

Electron-Electron Interaction in Plane Closed Semiconductor Nanostructures

I.V. Boyko^{1,*}, O.A. Bagrii-Zayats^{2,†}, H.B. Tsupryk¹, Y.M. Stoianov¹

¹ Ternopil National Technical University, 56, Ruska Str., 46001 Ternopil, Ukraine

² Ternopil State Medical University, 1, Voli Str., 46000 Ternopil, Ukraine

(Received 15 July 2018; revised manuscript received 07 December 2018; published online 18 December 2018)

In the model of rectangular potential wells and barriers and the model of effective masses for an electron, using the exact solutions of the nonlinear cubic Schrödinger equation, a quantum-mechanical theory of the stationary electronic spectrum and oscillator forces of quantum transitions taking into account electron-electron interaction in the Hartree-Fock approximation was developed.

The inclusion electron-electron interaction reduces the intensity of quantum transitions between the first electron states and reduces the value of detected energy, it is shown by an example of a two-well plane semiconductor nanostructure, that can function as an active zone of a quantum cascade detector.

Keywords: Quantum cascade laser, Quantum cascade detector, Electron-electron interaction, Cubic Schrödinger equation.

DOI: [10.21272/jnep.10\(6\).06001](https://doi.org/10.21272/jnep.10(6).06001)

PACS numbers: 73.21.Fg, 73.21.Cd, 74.55.+v

1. INTRODUCTION

In modern physics of semiconductor nanosystems, both experimentalists and theorists pay considerable attention to the study of physical processes occurring in quantum cascade detectors (QCD) [1, 2] and lasers (QCL) [3, 4]. Modern semiconductor compounds QCL and QCD have a number of functional advantages and features, including the ability to work in the infrared range of electromagnetic waves and within the wavelengths that fall into the so-called "window of transparency" of the atmosphere. So the study of the influence of dissipative processes, such as electron-phonon interaction, interaction with high-frequency electromagnetic field, interaction with constant magnetic and electric fields [5] is decisive in order to ensure the work efficiency of mentioned nanodevices.

Problems of the studying the processes of electron-electron interaction were considered mainly for open nanosystems [6-8], which allows us to apply the theory developed in these papers mainly to the QCL in which the active band and the injector function as interconnected within a single cascade, which was shown in papers [5, 8]. Concerning the QCD, the active zone of these nanodevices is separated from the rest of the cascade (extractor) by a thick potential barrier, which is due to the functional features of QCD [1, 2]. Taking this into account, electron-electron interaction processes will conveniently to investigate by considering a QCD separate active band in a closed nanostructure model.

In the present paper, using the Hartree-Fock approximation, we obtain a model Hamiltonian that takes into account the electronic interaction and obtains exact solutions of the stationary nonlinear Schrödinger equation. Using these solutions, the theory of stationary electronic states in two-element nanostructures is developed, taking into consideration of electron-electron interaction.

2. NONLINEAR SCHRÖDINGER EQUATION. ENERGY SPECTRUM OF AN ELECTRON

The plane closed two-well RTS (Fig. 1), which consists of two layers-potential wells of the semiconductor material $\text{In}_x\text{Ga}_{1-x}\text{As}$ and one layer – a potential barrier of semiconductor material $\text{In}_x\text{Ga}_{1-x}\text{As}$ located in the external environment is examined.

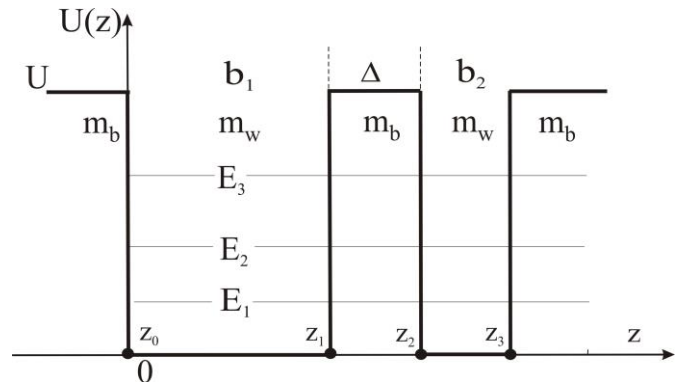


Fig. 1 – Geometric and energy schemes of two-well RTS

We introduce the Cartesian system of coordinates with the origin on the boundary between the external environment and the surface of the input potential well in such a way that its axis OZ will be directed perpendicular to the RTS layers.

