Sensors & Transducers

Tunneling Rate in Double Quantum Wells

* **Igor FILIKHIN, Sergei MATINYAN, Branislav VLAHOVIC**
North Carolina Central University, 1801 Fayetteville Str., Durham, NC 27707, USA,
Tel.: 919 530 6645, fax: 9195207252
* E-mail: ifilikhin@nccu.edu

Received: 16 October 2014 /Accepted: 28 November 2014 /Published: 31 December 2014

Abstract: We study spectral properties of electron tunneling in isolated double quantum wells (DQWs) in relation to the geometry variations of the double quantum well shapes. The tunneling rates in the double quantum wells for whole spectrum of confined electron states are calculated. The effect of the regularization of the tunneling rate along spectrum is searched by transformation of the geometry of quantum well in double quantum well from "regular" one to "chaotic" one. The cases of quantum billiards (infinite confinement) and InAs/GaAs quantum wells (finite confinement) are compared. The calculations presented do not generally support the recent proposed assumption about such effect. We show the strong influence of the geometry of quantum well boundaries on variations of tunneling rate along spectrum. *Copyright © 2014 IFSA Publishing, S. L.*

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 confined 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 interpreted 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 of Ref. [2] as an evidence of a regularization of the tunneling rate for DQW with chaotic geometry of QWs. 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 [3]. The systems with finite confinement are considered as well as InAs/GaAs QWs. We visualize features of the tunneling rate occurring in such DQW. Correlation between electron localization in the barrier between QWs and quasi-doublet energy splitting is studied. The factors of the effective mass anisotropy are 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

 http://www.sensorsportal.com/HTML/DIGEST/P_2551.htm

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:

$$(\hat{H} + V_c)\Psi(r) = E\Psi(r), \quad (1)$$

where $\hat{H}$ is the single band Hamiltonian operator $\hat{H} = -\nabla \frac{\hbar^2}{2m} \nabla$, 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 put here $\hbar^2 / 2m = 1$. The geometries of the considered DQW are shown in insets of the Fig. 1.

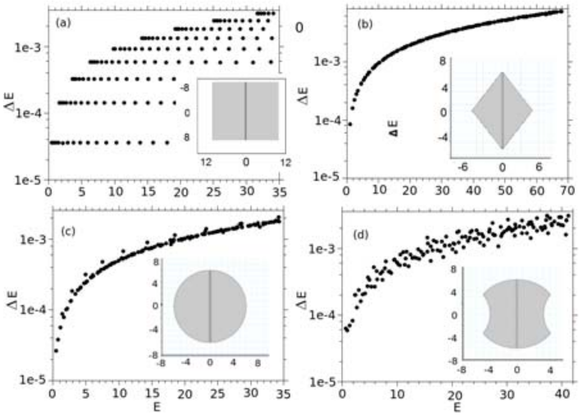

Fig. 1. Tunneling rates ΔE vs. energies E of electron confinement states for different shapes of DQWs: (a) rectangular, (b) triangle, (c) semi-circle, (d) semi-circle with cuts. Insets show corresponding DQW. All values are given in arbitrary units.

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]. The double billiard is represented as a two level quantum system. The consideration for such system can be found in [4] for one dimensional case. The electron spectrum is formed by a set of quasi-doublets. Evaluation of quasi-doublet energy splitting ΔE is performed using the following relation:

$$\Delta E \sim \int \Psi^{SL}(x,y) V_c(x,y) \Psi^{SR}(x,y) dxdy, \quad (2)$$

where $\Psi^{SL}(x,y)$ ($\Psi^{SR}(x,y)$) is the normalized wave function of the “single left” (“single right”) QW. The result of the integration depends on overlapping of the wave functions. Results of our calculations of ΔE are presented in Fig. 1 for each level of the spectrum.

