ELECTRON STATES IN THE ELECTROSTATICALLY FORMED QUANTUM DOTS* **

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In the article a simplified version of the Hartree method is proposed for calculation of electron states in a quantum dot. The results obtained by the use of the standard and the simplified Hartree methods are compared. Total energy of electrons confined in the quantum well allows to estimate capacitance of the dot.

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1. Introduction

One of the possible realizations of quantum dots are those formed electrostatically in an inverse heterostructure GaAs/$Al_xGa_{1-x}As$ [1]. Electron gas concentrates in the nearest neighbourhood of the heterostructure interplane. Because of strong electron localization in the direction z perpendicular to the plane of heterojunction, electron gas in the quantum dot is treated as a two-dimensional system. Voltage applied to the structure confines the gas in the remaining two directions and create the quantum dot.

2. Theoretical model

The confinement of electrons in directions x, y, parallel to the plane of electron gas, is modelled by parabolic potential $V(\boldsymbol{r}) = K_x x^2 + K_y y^2$ ($\boldsymbol{r} \equiv (x, y)$) inside the rectangular area S.

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2.1. Standard Hartree method

The idea of the Hartree method relies on iterative solving of the set of N effective mass equations for N electrons in a quantum dot. Each equation takes into account the effective potential energy which is unique for the electron being considered. Namely, for the i-th electron the effective mass equation in m-th step of the iterative procedure has the form:

$$\frac{-\hbar^2}{2m^*}\Delta\psi_i^{(m)}(\boldsymbol{r}_i)+\left(eV(\boldsymbol{r}_i)+eV_{\mathrm{H}_i}^{(m-1)}(\boldsymbol{r}_i)\right)\psi_i^{(m)}(\boldsymbol{r}_i)=E_i^{(m)}\psi_i^{(m)}(\boldsymbol{r}_i)\,, \quad (1)$$

where m^* is the effective mass of electron in Γ-valley of GaAs. The sum $\left(eV(\boldsymbol{r}_i)+eV_{\mathrm{H}_i}^{(m-1)}(\boldsymbol{r}_i)\right)$ describes the effective potential energy in which Hartree potential is calculated as:

$$V_{\mathrm{H}_i}^{(m-1)}=\int\limits_S\frac{\varrho_i^{(m-1)}(\boldsymbol{r}')}{4\pi\varepsilon\left|\boldsymbol{r}_i-\boldsymbol{r}'\right|}dS\,. \quad (2)$$

The quantity $\varrho_i^{(m-1)}$ is the charge density of all remaining electrons in a dot *i.e.* with the exception of the electron indexed i. $\varrho_i^{(m-1)}$ can be given in terms of electron wave functions in m and $m-1$ iterations.

$$\varrho_i^{(m-1)}(\boldsymbol{r})=e\sum_{j>i}^{1,N}\left|\psi_j^{(m-1)}(\boldsymbol{r})\right|^2+e\sum_{j<i}^{1,N}\left|\psi_j^{(m)}(\boldsymbol{r})\right|^2. \quad (3)$$

2.2. Simplified Hartree method

The idea of the simplification of the standard method relies on the assumption that all electrons in a dot feel identical potential. The latter is assumed as produced by all electrons accumulated in the well. As a result, in this case it is enough to solve iteratively **only one** effective mass equation

$$\frac{-\hbar^2}{2m^*}\Delta\psi^{(m)}(\boldsymbol{r})+\left(eV(\boldsymbol{r})+eV_{\mathrm{H}}^{(m-1)}(\boldsymbol{r})\right)\psi^{(m)}(\boldsymbol{r})=E^{(m)}\psi^{(m)}(\boldsymbol{r}) \quad (4)$$

which is valid for all N electrons in a dot. Hartree potential $V_{\mathrm{H}}^{(m-1)}$ is than given by the expression

$$V_{\mathrm{H}}^{(m-1)}=\int\limits_S\frac{\varrho^{(m-1)}(\boldsymbol{r}')}{4\pi\varepsilon\left|\boldsymbol{r}-\boldsymbol{r}'\right|}dS\,, \quad (5)$$

where the charge density $\varrho^{(m-1)}$ is the sum of charge densities of all electrons in a dot.

$$\varrho^{(m-1)}(\boldsymbol{r}) = e\sum_k 2^p \left|\psi_k^{(m-1)}(\boldsymbol{r})\right|^2. \tag{6}$$

Index k numbers the occupied energy levels in the quantum dot and p equals 1 or 0 depending on that whether the level is occupied by two electrons or by only one.

3. Results

The application of numerical methods for an eigenvalue problem allows to make use of both selfconsistent procedures described in the previous section. Results of calculations performed for a fixed number of electrons in the dot are shown in Fig. 1. The comparison shown in Fig. 1(b) justifies the conclusion that the simplified Hartree method gives results that are comparable with the results obtained with the help of the standard procedure.

