Tunneling Rate in Chaotic Quantum System

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ABSTRACT

We study spectrum properties of electron tunneling in isolated double quantum wells (DQWs) in relation to the geometry variations of the DQW shapes. The tunneling rate in DQW with chaotic and regular geometry was considered. The calculations presented do not support the recent proposed assumption about the regularization of the tunneling rate when the QW geometry in DQW is chaotic. We confirm the strong influence of the geometry of QW boundaries on the fluctuation of tunneling rate along the electron spectrum.

Keywords: quantum dots and wells, single electron states, tunneling, chaotic quantum billiards

1 INTRODUCTION

Relation between chaotic properties of the quantum objects and electron tunneling is considered to be important from technological point of view [1]. Semiconductor heterostructures such as quantum wells (QWs), quantum dots (QDs), and quantum rings (QRs) demonstrate atom-like structure of the electron spectrum, including several hundreds of confinement electron levels. In the case of a double quantum system, a single electron spectrum is composed of a set of symmetric and anti-symmetric state pairs (quasi-doublets). Energy splitting between members of the quasi-doublet is considered as the tunneling rate. We study electron spectra and electron tunneling in such quantum systems. In particular we compare the tunneling in double quantum well (DQW) with chaotic and regular geometry of the QW shapes, taking into account recently published results Ref. [2] as an evidence of a regularization of the tunneling rate for DQW with chaotic geometry. The regularization is interpreted as a characteristic of the tunneling rate taken along the total spectrum. Presented calculations do not support this explanation. However we confirm a strong influence of the QW geometry boundaries on the tunneling rate. A small violation of the symmetry drastically affects tunneling (see also [3]). The systems with finite confinement are considered as well as InAs/GaAs DQWs. We visualize a features of the tunneling rate occurring in such DQW. Correlation between electron localization in the barrier between QWs and quasi-doublet splitting for electron spectrum is studied. The factors of the effective mass anisotropy is also considered for Si/SiO_2 DQW.

2 QUANTUM BILLIARDS

We consider the two-dimensional double quantum wells (DQW) proposed in Ref. [2]. The wells in the DQW are separated by finite potential barrier which forms interior boundaries, since the exterior boundaries are infinite walls (like it is for the quantum billiard (QB)). The problem is mathematically formulated by the Schrödinger equation in two dimensions:

$$(\hat{H}+V_c)\Psi(r)=E\Psi(r). \qquad (1)$$

Here $\hat{H}$ is the single band Hamiltonian operator $\hat{H}=-\nabla\frac{\hbar^2}{2\mathrm{m}}\nabla$, m is the electron effective mass, and $V_c(r)$ is the confinement potential. $V_c(r)=0$ inside of the QWs, and is equal to V_c inside in the barrier. We use here definition $\hbar^2/2m=1$. The geometry of the considered DQW are shown in insets of the Fig. 1. The shape of each QWs corresponds to quantum billiard having regular (rectangular, triangle, semi-circle) or chaotic behavior (semi-circle with cut) (see for instance [3]. Results of the calculations are presented in Fig. 1. Evaluation of quasi-doublet energy splitting ΔE is performed using the following relation:

$$\Delta E \sim \int \Psi^{s_L}(x,y)V_c(x,y)\Psi^{s_R}(x,y)dxdy. \qquad (2)$$

Here $\Psi^{s_L}(x,y)$ ($\Psi^{s_R}(x,y)$) is normalized wave function of the “single left” (“single right”) QW. The consideration for one dimensional case can be found in [4]. The result of the integration depends on overlapping of the wave functions. The parameters that define this overlapping are the distance between QWs and spreading of the single wave function outside of the QW shape region, which depends on the energy of the levels, due to the asymptotic behavior of the wave function of confinement states. We write the asymptotics as follows:

$$\Psi^{s_R}(x,y) \sim A exp\left(-b\sqrt{(E_c-E)}x\right), \qquad (3)$$

where x is distance from a QW boundary, A and b are constants (or may weakly depend on y coordinate), E_c is the threshold of the continuous spectrum. It can be assumed that the value of logarithm of the tunneling rate $ln(\Delta E)$ depends on the energy as a linear function of $\sqrt{E}$. The appropriate value for evaluation of the integral (2) is the probability S to find an electron inside the barrier. The value of S is defined by contribution of "tails" of the wave functions outside QWs shape. Thus, the value $ln(S)$ depends on $\sqrt{E}$ linearly. This relation is approximately satisfied for levels which are far from bottom of the quantum well (see figures below). For the low-lying levels, the ΔE and S decrease with decreasing energy faster. Spectrum of "regular" DQW may be classified by "good" quantum numbers. For the geometry Fig. 1a) the energy is given by the relation: $E_{m,n} \sim (\hbar^2/2\mathrm{m})(n^2/L_y^2 + m^2/L_x^2)$. For the geometry Fig. 1c) the energy is given by the relation: $E_{n,l} \sim (\hbar^2/2\mathrm{m})(n+|l|)$, where n and l are radial and orbital quantum numbers. The difference of these cases ensures the difference for the behavior of the tunneling rate with the geometry 1a) and 1c) presented in Fig. 1. When we change geometry to use "chaotic" geometry for QW we have different energy dependence. There is more complicate dependence due to existing no "good" quantum numbers for the geometry. The calculations presented in Fig. 1 do not support recently proposed assumption [2] about regularization of the tunneling rate when the QW geometry in DQW is chaotic.