The parameters that define this overlapping (2) 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 confined states. We write the asymptotic as follows:

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

where x is the distance from a QW boundary, A and b are the 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, ΔE and *S* decrease with decreasing energy faster. Spectrum of "regular" DQW may be classified by "good" quantum numbers. For the geometry Fig. 1(a) the energy is given by the relation: $E_{m,n} \sim (\hbar^2 / 2m)(n^2 / L_y^2 + m^2 / L_x^2)$ with quantum numbers $|n|$, $|m|$=1, 2 ..., L_x, L_y define size of rectangular shaped QW. For the geometry Fig. 1(c) the energy is given by the relation: $E_{n,l} \sim (\hbar^2 / 2m)(n + |l|)$, 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 1(a) and 1(c) 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 such 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. One can set the transformations of the initial geometry (a) to geometry (b) and to (c) which do not violate “regular” geometry and which “regularize” of the initial tunneling rate (a).

Based on Fig. 1(c) - Fig. 1(d) and Fig. 2 one may see that the tunneling rates are correlated with the probability of the particle being at the barrier. It is not surprising due to relation (2), that 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.

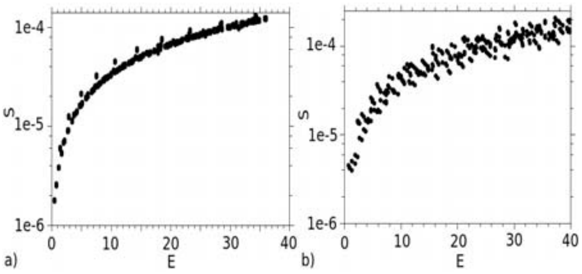

Fig. 2. The probability S of the particle being at the barrier. a) The spherical shaped DQW. b) The spherical shaped DQW with cuts.

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.

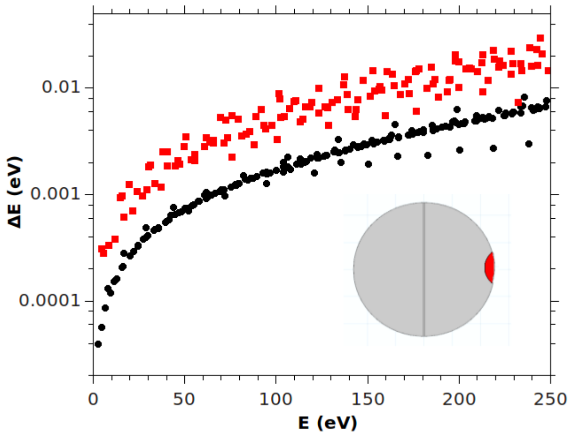

Fig. 3. Tunneling rate ΔE in a spherical shape quantum billiard (black circles) with asymmetric cut (red rectangles). The shape is shown in the inset. The cut is colored by red.

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.

3. InAs/GaAs Quantum Wells

Here, 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. 1(c) were increased by 9 times. The results of calculation for the tunneling rate are presented in Fig. 3 and Fig. 4 for rectangular and semi-circle shapes of QWs.

