

# Electron dynamical tunneling in the systems of double quantum dots and rings

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## ABSTRACT

Semiconductor heterostructures as quantum dots (QD) or quantum rings (QR) demonstrate discrete atom-like energy level structure. In the case of double QD (DQD) or double concentric QR (DCQR), a single electron spectrum is composed as a set of quasi-doublets. We study influence of these specific spectrum properties on electron tunneling which is related to the electron transport through DQD (DCQR). The double InAs/GaAs QDs (QRs) are considered within the single sub-band effective approach. The whole spectrum of the single electron is calculated for two and three dimensional quantum objects. We considered two type of dynamical tunneling in DQD. The first is related to tunneling in the system of two identical QDs; the second one occurs in the system of non-identical QDs. We study the effect of symmetry violation of DQD (DQR), the shape geometry on tunneling and show that violation of symmetry creates difficulties for tunneling.

**Keywords:** quantum dots and rings, single electron levels, anti-crossing of levels, electron localization

## 1 INTRODUCTION

In the present work we investigate the electron localization in double quantum dots (DQDs) and rings (DQRs). For DQD or DQR, a single electron spectrum is composed from sets of quasi-doublets. This property of a double quantum object is well known [1]. We study properties of this spectrum in relation to dynamical tunneling of a single electron. The tunneling is studied as function of distance between the objects: when distance is large, the electron is localized in one of the objects, when the distance decrease the electron is tunneling, the wave function is spread through the whole double system. We consider this electron tunneling related to the electron transport through DQD (DQR).

The InAs double QDs and QRs, embedded into the GaAs substrate are modeled. For these heterostructures, the well-established process of QDs formation by epitaxial growth and consecutive transformation of QDs into InAs/GaAs quantum rings (QR) has been reported in [2]. For the numerical modeling we apply an effective approach [3] in which the combined effect of strain, piezoelectricity and interband interactions are simulated by an effective potential. Quantum rings (QR) manifest specific electron behavior in the magnetic field [2]. Double concentric rings [4] are relatively new quantum objects which have potential

to have applications in nano science and nano-technology. In the present paper, we visualize interesting features occurring in double QR complex.

## 2 MODEL

We consider quantum dots and rings composed of InGaAs in a GaAs substrate. Two dimensional (2D) models are used. This heterostructure is modeled utilizing a  $kp$ -perturbation single sub-band approach with an energy dependent quasi-particle effective mass. The problem is mathematically formulated by the Schrödinger equation in two dimensions:

$$(\hat{H}_{kp} + V_c(\mathbf{r}) + V_s(\mathbf{r}))\Psi(\mathbf{r}) = E\Psi(\mathbf{r}). \quad (1)$$

Here  $\hat{H}_{kp}$  is the single band  $kp$ -Hamiltonian operator  $\hat{H}_{kp} = -\nabla \frac{\hbar^2}{2m^*} \nabla$ ,  $m^* = m^*(\mathbf{r}, E)$  is the electron effective mass which depends on both the energy and the position of the electron, and  $V_c(\mathbf{r})$  is the band gap potential.  $V_c(\mathbf{r}) = 0$  inside the QD (QR), and is equal to  $V_c$  outside the QD (QR), where  $V_c$  is defined by the conduction (or valence) band offset for the bulk. The band gap potential for the conduction band was chosen as  $V_c = 0.594$  eV. Bulk effective masses of InAs and GaAs are  $m_{0,1}^* = 0.024 m_0$  and  $m_{0,2}^* = 0.067 m_0$ , respectively, where  $m_0$  is the free electron mass.  $V_s(\mathbf{r})$  is the effective potential simulating the strain effect [3]. The effective potential  $V_s(\mathbf{r})$  has an attractive character and acts inside the volume of the QD. The magnitude of the potential can be chosen to reproduce experimental data. For example, the magnitude of  $V_s$  for the conduction band chosen in [3] is 0.21 eV. This value was obtained to reproduce results of the 8-th band  $kp$ -calculations of Ref [5] for InAs/GaAs QD. The Ben-Daniel-Duke boundary conditions are used on the interface of the material of QD and substrate.

