# Computer simulation of the non-uniform and anisotropic diamagnetic shift of electronic energy levels in double quantum dot molecules

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A B S T R A C T

In this study we calculated the lowest energy states of electrons confined in an asymmetrical *InAs/GaAs* double lens-shaped quantum dot molecule in external magnetic field. Based on the effective three-dimensional one electronic-band Hamiltonian approximation (with the energy and position dependent electronic effective mass) the electronic energy states of the system were computed by non-linear iterative method using Comsol MultiPhysics package. Our description allows us to simulate the semiconductor quantum dot molecule in arbitrary directed magnetic field. Simulation results clearly show that the diamagnetic shifts of the electronic energy levels are anisotropic and non-uniform. Therefore we demonstrate an opportunity to dynamically manipulate electronic states not only by varying the magnitude but also changing the direction of the magnetic field.

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## 1. Introduction

Recently studies on structural, electronic, and optical properties of semiconductor quantum dots attracted much attention from experimental and theoretical points of view (see for instance [1] and references therein). Advance in modern semiconductor technologies makes it possible to fabricate vertically stacked quantum dots of high quality and uniformity [2–4]. Stacked quantum dots allow us to form artificial quantum dot molecules (QDMs). Those semiconductor nano-objects are very attractive candidates for possible applications in the solid state quantum memory [5]. They are also considered as structural elements for new nano-structured metamaterials [6]. The quantum mechanical coherent coupling and forming of the molecular states in QDMs can be considered in complete analogy to real molecules. However artificial design of QDMs provides us with much wider opportunities to manipulate and reconfigure wave functions of electrons confined in QDMs. In order to control the quantum coupling between electronic quantum states localized in different dots one can adjust distance between dots (static approach). Another possibility to control dynamically the coherent coupling between dots is the application of external electromagnetic fields (known as dynamic approach) [7]. In this paper we simulated the electronic states of electrons confined in *InAs/GaAs* double QDMs assembled from the quantum dots with substantially different lateral radii [8] when the external magnetic field is applied to the system (see Fig. 1). In contrast to most of the known calculations we perform our simulations for several distances between dots in QDMs and few directions of the applied magnetic field.

## 2. Computational method

We theoretically consider the lowest energy states of electrons confined in the asymmetrical double *InAs/GaAs* lens-shaped quantum dot molecule. The molecule consists of two quantum dots with substantially different radii $\rho_L > \rho_S$ and heights $h_L < h_S$ ($L$ and $S$ stand for the "Large" and "Small" dots in the molecule). The inter-dot (base-to-base in the molecule) distance is $d$ (see Fig. 1). Therefore, our system is highly asymmetrical in $z$ direction. In our simulation the uniform external magnetic field can be applied in an arbitrary direction. To compute electronic energy states confined in the asymmetrical *InAs/GaAs* quantum dot molecule with three-dimensional hard-wall confinement potential we adopt the effective one-band Hamiltonian as in [8,9]:

$$\hat{H} = \frac{1}{2}\prod_{\mathbf{r}}\frac{1}{m(E,\mathbf{r})}\prod_{\mathbf{r}} + V(\mathbf{r}) + \frac{\mu_B}{2}g(E,\mathbf{r})\boldsymbol{\sigma}\cdot\mathbf{B} \qquad (1)$$

where $\prod_{\mathbf{r}} = -i\hbar\nabla_{\mathbf{r}} + e\mathbf{A}(\mathbf{r})$ is the electron momentum operator, $\nabla_{\mathbf{r}}$ is the spatial gradient, $\mathbf{A}(\mathbf{r})$ is the vector potential for the uniform arbitrary directed external magnetic field $\mathbf{B} = (B_x, B_y, B_z)$ and $\mathbf{B} = \text{curl}\mathbf{A}(\mathbf{r})$, $m(E,\mathbf{r})$ is the energy and position dependent electron effective mass:

$$\frac{1}{m(E,\mathbf{r})} = \frac{2P^2}{3\hbar^2}\left[\frac{2}{E + E_g(\mathbf{r}) - V(\mathbf{r})} + \frac{1}{E + E_g(\mathbf{r}) - V(\mathbf{r}) + \Delta(\mathbf{r})}\right]$$