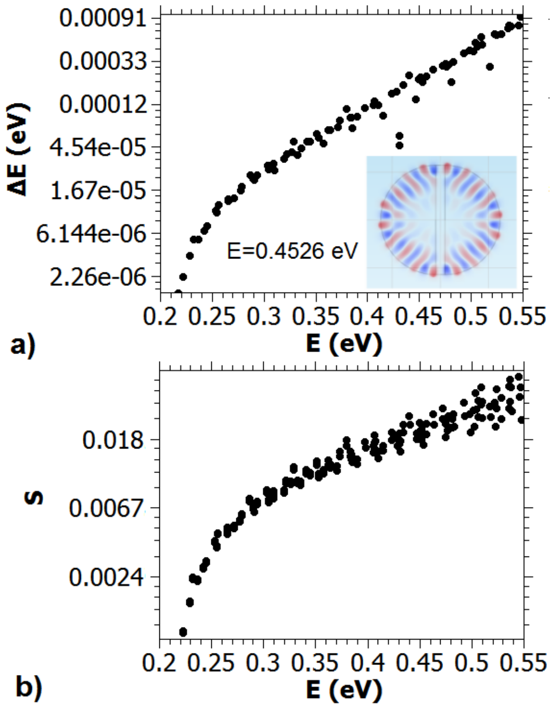

Fig. 4. Tunneling rates ΔE (a) and probability S (b) of the InAs/GaAs DQW semi-circle shaped, a=9 nm. Inset: The single electron wave function having mixing symmetry (“n =1” and “n =2”).

This calculation demonstrates behavior similar to what 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.

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.

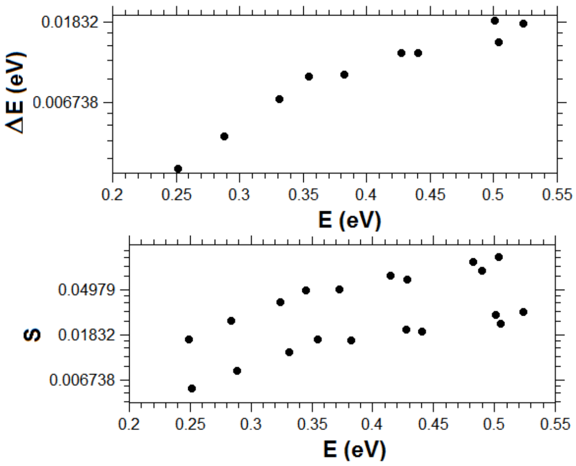

Fig. 5. The semi-circle shape InAs/GaAs DQW (see Fig. 1(c)). Tunneling rate ΔE , probability S of the particle being on the barrier.

In Fig. 6(a), the probability S is shown for rectangular shape of QWs. The results are close to one obtained for the quantum billiard (see Fig. 1). The large values of variations of funneling rate along the spectrum are obvious due to strong quantum number dependence. For symmetric cuts of each QW shown in inset of Fig. 6(b), the QW geometry becomes to chaotic one. However, the symmetry of the DQW geometry is kept. In the limits of strong coupling of QWs, chaotic properties of individual QW are disappeared in the DQW [3]. The visible "regularization of tunneling rate", which is demonstrated in Fig. 6(b), is attributed by geometry change (boundaries) most likely that the chaotic 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 Fig. 6), electron localization is randomly changed along spectrum. geometry of QWs.

In Fig. 7 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. 1(d) 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, in comparison with the regular shape of DQW, considered above.

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 normalized wave function of electron.

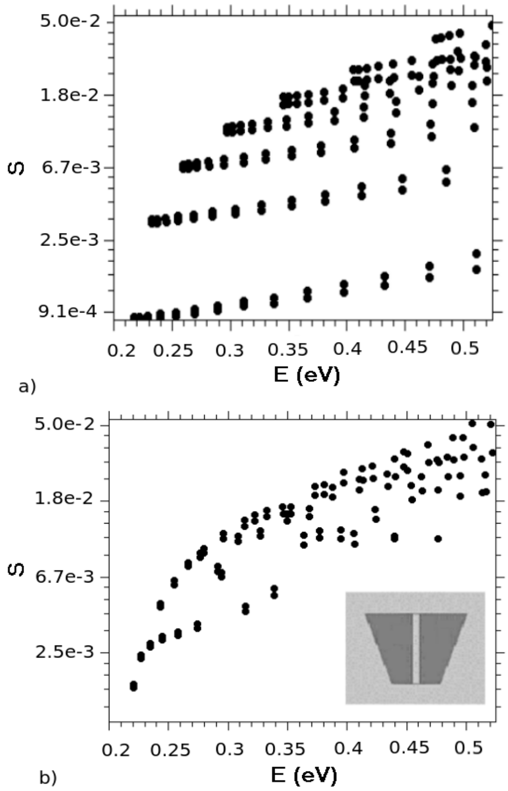

Fig. 6. The probability S of the InAs/GaAs DQW a) rectangular shaped (see Fig. 1), b) rectangular shaped with symmetric cuts. Here inter-dot distance is a=8 nm. Inset: the shape of DQW is shown.