Applying an electron to a model of rectangular potential wells and barriers with different effective electron masses in them (m_w, m_b), the effective electron mass in the RTS can be given as:

$$m(z) = m_w \sum_{p=0}^1 (\theta(z - z_{2p}) - \theta(z - z_{2p+1})) + m_b (\theta(-z) + \theta(z - z_1) - \theta(z - z_{21}) + \theta(z - z_3)), \quad (1)$$

The potential energy of an electron in the RTS is

* boyko.i.v.theory@gmail.com

† bagrijzayats@tdmu.edu.ua

given by the equation:

$$U(z) = U \left(\theta(-z) + \sum_{p=1}^3 \theta(z - z_p) \right), \quad (2)$$

where the coordinates of the boundaries of the RTS environment are indicated (Fig. 1)

$$z_0 = 0; z_1 = b_1; z_2 = b_1 + \Delta; z_3 = b_1 + \Delta + b_2, \quad (3)$$

$$\theta(z) = \begin{cases} 0, & z < 0, \\ 1, & z \geq 0 \end{cases} \text{ - Heaviside step function.}$$

The stationary wave functions and the energy spectrum of an electron in a closed RTS model are obtained by solving the stationary Schrödinger equation:

$$H(z)\Psi(z) = E \Psi(z), \quad (4)$$

where

$$H(z) = -\frac{\hbar^2}{2} \frac{\partial}{\partial z} \frac{1}{m(z)} \frac{\partial}{\partial z} + U(z) + U_{e-e}(z), \quad (5)$$

Hamiltonian of the electron of a quasistationary problem.

The energy of the electron-electron interaction $U_{e-e}(z)$ is based on the Hartree-Fock self-consistent potential, as in the case of open nanosystems [6, 8]. In this case $U_{e-e}(z)$ you can write in the form:

$$U_{e-e}(z) = \int V_{e-e}(z - z') |\Psi(z')|^2 dz', \quad (6)$$

where $V_{e-e}(z - z')$ - the potential of electron-electron interaction.

Considering the electron-electronic interaction under these conditions is local

$$V_{e-e}(z - z') = \nu \delta(z - z'), \quad (7)$$

from equations (6) and (7) the known [6-8] expression is obtained

$$U_{e-e}(z) = \int \nu \delta(z - z') |\Psi(z')|^2 dz' = \nu |\Psi(z)|^2. \quad (8)$$

The Schrödinger equation (4), taking into account (5) and (8), takes the form known as the cubic Schrödinger equation [9, 10]:

$$\left[-\frac{\hbar^2}{2} \frac{\partial}{\partial z} \frac{1}{m(z)} \frac{\partial}{\partial z} + U(z) + \nu |\Psi(z)|^2 \right] \Psi(z) = E \Psi(z), \quad (9)$$

where ν - is the potential of the electron-electron interaction, which is considered as a task parameter.

Given the explicit form $U(z)$ and the presence of inter-electron interaction only within the RTS, we obtain the system of Schrödinger equations to find the wave function $\Psi(z)$ of the stationary problem:

$$\begin{cases} \left(-\frac{\hbar^2}{2m_0} \frac{d^2}{dz^2} + U - E \right) \Psi(z) = 0, \\ -\infty \leq z < 0, \quad z_3 < z \leq +\infty, \\ \left(-\frac{\hbar^2}{2m_0} \frac{d^2}{dz^2} - E + \nu |\Psi(z)|^2 \right) \Psi(z) = 0, \\ z_0 \leq z \leq z_1, \quad z_2 \leq z \leq z_3, \\ \left(-\frac{\hbar^2}{2m_1} \frac{d^2}{dz^2} + U - E + \nu |\Psi(z)|^2 \right) \Psi(z) = 0, \quad z_1 \leq z \leq z_2. \end{cases} \quad (10)$$

The solutions of equations (10) must satisfy the conditions of the continuity of the wave function and the density of its flow at all limits of the system ($\eta \rightarrow +0$):

$$\left. \begin{aligned} & \Psi(z) \Big|_{z=z_p-\eta} = \Psi(z) \Big|_{z=z_p+\eta} \\ & \frac{1}{m(z)} \frac{d\Psi(z)}{dz} \Big|_{z=z_p-\eta} = \frac{1}{m(z)} \frac{d\Psi(z)}{dz} \Big|_{z=z_p+\eta} \end{aligned} \right\} \quad (11)$$

