NUMERICAL SIMULATIONS OF COUPLED QUANTUM DOTS

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ABSTRACT

In the work we present self-consistent solutions of Poisson and Schrödinger equations which describe electron states in coupled quantum dots. Results for two neighbouring quantum dots formed in an electrostatic way are discussed. Zero-dimensional electron gas is investigated in the structure proposed by Kastner [1] and presented in our earlier works [2–4]. In the work results of simulations performed in three- and two-dimensional space are shown. We included Hartree potential for modeling Coulomb interactions among electrons in the system. We also considered the exchange and correlation potentials which ensured that each discrete energy level was occupied by only one electron. The exchange and correlation potentials were taken into account with the help of the Local Density Approximation (LDA).

1. Introduction

Low-dimensional devices appear as very perspective for various applications in modern electronics. For example, zero-dimensional electron gas (0DEG), which is formed in quantum dots (QDs), gives many possibilities leading to miniaturization of electronic circuits together with reducing their power consumption. Furthermore, such miniaturized devices seem very promising in the aspect of making the use of electron spin.

In the work we study properties of two coupled quantum dots (CQDs) which are arranged in the structure based on GaAs/AlGaAs heterojunction (Fig. 1). The structure is slightly modified comparing to the original device which was firstly proposed by Kastner [1]. As it is shown in Fig. 1 voltages applied to metallic electrodes allow to create 2DEG (it can be done by the use of $U_{GS} > 0$) and to control

Fig. 1. The structure of two coupled quantum dots.

its density. The upper electrodes E, biased with voltages U_{ES1}, U_{ES2} of the same value ($U_{ES} < 0$), deplete the electron gas locally. It is being done mainly in the regions under the mentioned electrodes. Such a process is possible because of the character of the upper gate E and i-GaAs contact which forms Schottky barrier.

In our previous papers we studied electronic states of a single QD, formed in the same type of the structure [2–4]. We tested two types of numerical method for analyzing the problem in 2D space [2]. Now, our scope is to apply one of these methods and to describe electron states in a system of two QDs. Additionally, we supplemented the method by enclosing the influence of exchange and correlation effects.

2. Method

Potential distribution over the structure is described by Poisson equation in the form:

$$\Delta V(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\varepsilon}, \qquad \mathbf{r} = (x, y, z) \tag{1}$$

where $\rho(\mathbf{r})$ denotes charge density in the regions of 2DEG, neighbouring with source and drain − Fig.1. In order to find $V(\mathbf{r})$ values of the potential for metallic electrodes: G, D, S, E were specified. Undoped layers of AlGaAs and GaAs were treated as dielectrics with different electrical permitivities $\varepsilon = \varepsilon_0 \varepsilon_r$. For GaAs layers ε_r was taken as 12.85 and for AlGaAs region ε_r was equal to 13.18.

Because of the fact that charge density $\rho(\mathbf{r})$ is not known function, Eq. (1) must be solved in a self-consistent way.

We searched for the potential $V(\mathbf{r})$ in the form of single layer potentials:

$$V_k(p_k) = \frac{1}{4\pi\varepsilon_k} \int_{S_k} \frac{\sigma_{S_k}}{|\mathbf{r}|} ds_k \;; \qquad (2)$$

$$\text{where}: \quad k = \begin{cases} 1 - \text{for AlGaAs region,} \\ 2 - \text{for GaAs region.} \end{cases}$$

In the above equation σ_{S_k} describe charge densities corresponding to the single layer potentials at the surfaces S_k, which define the boundaries of k-th region. In the same equation $|\mathbf{r}|$ is the distance between any point p_k of k-th region and any point laying on the boundary surfaces of the region. To solve the Eqs. (1) and (2) boundary element method and Gauss method were used [4]. As a result three-dimensional potential distribution over the whole structure was obtained.

