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The energy eigenstates of two quantum dots systems placed at the air-semiconductor interface

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In this study, the nanostructured systems formed by two cylindrical quantum dots (QDs) it are considered - one is embedded into semiconductor substrate (GaAs) and the second is situated in air. Our particular interest was on evolution of the eigenstates of confined electrons with the distance between QDs. It was used a one-band model expression for Schrödinger equation [1] to characterize the energy of QDs electrons and that was solved using a finite element method for geometry discretization. The presence of the oscillating envelope function of the electrons for different distances between dots was observed. The wavelength corresponding to the system formed by two QDs is ranged in infrared domain.

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Keywords: Cylindrical quantum dots, Finite element method, Infrared domain

1. Introduction

The quantum dots are nanodevices created by confining free electrons in a semiconducting matrix. These droplets of confined "free electrons" present many and interesting electronic properties for future optical devices [1, 2]. The progress in quantum devices nanofabrication enabled to form an artificial molecule sharing electrons from two or more QDs. The couplings between QDs opens possibilities to design new quantum electron devices like electron splitters, based on physical effects that are usually encountered in quantum optics. In this paper, we have analyzed the energetic states of systems formed by two cylindrical quantum dots (QDs) of Carbon for the two cases:

1. case 1 – one dot with the fixed radius (QD2) is situated under the interface semiconductor – air (into the semiconductor matrix) and the second dot with the variable radius (QD1) is into air;
2. case 2 – QD1 is embedded in the semiconductor matrix and QD2 is situated on the interface semiconductor – air into air.

In order to compute the energetic states of QDs, we solve the 1-band Schrödinger equation in the effective mass approximation.

2. Theoretical background

The system of QDs formed by confined electrons in some spatial domains could be approximated with a group of free electrons in potential cylindrical holes. The energy eigenstates and associated eigenvalues of this QDs structure are given by the one-band Scrödinger equation in the effective mass approximation:

$$-\frac{\hbar^2}{2}\nabla\cdot\left(\frac{1}{m_e(\vec{x})}\nabla\Psi(\vec{x})\right)+V_e(\vec{x})\Psi(\vec{x})=E\,\Psi(\vec{x}) \qquad (1)$$

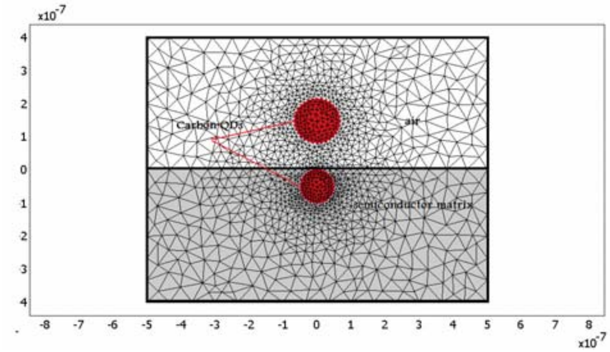
where $\hbar$, $m_e(\vec{x})$, $V_e(\vec{x})$, E, and $\Psi(\vec{x})\equiv\Psi(r,\theta,z)$ are Planck's constant divided by 2π, the position-dependent electron effective mass, the position-dependent band-edge potential energy, the electron energy, and the electron envelope function, respectively. Since cylindrical symmetry is assumed, it results that $\vec{x}=(r,\theta,z)$ are the cylindrical variables. From a physical point of view, the following two conditions should be satisfied on the boundary of each QD:

$$\Psi(\vec{x})\in C(Q),\ -\frac{1}{m_e^s}\nabla\Psi(\vec{x})\cdot\vec{n}=\frac{1}{m_e^b}\nabla\Psi(\vec{x})\cdot\vec{n} \quad (2)$$

where $m_e(\vec{x})=m_e^s$ is the electron effective mass in the QD-semiconductor structure and $m_e(\vec{x})=m_e^b$ is the electron effective mass in the barrier material, Q is the spatial domain of interest, C is the class of continuous functions and $\vec{n}$ is outer normal vector in the domain under consideration. Starting from the Schrödinger equation (1) with the conditions (2) and using finite element method (FEM), we can calculate the eigenvalues of electrons energy corresponding to QDs system. Because of the geometric symmetry, the problem was reduced at a bidimensional one. Consequently, the Schrödinger equation was written in a simplified form:

$$\nabla\times\nabla u+\alpha u+\beta\nabla u=\lambda E u$$

The equation was discretized on a domain that contains the system of QDs and part of the semiconductor matrix, and keeping account of the boundary conditions, a matricial eigenvalues and eigenfunctions problem is resulting. The discretization of the surface is realized with triangular elements, the position of the triangle nodes being an input for FEM algorithm. The distribution of the triangular elements is not uniform over the considered domain, the number of elements being higher close to the boundaries.Using the FEM for solving of Schrödinger equation it obtains a linear system of equations; the solutions are the density functions and the QD electrons energy eigenvalues.The boundary conditions consist in continuity conditions of density functions at the interfaces between different materials. The discretization domain is considered large enough as the influence of the offside boundaries could be ignored. The UMFPACK pack routines were used for solving the resulted unsymmetric sparse linear systems. Even if, from numerical solving of the eigenvalues and envelope functions problem, a big number of solution are obtained, only the energetic states below the ionization potential of semiconductor material are real. Up to this value of the potential, the electrons become free, and could go off from QD in semiconductor. One underlines that these energy bands do not represent the energy bands in a usual sense but they have been considered as possible solutions of the envelope function that satisfied the imposed boundary condition. These eigenvalues defines the discrete energy levels of electrons and the frequencies of emission/absorption energy transfer between QD and exterior.



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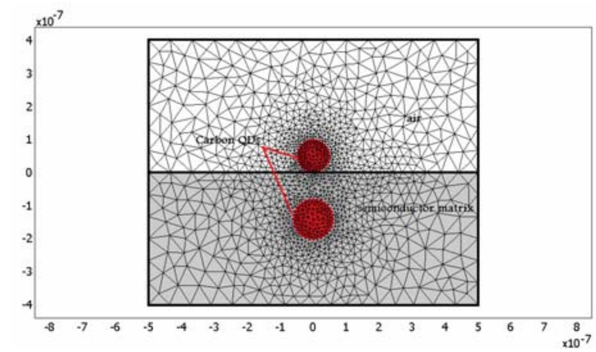

b

Fig. 1. The geometry of Carbon QDs.FEM discretization; (a) Case 1 - QD2 is situated under the interface GaAs matrix-air and QD1 is in air; (b) Case 2 - QD2 is situated on the interface GaAs matrix-air and QD1 is embedded in the semiconductor matrix.

3. The vertical cylindrical quantum dots systems

In the following, let's analyze a QDs system consisting of two cylindrical Carbon QDs, the first dot (QD1) having the variable radius in the range of $50 \div 100$ nm and the second dot (QD2) having the radius $R = 50nm$. In the case 1 the QD2 is situated under the interface air-semiconductor matrix in a fixed position and QD1 is placed in air, on the vertical direction to QD2 - Fig. 1(a) - while the second case, QD2 is situated on the interface air-semiconductor matrix in a fixed position and the QD1 is embedded in semiconductor matrix, on the vertical direction to QD2-Fig.1(b). The electric potentials are $V_{GaAs} = 0.697\, eV$ for the semiconductor substrate and $V_{Carbon} = 0.1eV$ for QDs. Firstly, the distance between QDs was fixed at $d = 90\, nm$ and the radius of the QD1 was modified. We was looking for a suitable radius of the QD1 for that both QDs have the same value of one energy eigenstate. In order to select the values of QD1 radius for that the QDs have the same eigenstate energy, the dependence the energy eigenstates for both QDs, as a system, with the QD1 radius was determined. The second purpose was to analyze the possibility to obtain the same value of the one eigenstates energy of both QDs for the different values of the distances between dots ($50 \div 90nm$).

3. 1 The QD1 is placed in air

From the multiplet eigenvalues of energy that correspond to this system, it was selected the first eigenstates close to the fundamental energy level. In Fig. 2 it is represented the dependence of the first three eigenstates energy of QD1 and QD2 with the QD1 radius. This figure shows that the value of QD1's energy decreases with the increase of the radius of the QD1. This behavior of QD1's energy leads to an increase of the wavelength with the increase of the QD1 radius. The value of QD2 energy is not significantly modified at the increase of the QD1 radius. For the case when the energy of the oscillation mode *n* of QD1 *En* is equal with the energy of the oscillation mode *m* of QD2 *Em* the total energy of the QDs system will be noted with *Enm*.The intersection points of the *En* and *Em* curves lead to the values of the QD1's radius (big dot) for that the QDs have the same value of the eigenstate energy *Enm* with different oscillation modes.

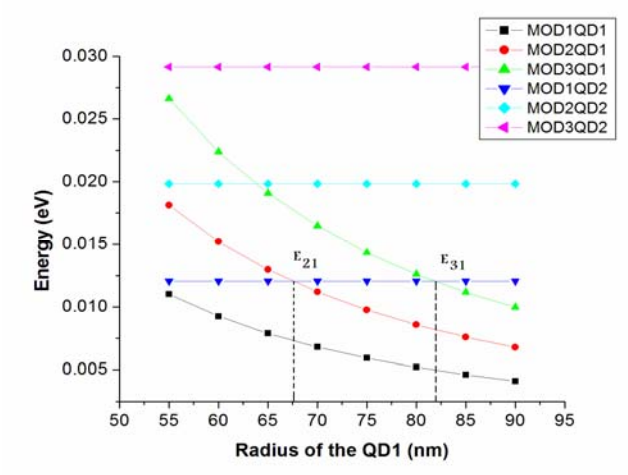

Fig.2 Evolution of the eigenstate energies with the radius of the QD1 for the distance between dots d = 80nm.