To describe tunneling of a single electron in double quantum object we have make some definition. Probability of localization of electron into region  $\Omega_\gamma$

( $\gamma=1, 2$ ) is defined by  $N_{n,\gamma} = \iint_{\Omega_\gamma} |\Phi_n(x, y)|^2 dx dy$ ,

where  $\Phi_n(x, y)$  is wave function of electron,  $n$  enumerates the states.  $\Omega_\gamma$  ( $\gamma=1, 2$ ) are area of QD (QR) shape (see Fig. 1) enumerated by  $\gamma$ . Let us define as tunneling measure parameter  $\sigma = \frac{N_{n,1} - N_{n,2}}{N_{n,1} + N_{n,2}}$ , with the range of  $[-1, 1]$ . Obviously, when  $\sigma = 0$ , the electron will be located in  $\Omega_1$  and  $\Omega_2$  with equal probability. The case  $|\sigma| \leq 1$  corresponds to the localization of the electron mainly in  $\Omega_1$  or  $\Omega_2$ .

### 3 CALCULATIONS

#### Identical quantum dots

Two dimensional InAs DQD with the radius  $R$  of each and inter-dot distance  $a$  embedded into GaAs substrate is considered. The single electron confinement spectrum of this DQD includes about 160 levels.

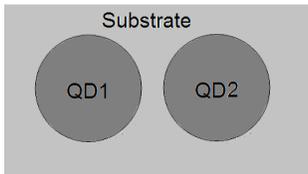


Figure 1. Two dimensional DQD. radius  $R$  is 40 nm; inter-dot distance is 10nm.

The inter-dot distance will be varying in this study. Visualization for the uniting tunneling is given in Fig. 2 where the parameter  $\sigma$  is presented along the energies of single electron spectrum in DQD for different inter-dot distances.

It is obvious that for enough large distances between the objects, electron is localized in one of the objects  $\sigma \approx 1$  ( $\sigma \approx -1$ ); when the distance decreases, the electron is tunneling so that its wave function is spread into the whole double system and  $\sigma \approx 0$ . The situation when all states have been tunneled appears for the inter-dot distances less than 10 nm. There are no tunneled states when  $a$  is larger than 40 nm. One can see that the obtained graph in Fig. 2 is symmetric relative the axis  $\sigma = 0$ . From Fig. 2 one can see that for each energy level (or very closed energy levels) there are four or two values of  $\sigma$ . There are quasi quadruplets or quasi doublets of the DQD spectrum. The spectrum has degeneracy order of two for each level when the QDs are independent. This degeneracy is due to the rotation symmetry of each (identical) QDs. Energy of the states can be approximated by the relation:  $E_{n,l} \sim \hbar/2m^*(n+|l|)$ , where  $n$  and  $l$  are radial and orbital quantum numbers. The state with  $l$  and  $-l$  are

degenerated. The states with  $\sigma$  between  $|\sigma|=1$  and  $\sigma \approx 0$  are tunneled states. There are quasi-doublets and quadruplets states in the electron spectrum. Examples of wave functions of such states is shown in Fig. 3.