Based on Fig. 1c)-d) and Fig. 2 one may see that the tunneling rates is correlated with the probability of the particle being at the barrier. It is not surprising, due to relation (2), the energy splitting is defined by overlapping of the basic functions. This overlapping is mostly in the barrier that establishes such correlation of this probability with the energy splitting.

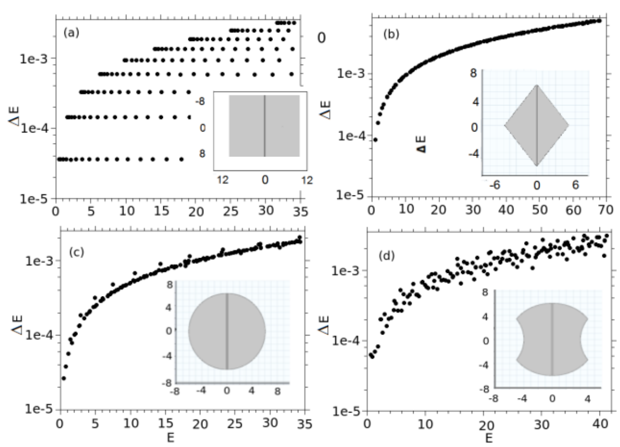

Figure 1. Tunneling rates ΔE vs. energies E of electron confinement states for different shaped DQWs: (a) rectangular, (b) triangle, (c) semi-circle, (d) semi-circle with cuts. Insets show corresponding DQW. All values are given in arbitrary units.

We varied the QW geometry to be chaotic one. Left-Right symmetry of DQW is violated by asymmetric cut as is shown in Fig. 3.

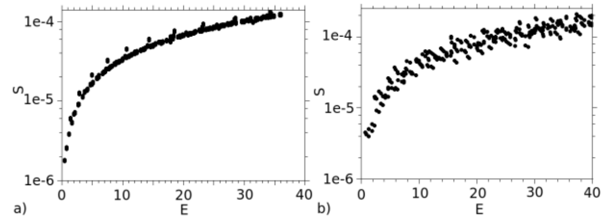

Figure 2. The probability S of the particle being at the barrier. a) The spherical shaped DQW. b) The spherical shaped DQW with cuts.

Tunneling rates ΔE calculated for chaotic geometry and regular geometry (presented in Fig. 3) differ and one can conclude that a regularization of the rate takes a place when we change the chaotic geometry to regular one.

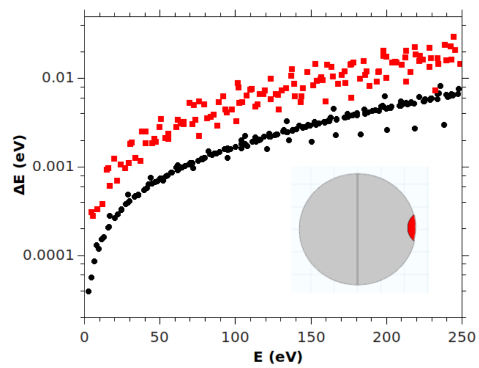

Figure 3. Tunneling rate ΔE in a spherical shape quantum billiard (black circles) with asymmetric cut (red rectangles). The shape is shown in the inset. The cut is colored by red.

3 INAS/GAAS DQW

We consider the InAs/GaAs QWs as an example of nano sized hetero-structures related to the considered above quantum billiards (QB). The effects occurred in QB may be found in such QWs. Note that the InAs/GaAs structures are well studied and have technological implementation. 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. We add extra potential on the left hand side of the Eq. (1) to simulate the strain effect [5]. The effective potential V_s has an attractive character and acts inside the QWs. The magnitude of the potential can be chosen to reproduce experimental data for the InAs/GaAs quantum dots. The magnitude of V_s for the conduction band chosen in [6] is 0.21 eV. The Ben-Daniel-Duke boundary conditions are used on the interface of the material of QW and substrate.

All sizes of the DQW shown in Fig. 1c) were increased by 9 times. The results of calculation for the tunneling rate are presented in Fig. 4.

