^2\varepsilon^2\hbar^2}$ as a scale energy and the

value $\frac{a_x}{\mu}$ as a scale length. Here $a_x = \frac{4\pi\varepsilon_0\varepsilon\hbar^2}{me^2}$ is the Bohr radius of the exciton, *m* is defined from a ratio $\frac{1}{m} = \frac{1}{m_e^*} + \frac{1}{m_h^*}$; $\mu \sim 0.01$ is a small parameter introduced in the system artificially to obtain the solutions including the interior transition layers.

In the dimensionless form the boundary value problem becomes the following:

$$\begin{cases} \mu^2 \frac{d^2\Psi e}{dz^2} = \left(V_e(z) - \varphi(z) - E_e\right)\Psi e + N\left|\Psi e\right|^{1/2}\Psi e \\ \mu^2 \frac{d^2\Psi h}{dz^2} = \left(V_h(z) + \varphi(z) - E_h\right)\Psi h + N\left|\Psi h\right|^{1/2}\Psi h \\ \frac{d^2\varphi}{dz^2} = K\left(\left|\Psi e\right|^2 - \left|\Psi h\right|^2\right). \end{cases} \tag{3}$$

Boundary conditions are the following:

$$\left.\frac{d\Psi e}{dz}\right|_{z=-\frac{\mu A}{a_x}} = \left.\frac{d\Psi e}{dz}\right|_{z=\frac{\mu A}{a_x}} = \left.\frac{d\Psi h}{dz}\right|_{z=-\frac{\mu A}{a_x}} = \left.\frac{d\Psi h}{dz}\right|_{z=\frac{\mu A}{a_x}} = 0; \quad \left.\frac{d\varphi}{dz}\right|_{z=-\frac{\mu A}{a_x}} = \left.\frac{d\varphi}{dz}\right|_{z=\frac{\mu A}{a_x}} = 0. \tag{4}$$

Here N – is a constant chosen in the course of numerical experiments that depends on the strained layer characteristics, $K = 4\pi\frac{n_0 \cdot a_x^2}{\mu} \sim 1$.

3. Asymptotic analysis

The research procedure of the systems of equations with a small parameter besides the derivatives is proposed in [7]. If we put $\mu = 0$ in the first two equations of the system (3), we obtain the so-called degenerate system:

$$\begin{cases} \left(V_e(z) - \bar{\varphi}(z) - E_e\right)\bar{\Psi} e + N\left|\bar{\Psi} e\right|^{1/2}\bar{\Psi} e = 0 \\ \left(V_h(z) + \bar{\varphi}(z) - E_h\right)\bar{\Psi} h + N\left|\bar{\Psi} h\right|^{1/2}\bar{\Psi} h = 0 \end{cases} \tag{5}$$

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The numerical solution of the system (3) is attracted to a stable solution of the degenerate system at a sufficient distance from the borders of the layer. The second equation (5) has two roots: $\bar{\Psi} h = (V_h(z) - \bar{\varphi}(z) + E_h)^2 \cdot N^{-2}$ and $\bar{\Psi} h = 0$. Outside the strained layer where $V_h(z) = 0$ the stable root is $\bar{\Psi} h^{(ex)} = 0$ and inside the layer the stable root is $\bar{\Psi} h^{(in)} = (V_h - \bar{\varphi}(z) + E_h)^2 \cdot N^{-2}$, i.e. the holes are concentrated within the layer. Outside the layer the stable root of the first equation (5) is $\bar{\Psi} e^{(ex)} = \left(\bar{\varphi}(z) + E_e\right)^2 \cdot N^{-2}$, that corresponds to the concentration of electrons outside the strained layer. Inside the layer where the inequality $V_e \geq \bar{\varphi}(z) + E_e$ is held the first equation (5) has a unique solution $\bar{\Psi} e^{(in)} = 0$ (the electrons are ejected from the layer). If $V_e < \bar{\varphi}(z) + E_e$ the zero root becomes unstable and there is the second, non-zero, root of the equation $\bar{\Psi} e^{(in)} = \left(-V_e + \bar{\varphi}(z) + E_e\right)^2 \cdot N^{-2}$,

which is stable in this case. This means that at sufficiently low height of the barrier the electrons can concentrate within the layer.

The potential energy in the zeroth approximation (in powers of the small parameter μ) can be determined from the third equation of system (3), with substituted squares of the wave functions $\bar{\Psi}e$ and $\bar{\Psi}h$ derived from a degenerate system. Using the zeroth approximation for the potential, we can determine the energy level for electrons E_e. In the present work we used the method of inverse iterations for this purpose. The holes energy level, E_h is obtained using the common technique for calculation of energy levels for a particle in a potential well.

4. The results of numerical experiments

The results of numerical experiments are shown in figure 1. In the figure the normalized density distribution of electrons (solid line) and holes (dashed line) crosswise the layer is represented. Vertical dashed lines indicate the boundaries of the SiGe layer. The main conclusions are the following.