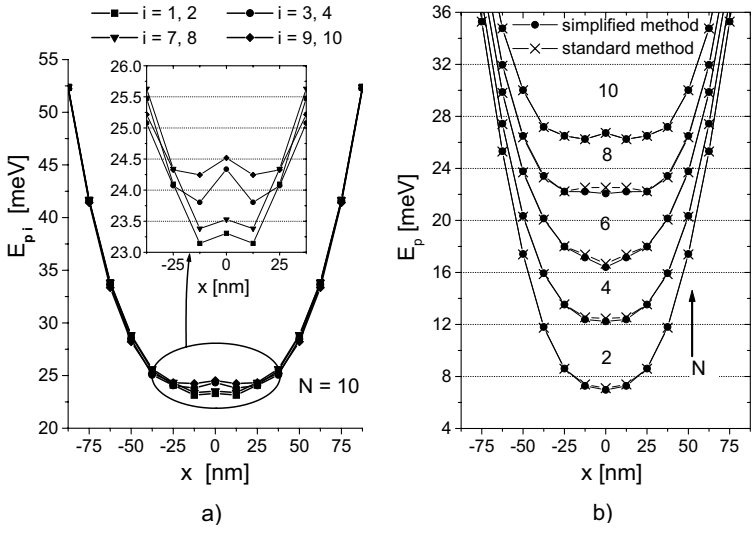

Fig. 1. (a) The effective potential energy E_{pi} being felt by i-th electron in the dot. It was obtained by the use of the standard Hartree method for $N = 10$. For two electrons occupying the same energy level the shapes of E_{pi} are identical. The crossections for $y = 0$ are shown. (b) Quantum wells obtained by the use of the simplified Hartree method (circles). The wells are compared to the wells given by $e(V(\boldsymbol{r}) + V_{\mathrm{H}}^{'}(\boldsymbol{r}))$ (crosses). Hartree potential $V_{\mathrm{H}}'(\boldsymbol{r})$ is calculated for the density $\varrho'(\boldsymbol{r}) = e\sum_i^{1,N} |\psi_i(\boldsymbol{r})|^2$ where $\psi_i(\boldsymbol{r})$ is the solution for the i-th electron in the dot found with the help of the standard Hartree method.

Also the energy spectra of the system obtained by the use of both selfconsistent methods only slightly differ one from each other. In Fig. 2(b) there are presented the values of the relative error $\delta = (E_{\mathrm{S}} - E_{\mathrm{ST}}) \,/\, E_{\mathrm{ST}}$ 100%. The symbols E_{S} and E_{ST} denote energy levels obtained by the use of the simplified and the standard Hartree methods, respectively. The maximum error of $\sim 4\%$ is observed for the lowest energy level.

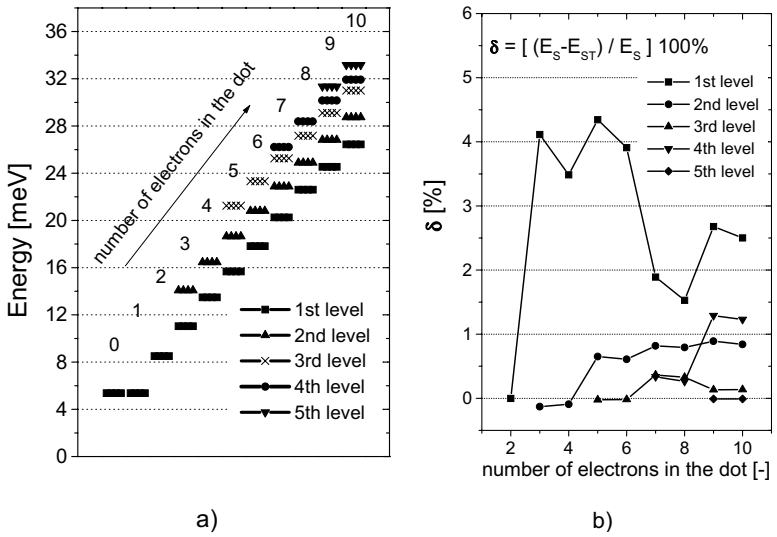

Fig. 2. (a) The lowest energy levels obtained by the use of the standard Hartree method. (b) Relative error for the energy levels obtained with the help of the simplified Hartree method.

The energy spectrum of a quantum dot allows to calculate the total energy E_{tot} of the electron system. For the standard Hartree method E_{tot} is just given by the sum $\sum_i^{1,N} E_i$. For the simplified Hartree method the total energy of the electron system is given by $E_{\mathrm{tot}} = \sum_k 2^p E_k$ where k and p has the same meaning as in Eq. (6).

The dependence $E_{\mathrm{tot}}\,(N)$ is nearly parabolic (see Fig. 3) so, the approximation with the polynom of the second order is used. From the relation $\frac{Q^2}{2C} = \left(\frac{e^2}{2C}\right) N^2$ we conclude that the coefficient 2,29 meV which stands with N^2 can be used to estimate the capacitance of the quantum dot $C = 3,49 \times 10^{-17} F$. The value is in good agreement with capacitances reported for quantum dots of comparable size [2].