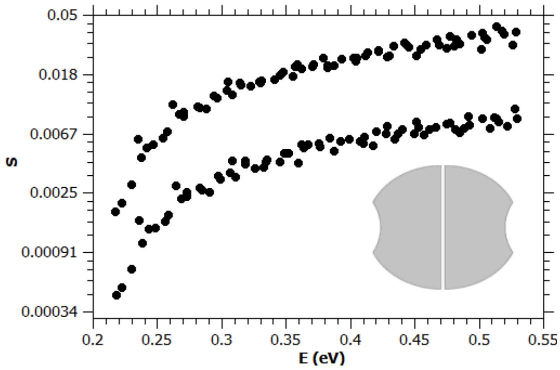

Fig. 7. The semi-circle shaped InAs/GaAs DQW with symmetrical cuts.

We define tunneling measure parameter

$$\sigma = (N_1 - N_2)/(N_1 + N_2), \tag{4}$$

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. In total 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.

The parameter σ is sensitive to the small geometry variations [8] violated reflexion symmetry of DQW. In Fig. 8, we present the results of calculations of the σ-parameter and the probability S for different geometries of the semi-circle shaped DQW with cuts (see Fig. 1(d)). The QWs in DQW are non-identical due to the ratio of the radii of the left and right cuts are R_{Left}/R_{Rigth} =5.99/6.0. In opposite to DQW with identical QWs and the same inter-dot distance, the spectrum of the asymmetric shape DQW includes mainly localized state. It is seen by σ-parameter in Fig. 8(a). Only few states in upper part of the spectrum are delocalized state. Decreasing of the inter-dot distance a returns the situation when all states are delocalized as shown in Fig. 7 (b) – Fig. 7 (c). One can conclude that the small violations of DQW shape symmetry affect the localized- delocalized states of the spectrum. The behavior of the tunneling rate along the spectrum is not essentially changed.

Also we can conclude from Fig. 7, that the coupling between quasi-doublet for weak and strong cases may be indicated by the difference of splitting of the probability S corresponding to states of quasi-doublets with "symmetric" and "anti-symmetric" wave functions.

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 calculations for S and the parameter σ in the case of strong violation of shape symmetry are presented in Fig. 9.

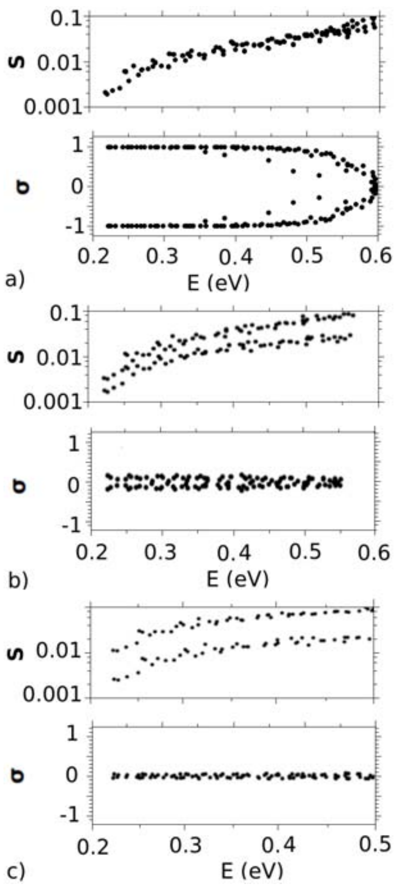

Fig. 8. Parameters S and σ for semi-circle DQW shaped with cuts (sizes of Fig. 1(d) scaled by $\times N$ factor) in cases of different inter-dot distances a) a=10.8 nm (x9) b) a=9.8 nm (x8), c) a=2.4 nm (x8). The ratio of the radii of the cuts is equal 5.99/6.0.