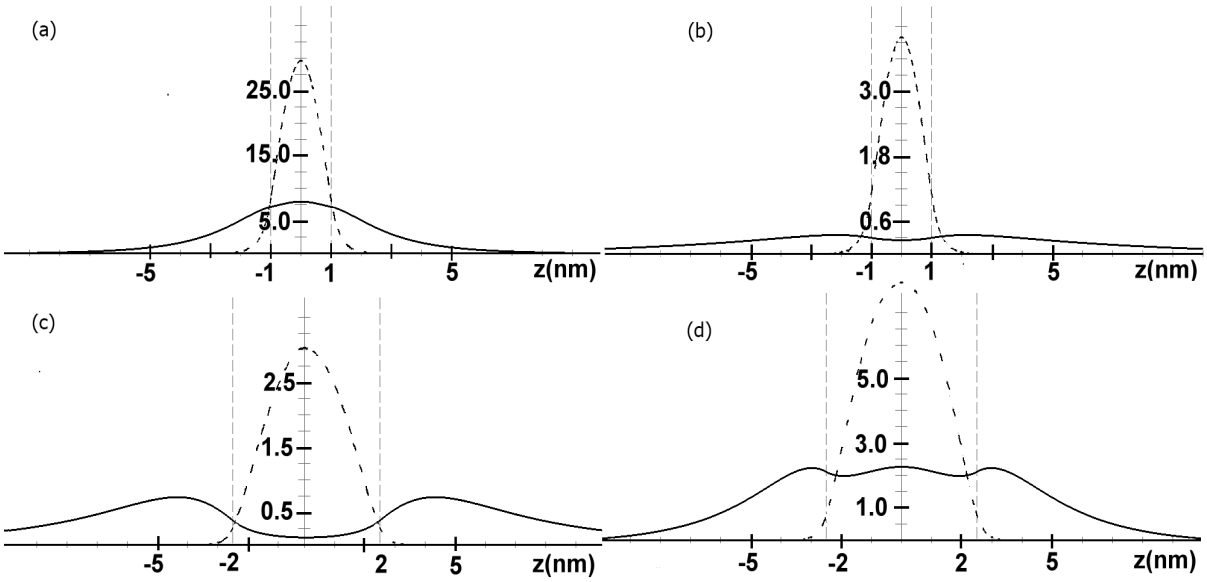

Figure1. Normalized density distribution of electrons (solid line) and holes (dashed line) crosswise the layer SiGe at different values of the layer width L, the barrier height V_e. and the parameter N. Vertical dashed lines indicate the boundaries of the SiGe layer.
(a) $L = 2$ nm, $V_e = 4$ meV, $N = 0.09$; (b) $L = 2$ nm, $V_e = 5$ meV, $N = 0.18$;
(c) $L = 5$ nm, $V_e = 10$ meV, $N = 0.081$; (d) $L = 5$ nm, $V_e = 10$ meV, $N = 0.055$.

At low barrier height ($V_e \leq 5$ meV, figure 1 (a)) and the arbitrary layer width the spatially direct EHS is implemented. Despite the barrier in the conduction band the maximum of the electron density is located in the center of the SiGe layer. (The wave function for holes in all cases is well localized in QW formed by SiGe layer in the valence band, however, the distribution of the electron and hole densities crosswise the layer does not coincide). This behavior of the electron wave function is qualitatively explained in [9] by the fact that for the concentrations of nonequilibrium carriers commonly used in the experiments the band bending caused by the Coulomb interaction of spatially separated electrons and holes creates a potential well for electrons in the SiGe layer (Hartree potential) comparable with the barrier height, in fact transforming these structures into a type-I heterostructure.

Note, that in such structures (at $x \approx 0.05$) for the layer width of 70 and 5 nm, respectively, the electron-hole liquid (EHL) was observed, which was spatially direct [10, 11].
With the increase of the barrier height (V_e = 5 meV, figure 1 (b)) the distribution of electrons crosswise the layer becomes double-peak. The transition to the dipolar EHS occurs. With further increase of the width and/or height of the barrier (V_e = 10 meV, L = 5 nm, figure 1 (c)) and not very high carrier density (low correlation interaction) the EHS becomes dipolar. Exactly in such structures upon the excitation the dipolar excitons and biexcitons must occur, and at high concentrations of nonequilibrium carriers the dipolar EHL must appear.

In the structure with the same parameters (figure 1 (d)) but higher correlative interaction (i.e. with higher density of nonequilibrium carriers) the two-component EHS is implemented. The holes are still well localized in the SiGe layer. The electron wave function has three maxima: two symmetric peaks in the Si layer and a less intense maximum at the center of the layer. In such a system the observation of the two-component excited state is possible.

5. Conclusion

The mathematical model that allows obtaining wave functions of electrons and holes and Coulomb potential in dependence on the parameters of the layer is proposed. In contrast to the common approach widely used in considerable literature, the proposed method allows to find the wave functions (and therefore the distribution of the carriers crosswise the layer) for all layers of the structure, both inside and outside the barrier layer, and does not require any additional artificial technique of smooth joining of the wave functions at the boundaries of the layers. The calculations showed that with decreasing barrier height and/or width the transition from the spatially indirect (dipolar) EHS to the spatially direct one occurs. The proposed model takes into account the effect of the correlation interaction on the wave functions and the density of distribution of the carriers crosswise the layers. This consideration is significant at high density of nonequilibrium carriers (i.e. at high level of excitation). It is shown that under certain parameters of the barrier at high carrier density the formation of both spatially direct and dipolar states is possible.

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