($p = 0, 1, 2, 3$)

Equations of the system (10) can be brought to the form:

$$\begin{cases} \frac{d^2\Psi(z)}{dz^2} - \chi_0^2\Psi(z) = 0, & -\infty \leq z < 0, \quad z_3 < z \leq +\infty, \\ \frac{d^2\Psi(z)}{dz^2} + k_0^2\Psi(z) - \frac{\alpha}{E} k_0^2\Psi^3(z) = 0, & z_0 \leq z \leq z_1, \quad z_2 \leq z \leq z_3, \\ \frac{d^2\Psi(z)}{dz^2} - \chi_1^2\Psi(z) - \frac{\alpha}{E} k_1^2\Psi^3(z) = 0, & z_1 \leq z \leq z_2. \end{cases} \quad (12)$$

where

$$\begin{aligned} k_0^2 &= \frac{2m_0 E}{\hbar^2}; \quad k_1^2 = \frac{2m_1 E}{\hbar^2}; \\ \chi_0^2 &= \frac{2m_0 U}{\hbar^2} - k_0^2; \quad \chi_1^2 = \frac{2m_1 U}{\hbar^2} - k_1^2, \end{aligned} \quad (13)$$

and taken into account, that $\Psi(E, z) = \Psi^*(E, z)$; $|\Psi(E, z)|^2 \Psi(E, z) = \Psi^3(E, z)$ for stationary electronic states.

Considering the necessity of fulfilling the condition of the finiteness of the wave function in the domains $(-\infty \leq z < 0) \cup (z_3 < z \leq +\infty)$ the solutions of equations (13) can be represented as:

$$\Psi(z) = \begin{cases} \Psi_0(z) = A_0 e^{\chi_0 z}, & -\infty \leq z < 0 \\ \Psi_1(z) = A_4 e^{-\chi_0 z}, & z_3 < z \leq +\infty. \end{cases} \quad (14)$$

Within the RTS, the Schrödinger equation can be reduced to the following form:

$$\left\{ \begin{array}{l} \frac{d^2\Psi(\zeta_1)}{d\zeta_1^2} + \Psi(\zeta_1) - \frac{\alpha}{E} \Psi^3(\zeta_1) = 0, \\ \zeta_1 = k_0 z, \quad z_0 \leq z \leq z_1, \quad z_2 \leq z \leq z_3, \\ \frac{d^2\Psi(\zeta_2)}{d\zeta_2^2} - \Psi(\zeta_2) - \frac{\alpha}{U-E} \Psi^3(\zeta_2) = 0, \\ \zeta_2 = \chi_1 z, \quad z_1 \leq z \leq z_2. \end{array} \right. \quad (15)$$

$$\left\{ \begin{array}{l} \Psi(z) = \sqrt{\frac{\sqrt{E(E-2\nu A_1)} - E}{\nu}} \operatorname{sn} \left((k_0 z - A_2) \sqrt{\frac{\nu}{E - \sqrt{E(E-2\nu A_1)}}}, \frac{E - \nu A_1 - \sqrt{E(E-2\nu A_1)}}{\nu A_1} \right), \quad z_0 \leq z \leq z_1, \quad z_2 \leq z \leq z_3, \\ \Psi(z) = \sqrt{\frac{(U-E) \left(\sqrt{1 + \frac{2\nu A_3}{U-E}} - 1 \right)}{\nu}} \operatorname{sn} \left(\frac{(\chi_1 z - A_4)}{\sqrt{2}} \sqrt{\frac{1 + \frac{2\nu A_3}{U-E}}{1 + \frac{2\nu A_3}{U-E}}}, \frac{1 - \sqrt{1 + \frac{2\nu A_3}{U-E}}}{1 + \sqrt{1 + \frac{2\nu A_3}{U-E}}} \right), \quad z_1 \leq z \leq z_2. \end{array} \right. \quad (16)$$