If voltages U_{GS} and U_{ES} have suitable values, two quantum wells arise in the regions between the pairs of electrodes E. Till now, we did not take into account the charge which may accumulate in these wells. The charge can be considered as $\sum_{i=0}^{N} \psi_i$. Wave functions ψ_i are the solutions of N Schrödinger equations which are written for each electron separately:

$$-\frac{\hbar^2}{2m_{GaAs}^{*\Gamma}} \Delta\psi_i(\mathbf{r}) + eV_{eff\,i}(\mathbf{r})\psi_i(\mathbf{r}) = E_i\psi_i(\mathbf{r}) \qquad (3)$$

Effective potential $V_{eff\,i}$ takes the form:

$$V_{eff\,i}(\mathbf{r}) = V(\mathbf{r}) + V_{H\,i}(\mathbf{r}) + V_{ex\,i}(\mathbf{r}) + V_{corr\,i}(\mathbf{r}) \qquad (4)$$

and regards to the influence of biasing voltages – throughout $V(\mathbf{r})$. It also includes Coulomb interaction among electrons in the system due to Hartree potential:

$$V_{H\,i}(\mathbf{r}) = \sum_{j=1;\,j\neq i}^{N} \int_{\Omega} \frac{|\psi_j(\mathbf{r})|^2}{4\pi\varepsilon|\mathbf{r} - \mathbf{r}_j|} d\Omega \qquad (5)$$

Finally it complies exchange and correlation effects according to the Local Density Approximation [5].

The expression for $V_{exi}(\mathbf{r})$ was chosen in the form which depends on the electron spin polarization. For electrons with spin up we used notation:

$$V_{ex\,i\uparrow}(\mathbf{r}) = -\frac{2\sqrt{2}}{\sqrt{\pi}} a_0 \left\{ \sqrt{\rho_{i\uparrow} + \rho_{i\downarrow}} \left[(1+\xi_i)^{3/2} + (1-\xi_i)^{3/2} \right] + \right.$$
$$\left. (\rho_{i\uparrow} + \rho_{i\downarrow})^{3/2} \frac{2\rho_{i\downarrow}}{(\rho_{i\uparrow} + \rho_{i\downarrow})^2} \left[\sqrt{1+\xi_i} - \sqrt{1-\xi_i} \right] \right\} \qquad (6)$$

and for electrons with spin down:

$$V_{ex\,i\downarrow}(\mathbf{r}) = -\frac{2\sqrt{2}}{\sqrt{\pi}} a_0 \left\{ \sqrt{\rho_{i\uparrow} + \rho_{i\downarrow}} \left[(1+\xi_i)^{3/2} + (1-\xi_i)^{3/2} \right] - \right.$$
$$\left. (\rho_{i\uparrow} + \rho_{i\downarrow})^{3/2} \frac{2\rho_{i\uparrow}}{(\rho_{i\uparrow} + \rho_{i\downarrow})^2} \left[\sqrt{1+\xi_i} - \sqrt{1-\xi_i} \right] \right\} \qquad (7)$$

The degree of polarization ξ_i is described as $(\rho_{i\uparrow} - \rho_{i\downarrow})/(\rho_{i\uparrow} + \rho_{i\downarrow})$, where $\rho_{i\uparrow}, \rho_{i\downarrow}$ are local electron densities, referring to electrons with spin up and spin down, with the exception of electron i. Bohr radius $a_0 = 4\pi\varepsilon\hbar^2/(m_{GaAs}^{*\Gamma} e^2) = 10.15$ nm is specific for GaAs due to the electron's effective mass $m_{GaAs}^{*\Gamma}$, which was taken as 0.067 of the free electron mass ($0.067m_0$).

Correlation effects were taken into account according to the potential:

$$V_{corr\,i}(\mathbf{r}) = -C_0 \frac{1 + d_1 w + d_2 w^2 + d_3 w^3 + d_4 w^4}{(1 + C_1 w + C_2 w^2 + C_3 w^3)^2} \qquad (8)$$

with values of coefficients: $d_1 = 2.26$, $d_2 = 2.635$, $d_3 = 2.007$; $d_4 = 0.70597$, and $C_0 = -0.3568$; $C_1 = 1.13$; $C_2 = 0.9052$; $C_3 = 0.4165$ [5].