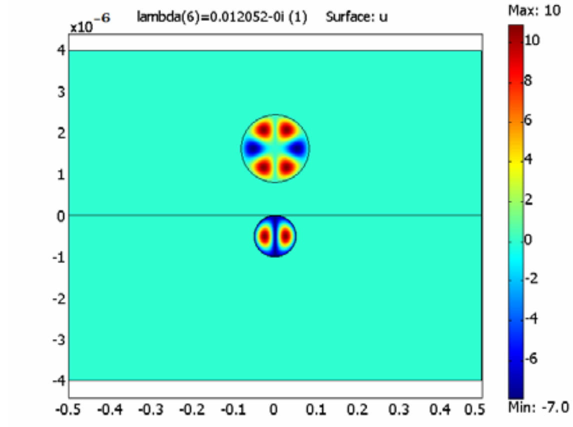

Fig.3 The envelope function representation corresponding to the eigenvalue of energy $E_{31} = 0.012052eV$ *for cylindrical quantum dots system. Radius of the QD1 is 81.86 nm and d = 80nm*

From the Fig. 2 the following the intersection points are obtained:

1. for the radius $R = 67.499nm$ of the QD1, it is obtained the same value of energy for the QDs system, $E_{21} = 0.012050eV$ but for this case the QD1 is in the second oscillation mode and QD2 in the first oscillation mode.

2. for the radius of QD1, $R = 81.86nm$, the same value of energy for the QDs system $E_{31} = 0.012052eV$ corresponds with the mode three of QD1 and mode one of QD2. There are few more possibilities to have the same energy for QDs eigenstates; the eigenstates with low value of energy are more stable and precise defined. Fig. 3 shows the case when the dots, being at the distance $d = 80\,nm$, have the energy, $E_{31} = 0.012052eV$. This configuration corresponds to the case when the radius of the QD1 is $R = 81.86\,nm$. As we can see on Fig.2, at a given distance between QDs, for a suitable radius of the QD1 we can obtain the same value of the system's energy, corresponding to the mode third of QD1 and mode one of QD2.The QDs system energy *Enm* is related with the distance between QDs and with the radius of the QD1. If the distance between QDs becomes infinity, the QDs act as isolated dot. Fig. 4 represents the evolution of energy E_{31} with distance between QDs $d = 10 \div 90nm$. As we seen in the Fig. 3 this energetic configuration corresponds with the mode three of QD1 and mode one of QD2.

The increase of the distance between QDs leads to the increase of the system's energy. In this figure we find for the given values of the distance between the QDs, the values of the QD1's radius corresponding to the same system's energy, E_{31}.The wavelength for this configuration is ranged in infrared domain. The behavior of system's energy leads to a decrease of the wavelength with the increase of distance between QDs.

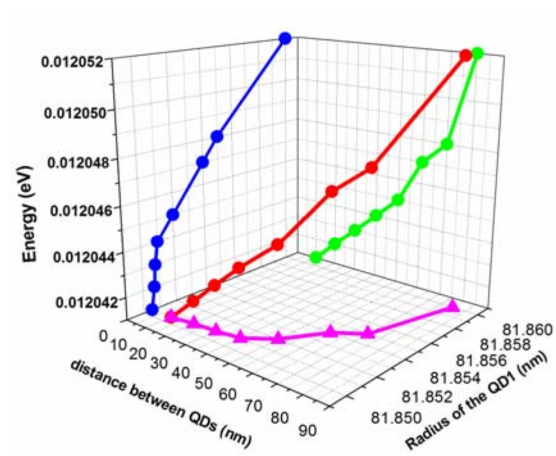

Fig. 4 Evolution with distance between QDs of the E_{31} *energy of the QDs system for the suitable radius of the QD1 for that the QDs system have the same value of Energy.*

Case 2 The QD1 embedded in the matrix

In the second case, the QD1 is embedded in the semiconductor matrix. Fig. 5 shows the dependence of the first three eigenstates energy of QD1 and QD2 with the QD1 radius.Value of QD1's energy decreases with the increase of the radius of the QD1. For the fundamental level, the intersection points of the *En* and *Em* curves lead to the values of the QD1's radius (big dot) for that the QDs have the same value of the eigenstate energy E_{21} and E_{31} with different oscillation modes.