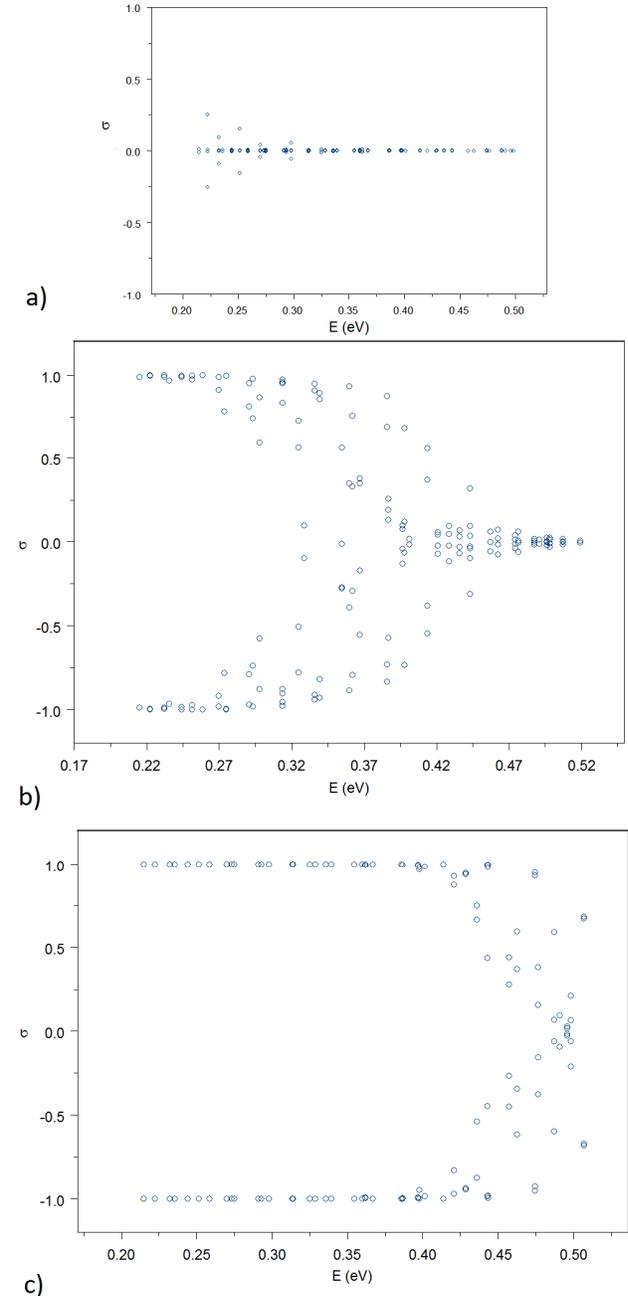


Figure 2.  $\sigma$ -parameter for 2D InGaAs/GaAs DQD along energy of the electron confined states: a) inter-dot distance  $a$  is 10 nm; b)  $a=20$  nm; c)  $a=30$  nm.

There is quasi quadruplet with energy about 0.487 eV. Note that the amplitude of the wave function can be different for left and right QDs. It means, particularly, that  $0 < |\sigma| < 1$  for these states.

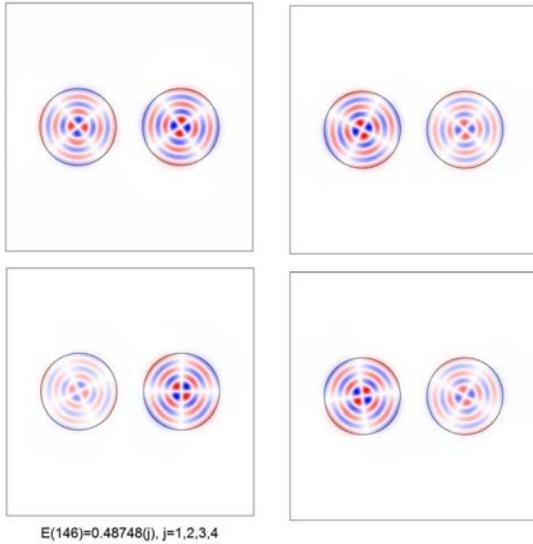


Figure 3. Countour plots of the wave functions of quasi-quadruplet in InAs/GaAs DQD.