Charge density distributions calculated by two versions of the Hartree method are shown in Fig. 4. Only slight differences are observed.

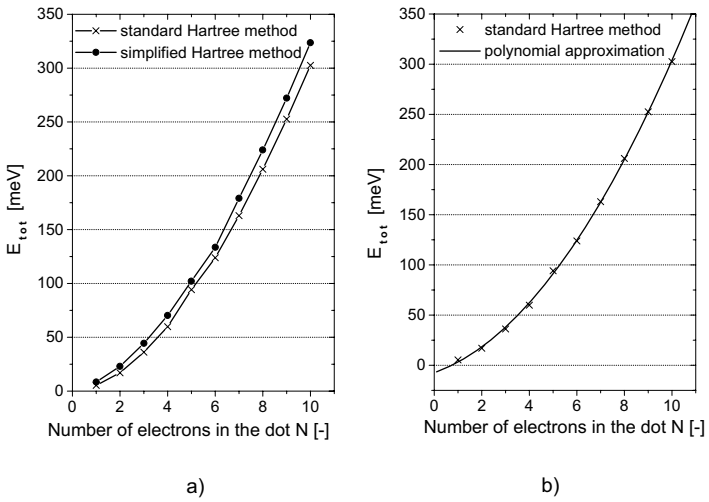

Fig. 3. (a) Total energy of electrons confined in the dot. Results obtained by the use of both Hartree methods are shown. (b) The approximation of the dependence $E_{\mathrm{tot}}(N)$ (crosses) with the polynom of the second order $E_{\mathrm{tot}} = 2,28598N^2 + 8,26386N - 7,38567$ (line) is presented.

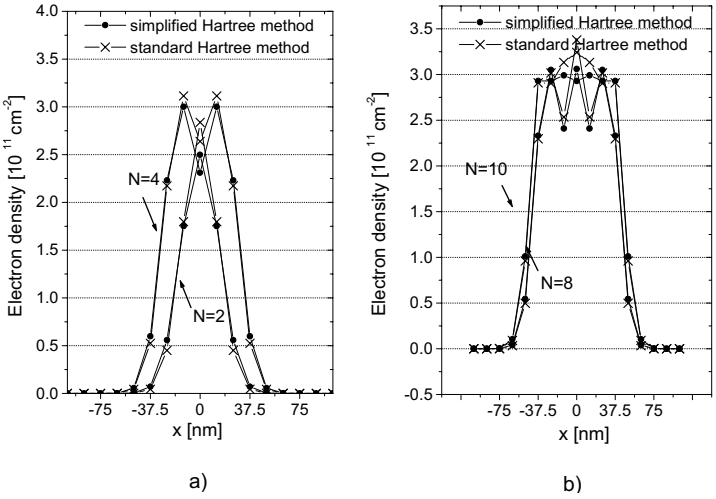

Fig. 4. Comparison of the electron densities calculated by the use of the standard and the simplified Hartree methods. The crossections for $y = 0$ are shown.

4. Conclusions

The selfconsistent Hartree method allows to take into account the influence of the electron charge on the quantum dot properties. The charge of confined electrons modifies in an essential way the energy spectrum of

a system. It also changes the shape of the potential well and the electron density in the well. Selfconsistent solution of the effective mass equation can be achieved in two ways: 1) each electron is treated individually 2) all of the electrons are treated as a whole.

The differences resulting from the application of the two different self-consistent procedures are inconsiderable. That means that the simplified Hartree method is good enough for calculation of electron states even for dots with a small number of electrons. Its main advantage relies on much simpler procedure which results in considerably shorter computational time.The effectivity of the modificated Hartree method compared to the effectivity of the standard method rises with increasing number of electrons in a dot. This is shown schematically in Fig. 5.

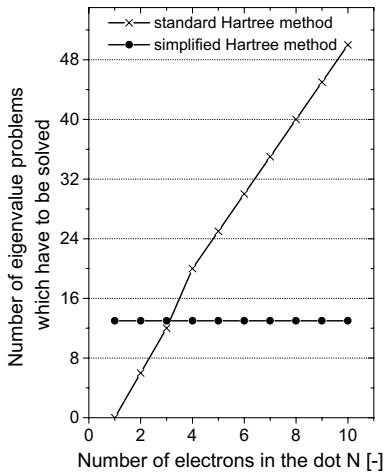

Fig. 5. The number of eigenvalue problems to be solved to achieve selfconsistency. There are compared the results for both versions of Hartree method for the same accuracy of selfconsistency.

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REFERENCES

[1] M.A. Kastner, *Rev. Mod. Phys.* **64**, 849 (1992).

[2] A. Kumar, S.E. Laux, F. Stern, *Phys. Rev.* **B42,** 5166 (1990).