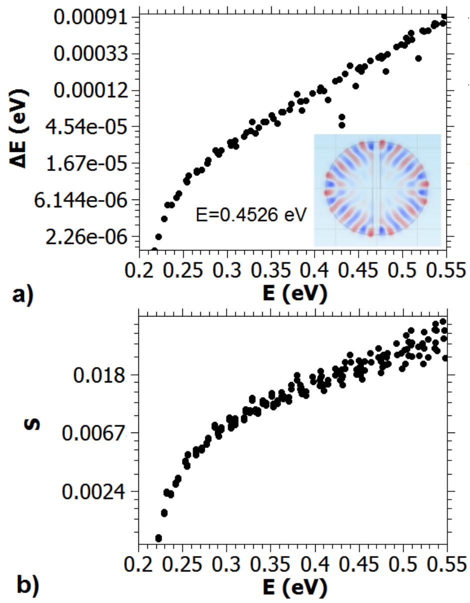

Figure 4. Tunneling rates ΔE (a) and probability S (b) of the InAs/GaAs DQW semi-circle shaped, a=9nm. Inset: The single electron wave function having mixing symmetry ("n=1" and "n=2").

This calculation demonstrates similar behavior which we see for QB above. The logarithmical dependence of tunneling rate for high-lying level is seen. The correlation between ΔE and S is well established. The new moment is existing levels with mixing of symmetry (shown in inset of Fig.4). This takes a place due to finite confinement in the InAs/GaAs hetero structure, when the energy spacing between levels become comparable with the quasi-doublet spacing and the level anti-crossing is possible.

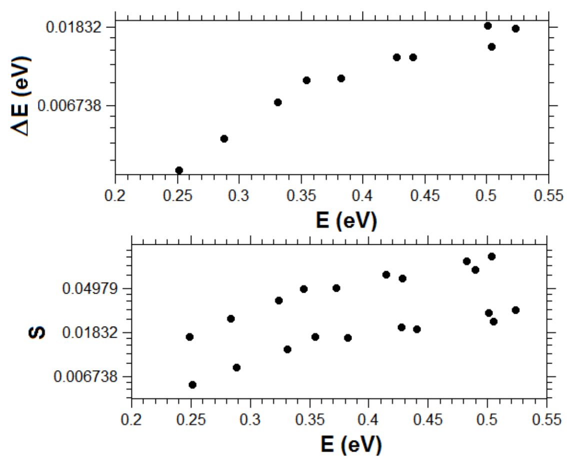

Figure 5. The semi-circle shape InAs/GaAs DQW (see Fig. 1c). Tunneling rate ΔE, probability S of the particle being on the barrier.

We decreased size of last DQW by 3 times to see the atom-like property of the hetero-structure. The results of the calculation are shown in Fig. 5. The probability S is split to two values for each quasi-doublet. The effect is known as the bounding and anti-bounding orbital effect in molecular physics [7]. The correlation between ΔE and S is clearly seen for this case.

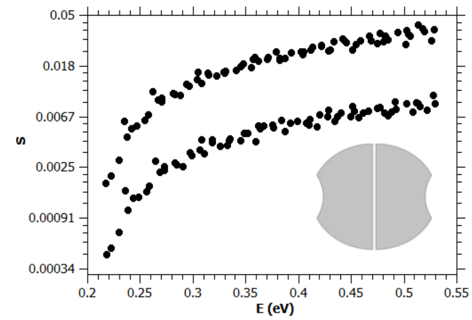

Figure 6. The semi-circle shaped InAs/GaAs DQW with symmetrical cuts.

In Fig. 6 we show calculated values of S for the semi-circle shape InAs/GaAs DQW with cuts (see inset). The shape size corresponds to the DQW shown in Fig. 1d) increased by 9 times. The geometry of each QW in DQW is chaotic, however the symmetry of the shape of whole system is not violated. We see that this does not affect the behavior of S, comparing with the regular shaped DQW, considered above.

We have seen for QB that the symmetry violation is the main factor which can de-regularize a tunneling rate. For the InAs/GaAs DQW, the results of calculation for the parameter S in the case of violation of shape symmetry are presented in Fig. 7. To describe localization of a single electron in this double quantum object we make some definition [8]. Probability of localization of electron in the region Ω_γ (γ=1, 2), related to the QW area is $N_\gamma = \iint_{\Omega_\gamma} |\Psi(x,y)|^2\, dxdy$, where $\Psi(x,y)$ is wave function of electron, and n numerates the states. We define tunneling measure parameter $\sigma = (N_1 - N_2)/(N_1 + N_2)$, with the range of [-1,1]. Obviously, when $\sigma = 0$, the electron will be located in left QW and right QW with equal probability (delocalized state). In the case $|\sigma| \leq 1$, electron is located in the left QW and the right QW simultaneously with different probability. Considering along the electron spectrum, σ-parameter demonstrates mirror symmetric location relative to the $\sigma = 0$ axis that reflects the quasi-doublet structure of the spectrum. For identical QWs in DQW, the electron is localized in one of the objects and $|\sigma| = 1$, when distance between the objects is large enough. The electron is tunneling, so that its wave function is spread over the whole double system and $|\sigma| \approx 0$, when the distance decreases.