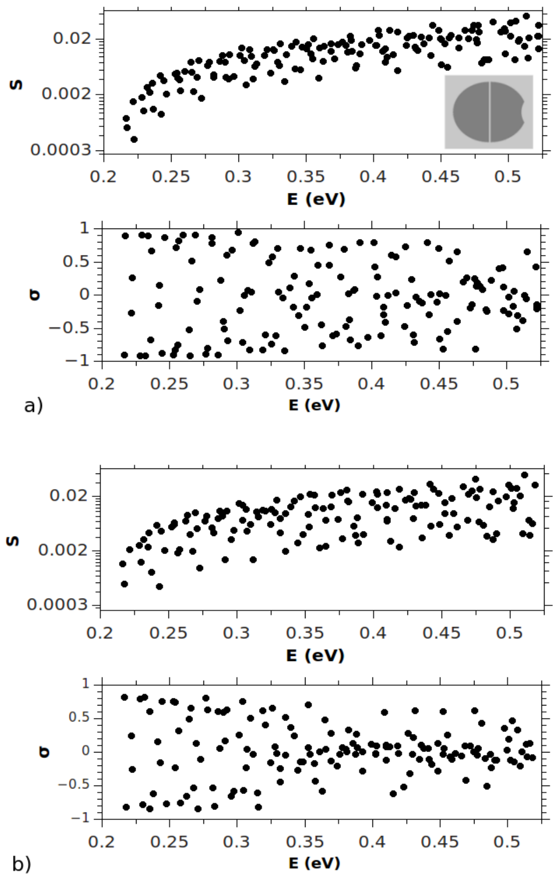

Fig. 9. Parameters S and σ for semi-spherical shaped InAs/GaAs QW with asymmetric cut. The DQW shape is shown in the inset. Distance between QWs is a) a =1.8 nm and b) a =1.4 nm.

The parameters S and corresponding tunneling rate (see also Fig. 3) demonstrate non-regular character along the spectrum with large and small deviations comparing with one for symmetric DWQ shown in Fig. 4, Fig. 7, Fig. 8. One can conclude that this behavior may be motivated by the irregular distribution of the localized-delocalized states in the spectrum (that is indicated by σ-parameters).

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. 1(c)) and the second one is the "chaotic" geometry (Fig. 1(d)). 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.

The results are presented in Fig. 10. One can conclude that the mass anisotropy effect for the tunneling rate deviation in the spectrum may be strong and is comparable with the considered DQD geometry variations. Weak asymmetry of DQW (see also Fig. 8) affects the distribution of the localized-delocalized states of the spectrum. The low-lying states become localized, mainly. Corresponding tunneling rate of the lower part of the spectrum demonstrate larger deviation than the upper part of the spectrum including many the delocalized states as is show in Fig. 11. The effect of the spreading is not large on background the dependence of the tunneling rate on quantum numbers and the mass anisotropy.

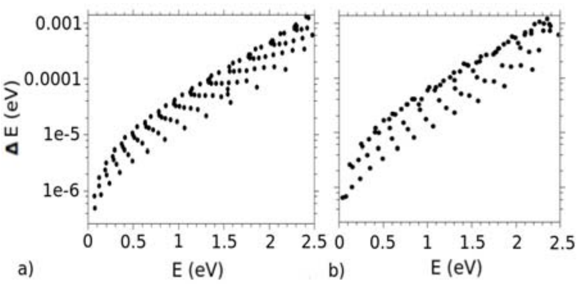

Fig. 10. Tunneling rates for the Si/SiO_2 DQWs. a) semi-circle shaped, b) semi-circle shaped with cuts. The DQD shape geometry is shown in Fig. 1 c-d) (sizes are in nm). The distance between QWs is 1 nm.

