phys. stat. sol. (c) **3**, No. 11, 3656–3659 (2006) / **DOI** 10.1002/pssc.200671565

Magnetically driven coupling of electronic states in quantum dot molecules

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Received 1 May 2006, revised 14 June 2006, accepted 18 July 2006
Published online 24 November 2006

PACS 73.21.La, 73.43.Cd

We consider lowest energy states of electrons confined in asymmetrical circular vertically stacked double *InAs/GaAs* quantum dot molecule. The energies where computed by using the effective three-dimensional one band Hamiltonian, the energy (non-parabolic) and position dependent electronic effective mass approximation, and the Ben Daniel-Duke boundary conditions with the finite hard wall confinement potential. We demonstrated theoretically a possibility to drive dynamically coupled electronic states (relocate electronic wave functions from one dot to another) by applying external magnetic field.

1 Introduction Recent advances in the fabrication of semiconductor nano-scale-objects stimulated much attention to the study of structural, optical, and electronic properties of semiconductor quantum dots (see for example [1]). Especially, during the last decade it has become possible to fabricate realistic semiconductor quantum dots in laboratories. Various experimental results demonstrate that *InAs/GaAs* quantum dots can have diverse shapes, such as disk, ellipsoid, or conical shapes with a circular top view cross section and a large area-to-height aspect ratio (see for instance [2, 3]). Coupled quantum dots allow us to form an artificial molecule. In this molecule we can adjust the inter-dot distance and through that to control coupling between electronic states localized in different dots. The ability to control coherent coupling between double quantum dots may open possibility for designing quantum logic gates (see [4, 5] and references therein). The inter-dot distance control is an example of a static approach to the gate's design. Another possibility to control dynamically the coupling lies in application of external fields [6]. In this work we demonstrate theoretically an opportunity to drive dynamically electronic states by applying external magnetic field to two vertically coupled *InAs/GaAs* quantum dots.

2 Theoretical model We consider lowest energy states of electrons confined in asymmetrical circular vertically stacked double *InAs/GaAs* quantum dot molecule [see insert (a) in Fig. 1]. The most important difference of this molecule from those usually discussed in literature is that our quantum dots have the same height h, but substantially different radii $r_L > r_U$ (L and U stand for the "lower" and "upper" dots). So, the system is highly asymmetrical in z-direction.

To simulate disk-shaped quantum dots we use the effective three-dimensional one-electronic-band Hamiltonian with hard-wall confinement potential (the energy and position-dependent electron effective mass approximation). The external magnetic field **B** is directed along the system axis z. In this approach the effective one-electronic-band Hamiltonian [7] is taken as the following

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

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where: $\mathbf{\Pi}_\mathbf{r}=-i\hbar\nabla_\mathbf{r}+e\mathbf{A}(\mathbf{r})$ is the electron momentum operator, $\nabla_\mathbf{r}$ is the spatial gradient, $\mathbf{A}(\mathbf{r})$ is the vector potential of the magnetic field $\mathbf{B}$=curl $\mathbf{A}(\mathbf{r})$, $m(E,\mathbf{r})$ is the energy and position dependent electron effective mass

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

and

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

is the Landé factor. In the equations above: $V(\mathbf{r})$ is the 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, σ is the vector of the Pauli matrixes, and m_0 and e are the free electron elementary mass and charge. The hard well confinement potential $V(\mathbf{r})$ can be presented as: $V_1 = 0$, if $\mathbf{r}$ is inside the dots (region $i = 1$); and $V_2 = V_0$, if $\mathbf{r}$ is outside the dots (region $i = 2$). V_0 is the band offset in InAs/GaAs heterostructures. The Ben Daniel-Duke boundary conditions [7] for the electron wave function are given by

$$\begin{aligned}&\Psi_1(\mathbf{r}_s)=\Psi_2(\mathbf{r}_s);\\&\frac{1}{m_1(E,\mathbf{r}_s)}\nabla|_{\mathbf{r}_n}\Psi_1(\mathbf{r}_s)=\frac{1}{m_2(E,\mathbf{r}_s)}\nabla|_{\mathbf{r}_n}\Psi_2(\mathbf{r}_s),\end{aligned}\tag{2}$$

where $\mathbf{r}_s$ and $\mathbf{r}_n$ denote, respectively, the position of the system interface and the normal direction to the interface.