The variable w is given as: $(a_0\sqrt{\pi\rho_i})^{-1/2}$. Charge density ρ_i is determined for the i-th electron in the system and concerns all remaining electrons in the wells.

Effective potential $V_{eff\,i}$ does not only confine electrons in the dots but simultaneously depends on the density distribution of 0DEG. For this reason self-consistent procedure must be performed. In the procedure both – potential and charge density distributions are adjusted to each other.

To solve Eq. (3) we used numerical methods of finding eigenvalues and eigenvectors for the real and symmetric eigenvalue problem.

Equations (3)–(8) were considered only in the plane of 2DEG. It was possible due to the verified feature of the potential $V(\mathbf{r})$ which confines electrons in z direction (perpendicular to heterointerface) much stronger than in 2DEG plane (x-y). In that case $\mathbf{r} = (x, y)$. Furthermore, the proper "slice" of the potential $V(x, y, z)$ must be chosen, i.e. $V(x, y) = V(x, y, z = z_{max})$. The value of z_{max} can be found on the basis of the Schrödinger equation solution in z direction:

$$-\frac{\hbar^2}{2} \frac{\partial}{\partial z}\left(\frac{1}{m^*} \frac{\partial\psi(z)}{\partial z} \right) + eV(z)\psi(z) = E_z\psi(z) \qquad (9)$$

where m^* is $0.067m_0$ for GaAs and $0.092m_0$ for AlGaAs layer. $V(z)$ is the potential $V(x_0, y_0, z)$ with co-ordinates x_0, y_0 corresponding to the central point of the dot.

As a result of calculations we obtained:
1) potential distribution over the whole structure $V(x,y,z)$ which originates from the biasing voltages;

2) energy spectrum of the system in the form $E_{xy} + E_{z1}$;
3) wave functions $\psi_i(x,y)$ and charge density ρ of all electrons accumulated in quantum wells,
4) degree of system polarization $\xi = (\rho_\uparrow - \rho_\downarrow)/(\rho_\uparrow - + \rho_\downarrow)$;
5) the strength of electron-electron interaction in the form of Hartree, exchange and correlation potentials.

3. Results

We simulated the structure with length $L = 1700$ nm, width $W = 600$ nm and height $H = 740$ nm. Figure 2a presents the top view of the model. Four upper electrodes E are identical. Configuration of the electrodes enables to model each dot in the arrangement independently. In Fig. 2a two axes of symmetry are marked. The symmetry of the structure was used to optimize calculations of the potential. Furthermore, the symmetry allows to expect symmetrical shape of the potential.

In Fig. 2b the side view of the device is presented. We marked the remaining parameters of the structure in it. Parameter z_e denotes the thickness of the electrodes E. Our earlier numerical research proves that the value of z_e influences the shape of the potential significantly. This is the reason for which the value of z_e must be assumed with a great care. For our calculations we took geometrical parameters of the structure (all expressed in nm) as follows: $z_b = 300$, $z_s = 50$, $z_e = 50$, $z_1 = 100$, $z_2 = 70$.
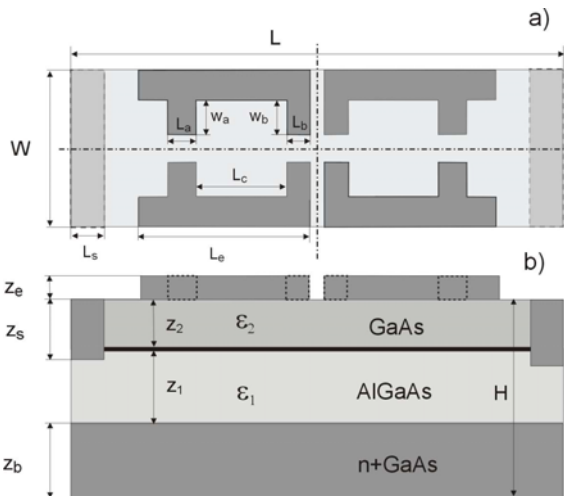

Fig. 2. Top view (a) and side view (b) of the device. In both figures geometrical parameters of the numerical model are marked.