and

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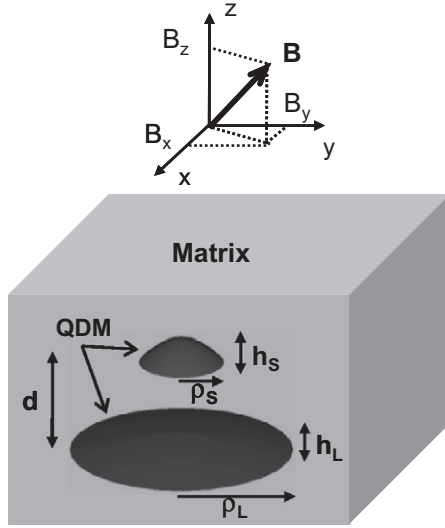  E-mail addresses: leminhthu_1981@yahoo.com, minhthule1981@gmail.com (L.M. Thu).

**Fig. 1.** Schematic of the asymmetrical *InAs/GaAs* semiconductor double quantum dot molecule in uniform arbitrary directed external magnetic field.

$$g(E, \mathbf{r}) = 2\left[1 - \frac{m_0}{m(E, \mathbf{r})}\frac{\Delta(\mathbf{r})}{3(E + E_g(\mathbf{r})) + 2\Delta(\mathbf{r})}\right]$$

is the electronic Landé factor. In the equations above: $V(\mathbf{r})$ is the electron's confinement potential, $E_g(\mathbf{r})$ and $\Delta(\mathbf{r})$ stand for the position dependent band gap and spin–orbit splitting in the valence band, $P$ is the momentum matrix element, $\boldsymbol{\sigma}$ is the vector of the Pauli matrixes, $\mu_B$ stands for the Bohr magneton, $m_0$ and $e$ are the free electron elementary mass and charge. The hard-wall confinement potential can be presented as: $V(\mathbf{r}) = 0$, if $\mathbf{r}$ is inside the dots; and $V(\mathbf{r}) = V_0$, if $\mathbf{r}$ is outside the dots ($V_0$ is the electronic band offset in *InAs/GaAs* heterostructures). For the electrons confined in the QDM the envelop wave functions $F(\mathbf{r})$ should satisfy the Schrödinger equation

$$HF(\mathbf{r}) = EF(\mathbf{r}) \qquad (2)$$

Since we are dealing with the hard-wall confinement potential, the Ben Daniel-Duke boundary conditions [9] for the wave functions in Schrödinger equation has to be imposed on the boundary between two materials. The Ben Daniel-Duke boundary conditions for electron wave functions are given by

$$F(\mathbf{r})|_{in} = F(\mathbf{r})|_{out}$$
$$\frac{1}{m(E, \mathbf{r})}\nabla_{\mathbf{r}}F(\mathbf{r}) \cdot \mathbf{n}|_{in} = \frac{1}{m(E, \mathbf{r})}\nabla_{\mathbf{r}}F(\mathbf{r}) \cdot \mathbf{n}|_{out} \qquad (3)$$

Here subscribe "*in*" and "*out*" denote the different sides of the interface (*InAs* and *GaAs* respectively) and $\mathbf{n}$ is the outward normal unit vector at the boundary. Solving the Schrödinger equation with the Ben Daniel-Duke boundary conditions we can find the energy states of electrons confined in the QDM.

In our simulations we use realistic semiconductor material parameters and dimension of the dots in the molecule known in literature [8,10–12]. Our molecule consists of two quantum dots with substantially different radii $\rho_L > \rho_S$ and height $h_L < h_S$ (*L* and *S* stand for "Large" and "Small" dot in Fig. 1). The simulations were performed for the double QDM with geometry parameters [4,8]: $\rho_L = 25$ nm, $\rho_S = 9.5$ nm, $h_L = 3$ nm, $h_S = 4$ nm, and few inter-dot distances (base-to-base) $d_1 = 20$ nm, $d_2 = 10$ nm and $d_3 = 5$ nm.

The material parameters for the *InAs/GaAs* quantum dot molecule are taken from Ref. [10] with correction for strained *InAs* inside the dot: $E_{gInAs} = 0.842$ eV, $\Delta_{InAs} = 0.39$ eV, $m_{eInAs} = 0.044$ $m_0$. For the *GaAs* surrounding matrix we take the data from [11]:

$E_{gGaAs} = 1.52$ eV, $\Delta_{GaAs} = 0.341$ eV, $m_{eGaAs} = 0.067$ $m_0$. Using these parameters the band offset of conduction band can be found as: $V_0 = 0.474$ eV. The energy states of electrons confined in QDM are obtained numerically form solutions of Schrödinger equation (1) with Ben Daniel-Duke boundary conditions (3) by the non-linear iterative method [13–15] using the Comsol MultiPhysics package (www.comsol.com).