From the boundary conditions (11) we obtain a dispersion equation, from which the stationary spectrum of an electron E_n is determined. Since the RTS is closed, the condition of valuation must be fulfilled:

$$\int_{-\infty}^{\infty} |\Psi(E, z)|^2 dz = 1, \quad (17)$$

together with the boundary conditions (11), which allows us to determine all the coefficients A_0, A_1, A_2, A_3, A_4 , and hence the complete wave function of the electron:

$$\begin{aligned} \Psi(E_n, z) = & \Psi_0(E_n, z)\theta(-z) + \\ & + \sum_{p=1}^3 \Psi_p(E_n, z) [\theta(z - z_{p-1}) - \theta(z - z_p)] +, \quad (18) \\ & + \Psi_4(E_n, z)\theta(z - z_3), \quad z_0 = 0 \end{aligned}$$

where the wave functions in the corresponding areas of the RTS are determined by the relations (15) and (16).

3. DISCUSSION OF THE RESULTS

Using the developed theory, the calculation of the stationary electronic spectrum and the oscillators forces of the quantum transition in a two-well closed RTS with $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ – potential wells and $\text{In}_{0.52}\text{Al}_{0.48}\text{As}$ – potential barriers with taking into consideration the influence between the electron interaction was performed. The geometric parameters of the RTS: the widths of the potential wells: $b_1 = b_2 = 5.3$ nm, the thickness of the potential barrier: $\Delta = 3$ nm. Physical parameters of the RTS: the effective mass of the electron in potential wells $m_0 = 0.046m_e$ and barriers $m_1 = 0.089m_e$, respectively, the height of the potential barrier $U = 516$ meV, m_e is the mass of the free electron.

Calculations of the stationary spectrum E_n and oscillator forces $f_{nm'}$ of quantum transitions were performed depending on the position $d = b_1 + b_2$ of the internal potential barrier in the total potential well. The values of the parameter ν were selected in relation to

The exact solutions of the equations (15) are known, they can be represented by Jacobi elliptic functions $\operatorname{sn}(x, k)$ [11]:

the energy value $E_1 = E_1(d/2)$ equal to: $0.01E_1, 0.1E_1, E_1$. The results of those calculations and calculations performed without taking into account the electronic interaction are presented at the Fig. 2 a, b.

Fig. 2 shows, that for all values of the parameter ν the dependence $E_n = E_n(d)$ for the first two stationary electronic states are qualitatively identical: each of the dependences forms respectively one and two maxima for the first and second states respectively. In this case,

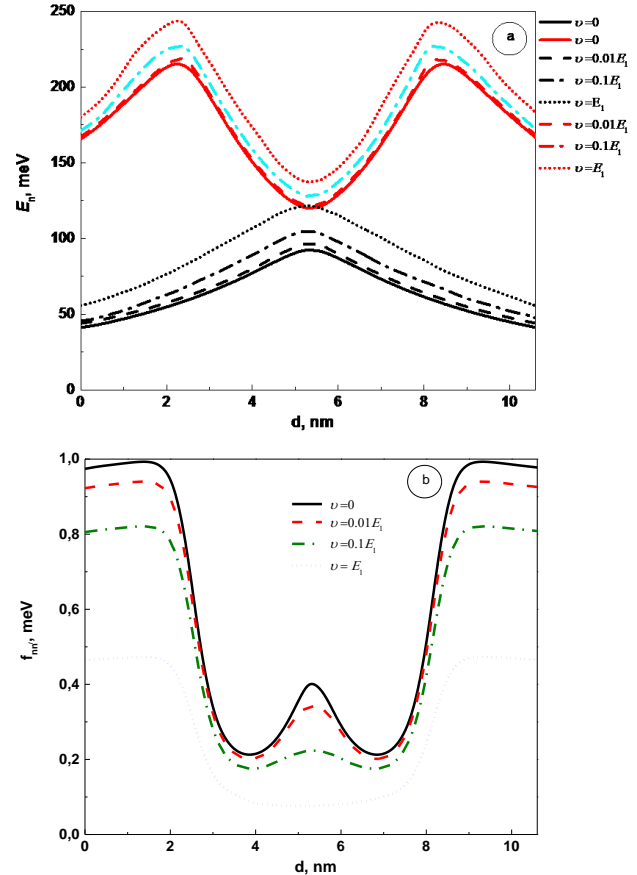


Fig. 2 – The dependences of the stationary electron spectrum and the forces of oscillators of quantum transitions from the potential barrier position $d = b_1 + b_2$

the calculated values of the energies of the corresponding states for the same value of magnitude d are different, they increase with increasing value ν . As can be seen from Fig. 2a, for small values ν , the calculated dependencies are close to those calculated without including electron-electron interaction. With increasing ν , the magnitudes of the energies of the first stationary state increase more than the energy of the second stationary state, so the values of the energies of quantum transitions between stationary states decrease.