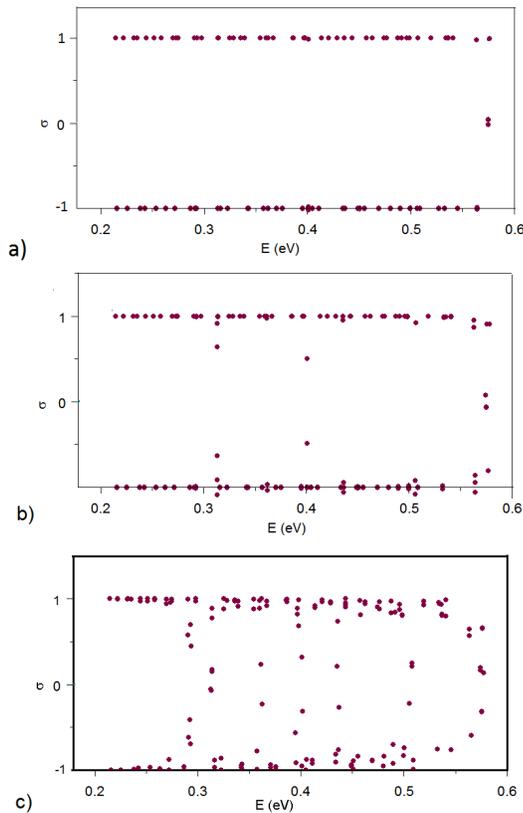


Figure 4.  $\sigma$ -parameter for 2D InGaAs/GaAs DQD along energy of the electron confined states: a) inter-dot distance  $a$  is 10 nm; b)  $a = 6$  nm; c)  $a = 2$  nm.

When the inter-dot distance decreases from the maximal distance (no electron tunneling) the tunneling happens through the higher electron levels of the spectrum, sequentially. At the minimal distances all electron states are

tunneled states. It occurs for the case of identical QDs in DQD.

### Non-identical quantum dots

If DQD includes two non-identical quantum dots with the radius  $R_1$  and  $R_2$  then the type of the tunneling changes. In Fig. 4 the results of the calculations for DQD with  $R_1 = 40$  nm and  $R_2 = 35$  nm are presented for different values of the inter-dot distance  $a$ : when  $a$  is large (about 10 nm) the tunneling occurs for few-levels, decreasing distance leads to increasing of the tunneling. In opposite to the “identical dots” tunneling, when tunneled spectrum is consequently going from upper edge of the potential well, the “non-identical dots” tunneling has discontinuous character and may begin from the region which is relatively far from upper edge of the potential well. The last tunneling proceeds through the levels having the same type of symmetry (rotation symmetry in this case) by anti-crossing. In the spectra of the non-identical QDs such states are placed irregularly due to the difference of the both spectra ( $R_1 \neq R_2$ ). Important difference of the tunneling in non-identical QD system is shortest distance for which the tunneling occurred: 10-40 nm for identical QDs, and 0-10 nm for non-identical QDs.

### Chaotic DQD

It is interesting to consider DQD including two identical quantum dots with asymmetrical shapes (see Fig. 5), which leads to chaotic properties of the electron spectrum [7] for the single QR. Again we study the effects related to the inter-dot distance  $a$



Figure 5. Double quantum dot with chaotic shape.

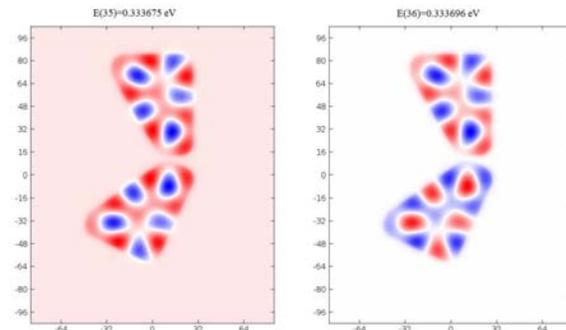


Figure 6. Countour plots of the quasi-doublet wave functions in the chaotic InAs/GaAs DQD: (left) symmetric; (right) anti-symmetric. The sizes are given in nm. The angle of the rotation  $\vartheta$  for lower QD is  $\sim 25$  deg.

The chaos may be related to the behavior of the energy splitting between the quasi-doublet [6]. We calculate the energy of quasi-doublet splitting as a function of inter-dot distance in DQD. The results of this calculation are presented in Fig. 6 and 7. In Fig. 6 the wave functions of the quasi-doublet are shown for case when the lower QD has been rotated relatively to upper QD for the angle  $\vartheta$ . This non zero  $\vartheta$  makes the system as chaotic one.