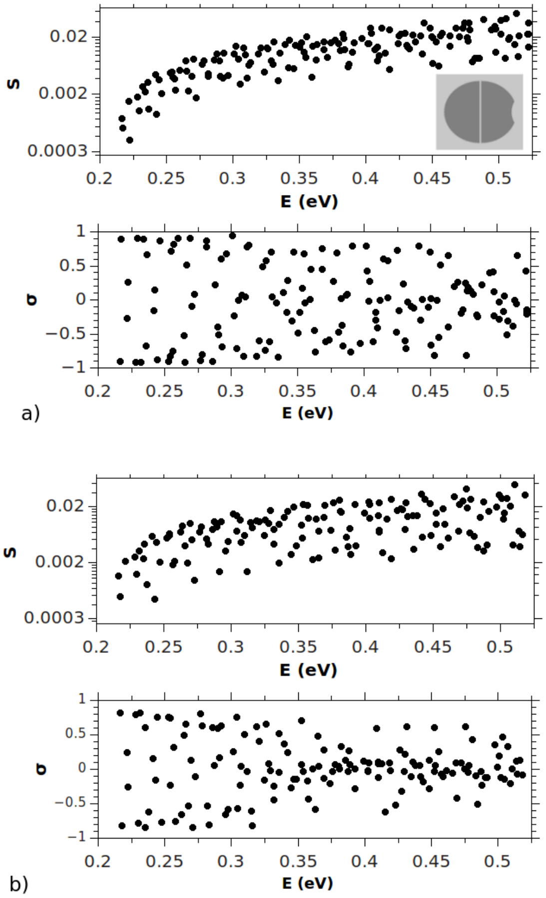

Figure 7. Parameters S and σ for semi-spherical shaped InAs/GaAs QW with asymmetric cut. The DQW shape is shown in the inset. Distance between QWs is a) a =1.8 nm and b) a =1.4 nm

Distance between QWs is changed in these calculations. We detect the effect of violation of the symmetry: the regular behavior of S as a function of confined energy is broken (see Fig. 4 and 6), an electron localization is randomly changed along spectrum.

4 SI/SIO$_2$ DQW AND MASS ANISOTROPY

In this section we consider another factor which may affect tunneling rate. The effective electron mass in the Si/SiO$_2$ DQWs has strong anisotropy $m_{Si,\perp}/m_{Si||} < 1$. Based on the model for the Si/SiO$_2$ QD proposed in [9, 10] we compare tunneling rate for two variants of the DQW geometry. The first one is the regular geometry (Fig. 1c) and the second one is the "chaotic" geometry (Fig. 1d). The band gap potential for the conduction band is V_c =3.276 eV. Bulk effective masses of Si and SiO$_2$ are m_{Si} =($m_{Si,\perp}$ =0.19 m_0 , $m_{Si||}$ =0.91 m_0) and m_{SiO_2} =1.0 m_0 respectively. We assumed that, in the QWs, the effective mass m_{Si} is equal $m_{Si,\perp}$ along x-direction and $m_{Si} = m_{Si||}$ -along y-direction.

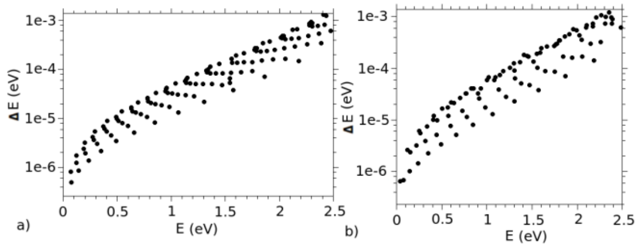

Figure 8. Tunneling rates for the Si/SiO$_2$ DQWs. a) semi-circle shaped, b) semi-circle shaped with cuts. The DQD shape geometry is shown in Fig. 1 c-d) (sizes are in nm). The distance between QWs is 1 nm.

The results are presented in Fig. 8. One can conclude that the mass anisotropy effect for the tunneling rate may be strong and is comparable with the considered DQD geometry variations.

5 CONCLUSION

We studied spectrum properties of electron tunneling in double quantum wells. We found that regularization of the tunneling rate is generally possible when the geometry is changed from chaotic (asymmetric) to regular (symmetric) one. We confirmed strong influence of geometry QW boundaries on the fluctuation of the rate along the electron spectrum. We have shown that the probability S of the particle being in the barrier may be a useful addition to ΔE in theoretical analysis of tunneling in chaotic quantum systems

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