Because of the cylindrical symmetry of the system ($\mathbf{B}\|\mathbf{z}$) we can treat the problem (1)-(2) in cylindrical coordinates (ρ, z, ϕ) and the wave function can be represented as

$$\Psi(\mathbf{r})=\Phi(\rho,z)\exp(il\phi)\ ,$$

where l=0,±,1,±2,… is the orbital quantum number. The problem remains two-dimensional in (ρ, z) plane because of the coordinate dependence of the effective mass, Landé factor and confinement potential

$$\begin{aligned}&-\frac{\hbar^2}{2m_i(E)}\left(\frac{\partial^2}{\partial z^2}+\frac{\partial^2}{\partial\rho^2}+\frac{\partial}{\partial\rho}-\frac{l^2}{\rho^2}\right)\Phi^i_{\{n,l,s\}}(\rho,z)\\&+\left[V_i+\frac{m_i(E)\Omega_i^2(E)\rho^2}{8}+\frac{1}{2}l\hbar\Omega_i(E)+\frac{s\mu_B}{2}g_i(E)B\right]\Phi^i_{\{n,l,s\}}(\rho,z)=E_{\{n,l,s\}}\Phi^i_{\{n,l,s\}}(\rho,z),\\&\rho,z\in i=1,2,\end{aligned}\tag{3}$$

where

$$\Omega_i(E)=\frac{eB}{m_i(E)}\,.$$

In Eq. (3) n and s refer to the main quantum number and spin orientation along z-axis correspondingly. The boundary conditions (2) can be written as the following

$$\begin{aligned}&\Phi^1_{\{n,l,s\}}(\rho,z)=\Phi^2_{\{n,l,s\}}(\rho,z),\ z=f_s(\rho),\\&\frac{1}{m_1(E_{\{n,l,s\}})}\left\{\frac{\partial\Phi^1_{\{n,l,s\}}(\rho,z)}{\partial\rho}+\frac{df_s(\rho)}{d\rho}\frac{\partial\Phi^1_{\{n,l,s\}}(\rho,z)}{\partial z}\right\}\Bigg|_{z=f_s(\rho)}\\&=\frac{1}{m_2(E_{\{n,l,s\}})}\left\{\frac{\partial\Phi^2_{\{n,l,s\}}(\rho,z)}{\partial\rho}+\frac{df_s(\rho)}{d\rho}\frac{\partial\Phi^2_{\{n,l,s\}}(\rho,z)}{\partial z}\right\}\Bigg|_{z=f_s(\rho)},\end{aligned}$$

where $z = f_s(\rho)$ presents on (ρ, z) plane the generator contour of the molecule. The solutions of the two-dimensional problem in this work are found by the nonlinear iterative method described somewhere else [8–10].

3 Results and discussion In the following our discussion will focus on *InAs/GaAs* double dot molecule with the material parameters for *InAs*: $E_{1g} = 0.42$ eV, $\Delta_1 = 0.38$ eV, $m_1(0) = 0.024m_0$; and for *GaAs*: $E_{2g} = 1.52$ eV, $\Delta_2 = 0.34$ eV, $m_2(0) = 0.067m_0$ The band offset parameter is taken as $V_0 = 0.77$ eV. Here we present our calculation results for lowest energy states of the system with $h = 10$ nm, $r_L = 4r_U = 40$ nm, and inter-dot distance 6 nm ($z_U - z_L = 16$ nm). For the clarity reasons we consider here only the lowest ground energy states of the molecule with angular momentum $l = 0$. We also do not discuss here Zeeman spin-splitting for the electronic states (so, $g_{1,2} = 0$ and because of that we use notation "$s = 0$"). It should be noticed that g-factor itself in semiconductor nano-structures is still a very controversial issue [11]. But in the first approximation Zeeman spin-splitting should not affect much effects described below. We will describe states with $l \neq 0$ and $g \neq 0$ in the future works.

Figure 1 shows the energy dependence on the external magnetic field for three lowest energy states ({1,0,0}, {2,0,0}, and {3,0,0}) of the system. The most remarkable result is anti-crossing between the second ({2,0,0}) and third ({3,0,0}) states (states of the same symmetry) for the system with given parameters. The anti-crossing leads to relocation of the wave functions from one dot to another. The wave function of the third state relocates from the upper dot [position z_U, insert (b) in Fig. 1] to lower [position z_L, insert (c)]. Opposite relocation can be traced for the second state: from position z_L, [insert (e)] to position z_U [insert (d)].