## 3. Simulation results and discussion

We present our calculation for few distances between quantum dots in the molecule: $d_1 = 20$ nm, $d_2 = 10$ nm and $d_3 = 5$ nm with uniform external magnetic field directed in three directions: $\mathbf{B}_{\{1\}} = (0, 0, B\mathbf{z})$, $\mathbf{B}_{\{2\}} = \frac{1}{\sqrt{2}}(0, B\mathbf{y}, B\mathbf{z})$, and $\mathbf{B}_{\{3\}} = (0, B\mathbf{y}, 0)$. Combination of the distance $d$ and directions of magnetic field $\mathbf{B}$ gives us nine configurations for our system: $[d_i, \mathbf{B}_{\{j\}}]$, where $i, j = 1, 2, 3$. For those configurations, we simulate the lowest confined electronic energy states. The results are shown in Figs. 2–4. When the distance between dots in the molecule is large enough, the tunnel coupling between dots is weak. Therefore, in $[d_1, \mathbf{B}_{\{1\}}]$ configuration the diamagnetic shifts of electronic energies become non-uniform because of the non-uniformity of the QDMs geometry in the z-direction. This leads to the anticrossing at $B_{AC} = 10.7$ T for electronic energy of two lowest states $e_1$ and $e_2$ (see Fig. 2a). The details of the anticrossing were found and discussed in Ref. [8]. An important aspect is that the anticrossing manifests a redistribution of the electronic wave function inside the quantum dot molecule: the electronic wave function of the state $e_1$ at the anticrossing point relocates from the large dot to the small one whereas the wave function of the state $e_2$ relocates in the opposite direction. When the magnetic field direction changes from $\mathbf{B}_{\{1\}}$ to $\mathbf{B}_{\{2\}}$ the anticrossing point shifts to a larger magnitude of the magnetic field (Fig. 2b). When $\mathbf{B} = \mathbf{B}_{\{3\}}$ (magnetic field is parallel to the *xy*-plane) the anticrossing disappears (Fig. 2c). The electronic wave functions localized in the large and small dots are under strong confinement in z-direction. Therefore, in this last configuration ($[d_1, \mathbf{B}_{\{3\}}]$) the wave functions hardly can be controlled by external magnetic
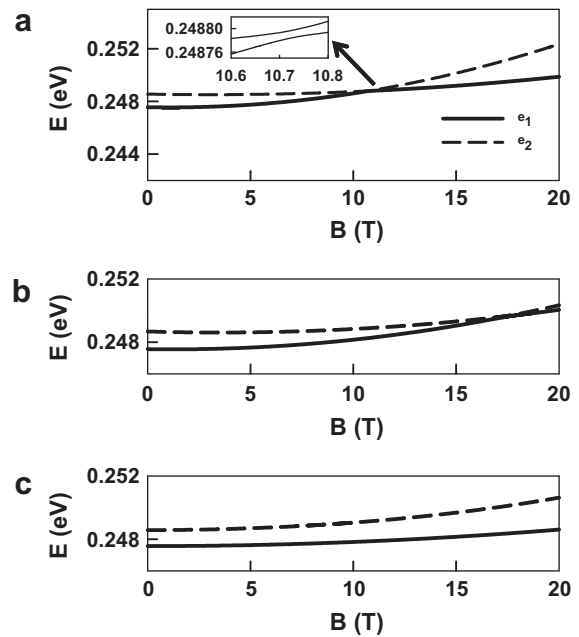