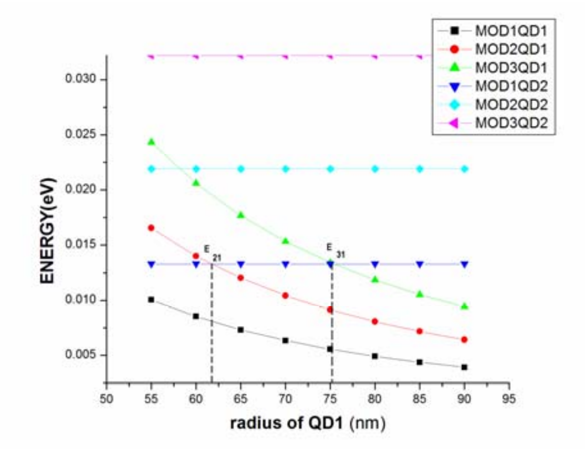

Fig.5 Evolution of the eigenstates energies with the radius of the QD1 for the distance between dots d = 80nm.

In the Fig. 5 the following intersection points are obtained: (1) for the radius $R = 61.62nm$ of the QD1, it is obtained the same value of energy for the QDs system, $E_{21} = 0.013322eV$ but for this case the QD1 is in the second oscillation mode and QD2 in the first oscillation mode;(2) for the radius of QD1, $R = 75.29\,nm$, the same value of energy for the QDs system $E_{31} = 0.013325eV$ corresponds with the mode three of QD1 and mode one of QD2. There are few more possibilities to have the same energy for QDs eigenstates; the eigenstates with low value of energy are more stable and precise defined. Fig.7 shows the case when the dots, being at the distance $d = 80\,nm$, have the energy, $E_{31} = 0.013325eV$. This configuration corresponds to the case when the radius of the QD1 is $R = 75.29\,nm$. As we can see on figure Fig.6, at a given distance between QDs, for a suitable radius of the QD1 we can obtain the same value of the system's energy, corresponding to the mode third of QD1 and mode one of QD2. Fig. 9 represents the evolution of energy E_{31} with distance between QDs $d = 10 \div 90nm$. As we seen in the Fig. 7 this energetic configuration corresponds with the mode three of QD1 and mode one of QD2. The increase of the distance between QDs leads to the increase of the system's energy. In this figure we find for the given values of the distance between the QDs, the values of the QD1's radius corresponding to the same system's energy, E_{31}.

4. Conclusions

The eigenstates of confined electrons depend on both the distance between dots and their radius. The eigenstates energy of confined electrons is bigger for smaller radius of QDs. The wavelength corresponding to the system formed by QDs is ranged in infrared domain. For the suitable values of the QD1's radius it can be found the same values of the energy for both dots that are in different oscillation modes.

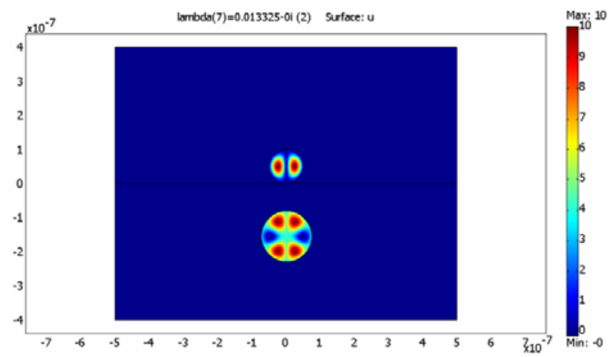

Fig. 6 The envelope function representation corresponding to the eigenvalue of energy $E_{31} = 0.013325eV$ for cylindrical quantum dots system. Radius of the QD1 is 75.29 nm and d = 80 nm

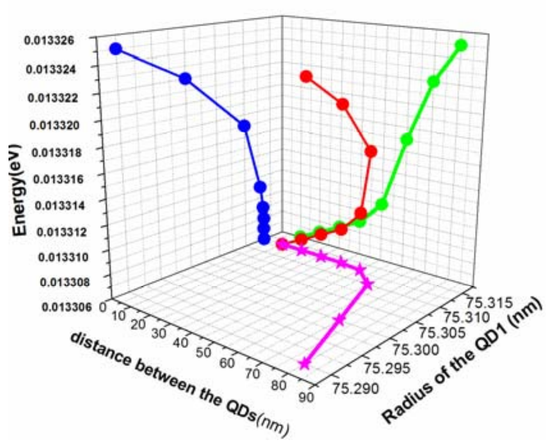

Fig. 7 Evolution with distance between QDs of the E_{31} energy of the QDs system for the suitable radius of the QD1 for that the QDs system have the same value of energy

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