To study the influence of electron-electron interaction on the intensity of quantum transitions between the first and the second stationary states of nanosystems, dependences of the oscillator strengths of quantum transitions $f_{12} = f_{12}(d)$ were calculated. Fig. 2b shows that for small values ν the oscillator's force actually repeats the dependence calculated without taking into account the electron-electron interaction. Further increase ν leads to a significant decreasing of the

oscillator force value, and the intensity of the quantum transitions. Consequently, we can conclude that electron-electron interaction can act as a significant dissipative factor, which in particular, in QCD can cause deviations in the operation of the nanodevice not allowing the detection of the required frequencies of electromagnetic waves and deducing the QCD of the coherent state.

4. CONCLUSIONS

In presented paper, with the use of found solutions of the stationary nonlinear Schrödinger equation, the quantum-mechanical theory of stationary electronic states and the forces of oscillators of quantum transitions in a two-well closed plane nanosystem with the influence of electronic interaction has been developed.

The electron-electron interaction causes a decrease in the energy of the quantum transition and the intensity of these transitions, it is shown in this paper.

Електрон-електронна взаємодія у плоских закритих напівпровідникових наноструктурах

I.V. Бойко¹, О.А. Багрій-Заяць², Г.Б. Цуприк¹, Ю.М. Стоянов¹

¹ Тернопільський національний технічний університет імені Івана Пулюя,
вул. Руська, 56, 46001 Тернопіль, Україна

² ДВНЗ «Тернопільський державний медичний університет імені Івана Горбачовського МОЗ України»,
м-н Волі, 1, 46000 Тернопіль, Україна

У моделі прямокутних потенціальних ям та бар'єрів та моделі ефективних мас для електрона, з використанням отриманих точних розв'язків нелінійного кубічного рівняння Шредінгера, розвинена квантово-механічна теорія стаціонарного електронного спектру та сил осциляторів квантових переходів з урахуванням електрон-електронної взаємодії у наближенні Хартрі-Фока. На прикладі двоямної плоскої напівпровідникової наноструктури, що може функціонувати як активна зона квантового каскадного детектора показано, що врахування між електронної взаємодії зменшує інтенсивність квантових переходів між першими електронними станами та зменшує величину детектованої енергії.

Ключові слова: Квантовий каскадний лазер, Квантовий каскадний детектор, Електрон-електронна взаємодія, Кубічне рівняння Шредінгера.

REFERENCES

1. P. Reininger, B. Schwarz, A. Harrer, T. Zederbauer, H. Detz, A. M. Andrews, R. Gansch, W. Schrenk G. Strasser, *Appl. Phys. Lett.* **103**, 241103 (2013).
2. T. Dougakiuchi, K. Fujita, T. Hirohata, A. Ito, M. Hitaka, T. Edamura, *Appl. Phys. Lett.* **109**, 261107 (2016).
3. C. Kumar, N. Patell, R. Barron-Jimenez, I. Dunayevskiy, G. Tsvid, A. Lyakh, *Appl. Phys. Lett.* **110**, 031104 (2017).
4. S. Singh, R. Kamoua, *J. Appl. Phys.* **110**, 213106 (2014).
5. M. Tkach, Ju. O. Seti, I. Boyko, O. Voitsekhivska, *Condens. Matt. Phys.* **13**, 33701 (2013).
6. V.F. Elesin, *JETP* **495**, 114 (2002).
7. V.F. Elesin, Yu. Kateev, M.A. Remnev, *Semiconductors* **43**, 257 (2009).
8. M. V. Tkach, Ju. O. Seti, I. V. Boyko, *Ukr. J. Phys.* **57**, 849-859 (2012).
9. L. D. Carr, C. W. Clark, W. P. Reinhardt, *Phys. Rev. A* **62**, 063610 (2000).
10. K. Rapedius, D. Witthaut, H. J. Korsch, *Phys. Rev. A* **73**, 033608 (2006).
11. M. Abramowitz, I. Stegun, *Handbook of mathematical functions* (New York: Dover Publications: 1970).