7. Conclusions

We studied spectral 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 of QW boundaries on the deviations of the rate along electron spectrum. We have shown that the probability S of the particle being in the barrier may be a useful addition to the tunneling rate ΔE in theoretical analysis of tunneling in chaotic quantum systems.

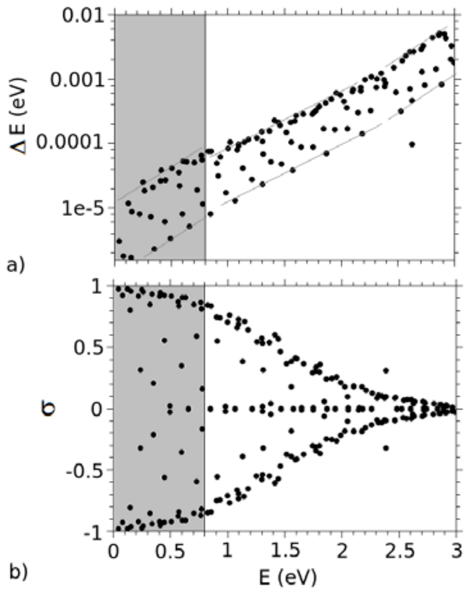

Fig. 11. Tunneling rate and parameters σ for Si/SiO_2 DQW with semi-circle shapes and asymmetric cuts. The part of the spectrum where the states are strong localized in one QW or another QW is marked by gray color accent.

Acknowledgements

This work is supported by the NSF (HRD-1345219) and NASA (NNX09AV07A).

References

[1]. L. A. Ponomarenko, *at al.*, Chaotic Dirac Billiard in Graphene Quantum Dots, *Science*, Vol. 320, No. 5874, 2008, pp. 356-358.

[2]. L. M. Pecora, H. Lee, D.-Ho Wu, Th. Antonsen, M.-Jer Lee, E. Ott, Chaos regularization of quantum tunneling rates, *Physical Review E*, Vol. 83, 2011, pp. 065201(R)- 065204(R).

[3]. I. Filikhin, S. G. Matinyan, B. Vlahovic, Disappearance of quantum chaos in coupled chaotic quantum dots, *Physics Letters A*, Vol. 375, 2011, pp. 620-623.

[4]. G. Bastard, Wave Mechanics Applied to Semiconductor Heterostructures, *Halsted Press*, 1988.

[5]. I. Filikhin, V. M. Suslov, B. Vlahovic, Modeling of InAs⁄GaAs quantum ring capacitance spectroscopy in the non-parabolic approximation, *Physical Review B,* Vol. 73, 2006, pp. 205332-205334.

[6]. I. Filikhin, V. M. Suslov, M. Wu, B. Vlahovic, InGaAs/GaAs quantum dots within an effective approach, *Physica E,* Vol. 41, 2009, pp. 1358-1363.

[7]. P. W. Atkins, Atkins Physical Chemistry, 7th ed., *Oxford*, 2002.

[8]. I. Filikhin, S. G. Matinyan, B. Vlahovic, Electron tunneling in double quantum dots and rings, *Journal*

of Physics: Conference Series, Vol. 393, 2012, pp. 012012-012014; I. Filikhin, S. Matinyan, B. Vlahovic, Electron Spectrum, Localization and Tunneling in Double Nanoscale Structures, *Mathematical Modelling and Geometry*, Vol. 2, No. 2, 2014, pp. 1-18.

[9]. A. S. Moskalenko, J. Berakdar, A. A. Prokofiev, I. N. Yassievich, Single-particle states in spherical Si/SiO_2 quantum dots, *Physical Review B*, Vol. 76, 2007, pp. 085427-085429.

[10]. I. Filikhin, S. Matinyan, B. K. Schmid, B. Vlahovic, Electronic and level statistics properties of Si/SiO_2 quantum dots, *Physica E,* Vol. 42, 2010, pp. 1979-1983.