In our calculations voltages U_{GS} and $U_{ES1} = U_{ES2}$ were taken as 390 mV and −245 mV, respectively. They allowed to create two quantum wells with the same geometry and depth. The Table 1 shows remaining parameters of the structure and their values.

Table 1. The values of the simulations parameters

Basic parameters of the structure			
$L = 1700$ nm	$z_b = 300$ nm	$L_a = 100$ nm	$L_s = 100$ nm
$W = 600$ nm	$z_s = 50$ nm	$L_b = 50$ nm	$w_a = 150$ nm
$H = 740$ nm	$z_e = 50$ nm	$L_c = 500$ nm	$w_b = 150$ nm
$z_1 = 100$ nm	$z_2 = 70$ nm	$L_e = 650$ nm	

The calculation of the potential $V(\mathbf{r})$ was performed with the use of 3D discretization mesh. The distance between points of the mesh in z direction was equal to 0.25 nm and in the both remaining directions (x and y) it was 5 nm. For the simulated device the mesh had a colossal number of the points, therefore only Boundary Element Method and single layer potential functions permit to realize simulations in relatively short time. The potential in every point of the mesh was calculated with the accuracy of 10^{-2} meV and boundary conditions were fulfilled with the accuracy of 10^{-4} %.

Analysis of the Eq. (9) shows that the base energy level E_{z1} is located at −4.2 meV that is 17.7 meV over the bottom of the well (Fig. 3). All energies obtained from calculations are referred to zero which is also the potential of source. As it is shown in Fig. 3, the maximum of wave function $\psi_1(z)$ is very close to heterojunction. Location of the maximum at 608.75 nm determined the selection of $V(x,y,z_{max})$ for further analysis in xy plane. Figure 4 presents the potential which was taken into account in our two-dimensional problem. In this figure also the central point of quantum dot $(x_0, y_0) = (-325$ nm, $0)$ is marked. Potential $V(z)$ for the point was shown in Fig. 3.
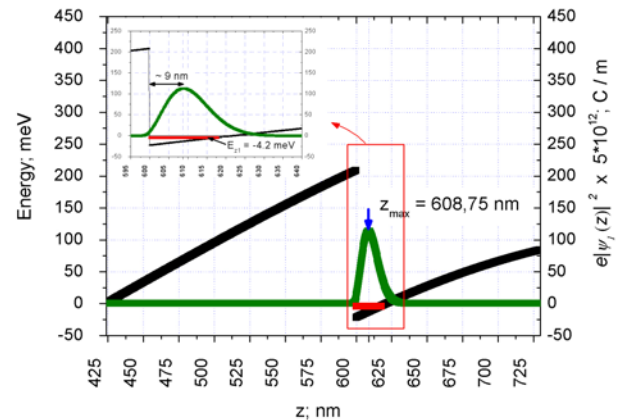

Fig. 3. Quantum well formed at the GaAs/AlGaAs interface (black line and left axis). Energy of the ground state E_{z1} (red line) and corresponding wave function $\psi_1(z)$ (green line and right axis). The inset shows the neighbourhood of the hetero-junction.

Self-consistent solutions of Eq. (3) were found. They are wave functions ψ_i and energy levels $E_{x,y}$ for 4 electrons in CQDs. Solutions respect the assumed convergence criterion. In our case that means that the difference of $V_{eff\,i}$ in two subsequent iterative steps was lower than 0.1% at any point of the discretization mesh.
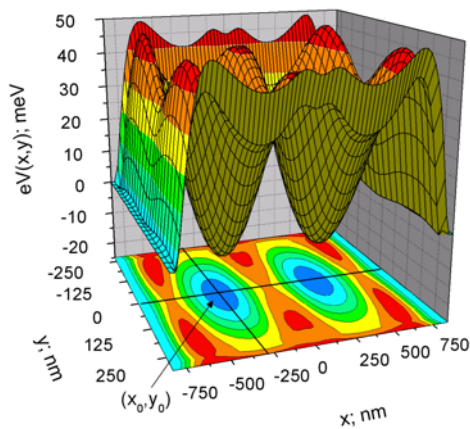
Fig. 4. Potential $V(x,y)$ which forms CQDs.