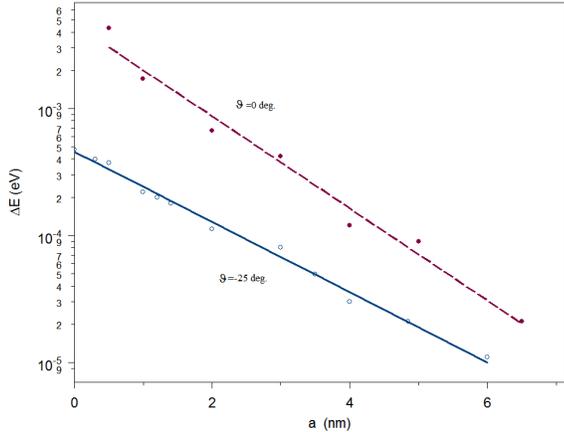


Figure 7. Energy of quasi-doublet splitting as a function of inter-dot distance in DQD (see Fig. 3) for different angle of the rotation for the bottom QD.

The dependence of the energy splitting on inter-dot distance is logarithmical. The same dependence we have for regular DQD with identical QDs. The chaos has no influence on this dependence.

### Double quantum ring complex

For InAs DQR complex (having weak chaotic properties due to a shift of the centers of the inner and outer circles) that includes two identical quantum rings located laterally, one can find a mixed type of the electron tunneling.



Figure 8. DQR complex.

Energy of a single electron in QR is defined by the following relation:

$$E_{n,l} \sim \hbar / 2m * (n^2 / W^2 + l^2 / R^2), W \ll R, \quad \text{where}$$

$W$  is the width of the QR, the single electron levels in QR separated by the bands  $n=1,2,3,\dots$ , with in-band states with  $|l|=0,1,2,\dots$ . Because  $W < R$  the density function of the electron energy spectrum has local maximum when each band  $n=1,2,3,\dots$  is started and the orbital momentum  $l$  is

decreasing  $|l|=0,1,2,\dots$  (see Fig. 9). That allows us to separate the bands corresponding to different  $n$  as it is shown in Fig. 9.

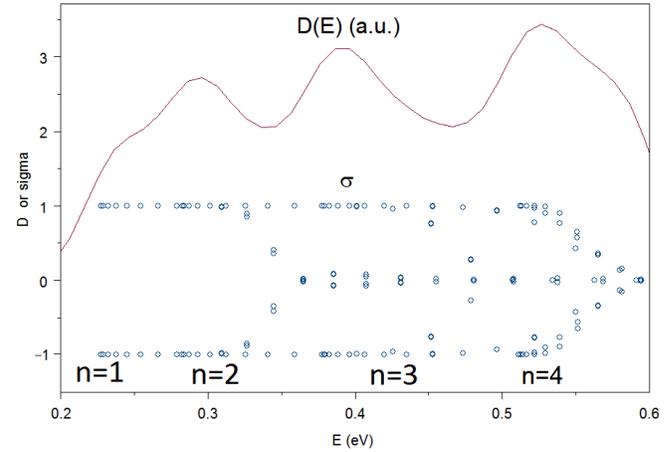


Figure 9.  $\sigma$ -parameter for 2D InGaAs/GaAs DQR along energy of the electron confined states (open circles). Density of the states  $D(E)$  is shown by solid line.

## 4 CONCLUSION

Concluding, we say that there are two types of dynamical tunneling in nano-sized double quantum objects. The first is related to tunneling in the system of two identical QDs; the second one occurs in double system of non-identical QDs or DQR. The tunneling is going through the levels having the same type of symmetry. The violation of symmetry of DQD (DQR) shape geometry creates difficulties for tunneling. Choosing the “chaotic” shape for DQD does not change the type of the tunneling and, in particular, does not lead to the enhancing of the tunneling.

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