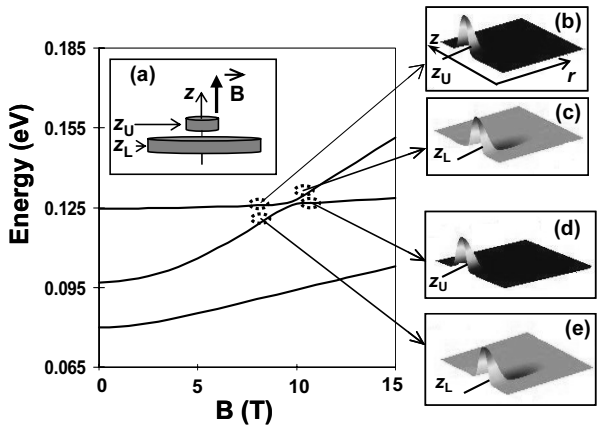

Fig. 1 Asymmetrical double dot molecule in magnetic field: (a) concept of the system. (b)-(e) locations the wave functions before the level's anti-crossing. (c)-(d) locations the wave functions after the level's anti-crossing.

This result can be understood on the base of the traditional approach to the diamagnetic shift theory in nano-sized three-dimensional systems [7]. In the first approximation of the perturbation theory the diamagnetic shifts of the states $\{n,0,0\}$ can be presented as

$$\delta E_{\{n,0,0\}}(B) = E_{\{n,0,0\}}(B) - E_{\{n,0,0\}}(0) \approx C_{\{n,0,0\}} B^2 ,$$

where

$$C_{\{n,0,0\}} = \frac{e^2}{8} \left\langle \frac{\rho^2}{m\left[\rho, z, E_{\{n,0,0\}}(0)\right]} \right\rangle ,$$

and $\langle\ \rangle$ denotes the quantity being averaged with the state wave function at zero magnetic field. It can be seen from Fig. 1 that the state {2,0,0} is adjusted (by choosing of a proper h and distance between dots) to correspond to the wave function located in the lower dot (the dot with large r_L) at $B = 0$. In the same

time, the state {3,0,0} corresponds to the wave function located in the upper dot (the dot with small r_U) at $B = 0$. The distance between those to levels in our system is

$$\Delta E(B) = E_{\{3,0,0\}}(B) - E_{\{2,0,0\}}(B) \approx [E_{\{3,0,0\}}(0) - E_{\{2,0,0\}}(0)] + (C_{\{3,0,0\}} - C_{\{2,0,0\}}) \cdot B^2. \quad (4)$$

For our double dot molecule $C_{\{3,0,+1\}} \approx 2.2\times10^{-5}$ eV/T and $C_{\{2,0,+1\}} \approx 3.6\times10^{-4}$ eV/T. It follows from Eq. (4) that those two levels should converge when magnetic field is increasing. Finally, having the same symmetry the levels anti-cross according to the general theory. So, the magnetic field acts as a dynamic coupling factor for energy states localized in different dots on the analogy of the inter-dot distance in the static approach [4].

4 Conclusion In summary, in this work we calculated single electron energy states for a realistic three-dimensional model of *InAs/GaAs* asymmetrical vertical double dot molecule in external magnetic field. We use the effective three-dimensional one band Hamiltonian, the energy and position dependent electronic effective mass approximation, and the Ben Daniel-Duke boundary conditions with the finite hard wall confinement potential. We demonstrated theoretically a possibility to drive dynamically coupled electronic states (relocate electronic wave functions from one dot to another) by applying external magnetic field. This can be potentially interesting in quantum information processing.

We would like to point out that the model and calculation results presented here can be used as a starting point for further theoretical investigations (including exited states and Zeeman splitting). We stress that our theoretical model is already very close to the demonstrated recently vertically aligned *InAs* stacked quantum dot arrays [12] and it is adjustable in respect to the system's parameters. On the other hand, the main idea to use external magnetic field like a dynamical coupling factor for energy states in highly non-symmetrical nano-systems is more general and potentially very reach.

Acknowledgements This work is supported by the National Science Council of Taiwan under contract NSC-94-2112-M-009-037.

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