Figure 5 presents cross-section of charge density distribution, calculated as $e\sum_{i=1}^{N=4}|\psi_i(x,y)|^2$ and corresponding distribution of potential energy $eV_{eff}(x,y)$. In the same figure occupied energy levels E_0 and E_1 are shown. The were determined as $E_{z1} + E_{x,y}$. The levels E_0 and E_1 only slightly differ to each other and they are identical in both wells. Each of the level is occupied by only one electron. This is the consequence of calculations including the exchange potential. It should be noted that the exchange term always gives negative contribution to the total energy of 0DEG.
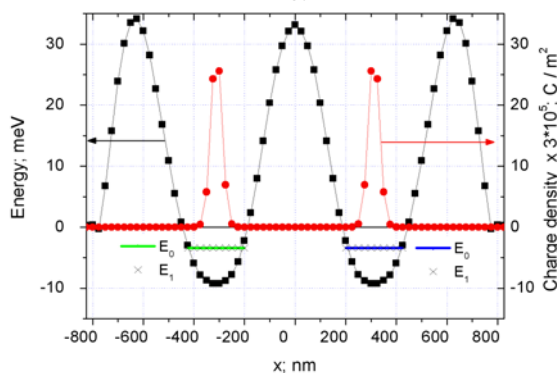

Fig. 5. Cross-sections of charge density (red circles) and potential distribution (black squares) after self-consistent procedure, performed in *xy* plane. There are also energy levels E_0, E_1 marked in each quantum well.

It can be seen that charge density in both dots has slightly larger values at the sides where it "feels" the neighbouring dot. We expected the interaction between charges accumulated in two wells but rather opposite effect to that what we have observed. It can be explained if we consider rather small distance between the outer barriers of the potential and the boundaries of the structure. In calculations (solution of the Eq. (3)) we assumed boundary conditions which state that wave functions decay at the boundaries of the model. It corresponds to the hard walls of the potential. In our case the influence of the boundary conditions is stronger than interaction of two neighbouring dots. Moreover, the upper electrodes E, polarized with the potential U_{ES}, form quite wide potential barrier between the dots. Two wells are separated by the distance of about 360 nm

at energy equal to zero. The bottoms of the wells are separated by 650 nm. Distance between these wells is too large to cause a significant interdot interaction.

Total charge density ρ is the sum of densities found for electrons with spin up ($\rho_\uparrow$) and spin down ($\rho_\downarrow$). In our case $N = 4$ so each of the wells contains two electrons with opposite spins. Figure 6 presents the degree of polarization determined for considered CQDs.
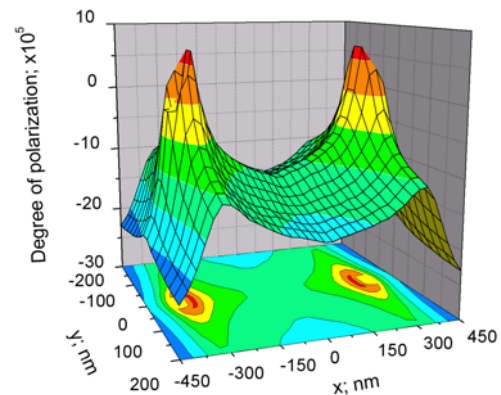

Fig. 6. Polarization of the electron gas confined in two quantum wells.

4. Conclusion

In the paper we presented results of simulations performed for two coupled quantum dots. We found the potential distribution for the structure and electronic states in two quantum wells. We included exchange and correlation interaction between electrons in the system. In our case the interdot interaction is not observed. The dots are too far from each other and the influence of boundary conditions (hard walls of the potential) is too strong.

It appears interesting to test how the distance between the dots affects the charge density distribution and spin polarization of the system. This will be the next step of our simulations.

CQDs provide the opportunity to tune the interdot tunneling. In the structure which we considered it can be done by modification of U_{ES2} in relation to U_{ES1}. We want to expand our research in that direction and to find $I(V)$ characteristics of the system.

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