**Fig. 2.** Magnetic field dependence of the lowest electronic energy levels of the double QDM for $d_1 = 20$ nm at different directions of the magnetic field: (a) $\mathbf{B} = \mathbf{B}_{\{1\}}$; (b) $\mathbf{B} = \mathbf{B}_{\{2\}}$; (c) $\mathbf{B} = \mathbf{B}_{\{3\}}$ (inset: anticrossing region).
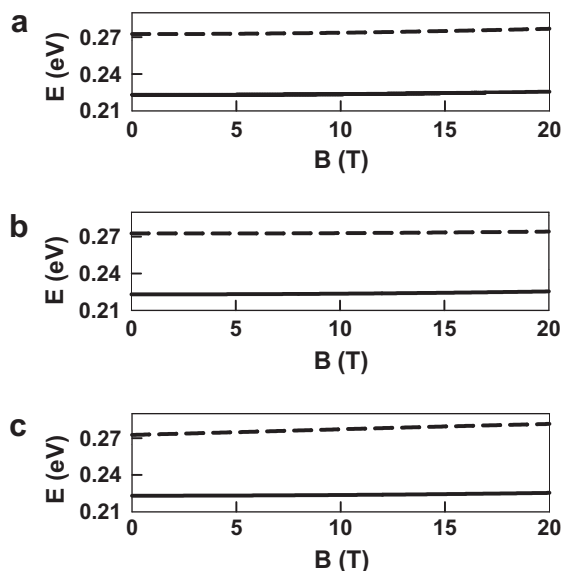
**Fig. 3.** Magnetic field dependence of the lowest electronic energy levels of the double QDM for $d_3 = 5$ nm (description of the levels and magnetic field directions see in Fig. 2).
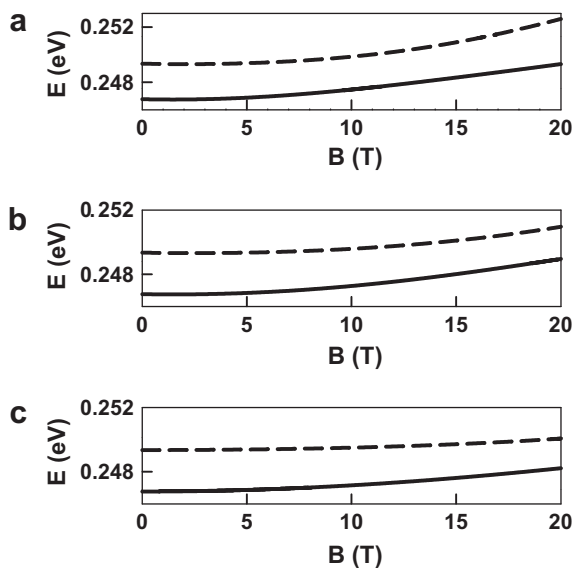


**Fig. 4.** Magnetic field dependence of the lowest electronic energy levels of the double QDM for $d_2 = 10$ nm (description of the levels and magnetic field directions see in Fig. 2).

fields. So, change in the direction of magnetic field from $\mathbf{B}_{\{1\}}$ to $\mathbf{B}_{\{3\}}$ shifts the anticrossing point and gradually removes it. This means that one can manipulate electronic states in double QDMs by varying the magnitude and changing direction of the magnetic field as well.

The small distance between dots in the molecule ($d_3 = 5$ nm) brings strong tunnel coupling between dots and leads to the strong hybridization between two electronic states $e_1$ and $e_2$. This generates molecular electronic states with symmetric and anti-symmetric wave function configurations along $z$-direction [8,12]. The diamagnetic shifts of electronic energies become uniform (even for $\mathbf{B}_{\{1\}}$) and this leads to the disappearance of the anti-crossing (Fig. 3a). The system with distance $d_2 = 10$ nm presents an intermediate case between the large and small distances. In this configuration we can see a combination of the anticrossing and hybridization. It leads to a weak convergence of the electronic energies and the anticrossing disappears even for $\mathbf{B} = \mathbf{B}_{\{1\}}$ (see Fig. 4a). Clearly, the reduction of the distance between dots conventionally hybridizes electronic states from different dots and this finally forms typical molecular states in the QDM (see Figs. 3 and 4).

In conclusion, we calculated the lowest electronic energy states for a realistic three-dimensional model of asymmetrical lens-shaped double *InAs/GaAs* quantum dot molecule in the uniform arbitrary directed external magnetic field for few distance between dots in the molecule. The simulation results clearly show that the diamagnetic shifts of the electronic energy levels are considerably different for different distances. In addition the application of the magnetic filed in various directions generates anisotropy in the diamagnetic shifts. Energy states of electrons confined in QDMs can be manipulated by adjusting the distance between dots in the molecule (statically) or application external magnetic field (dynamically). Moreover, one can dynamically manipulate electronic states not only by varying the magnitude but also changing the direction of the external magnetic filed. The results can be useful in modeling and investigation of the magnetic properties of QDMs.

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