Energy levels and chaos

CREST Research Project 1: Computer modeling and design and formation and characterization of novel nanostructured materials and nanodevices;

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Dimensions in Meso- and Nanoworld

At 1980-ies: **Bulk** Semiconductor --- Quantum **Wells** (QW) (D = 2) --- Quantum **Wires** (D -1 = 1) --- Quantum **Dots** (QD) --- atom:

Localization in ALL 3D
Breakdown of usual band structure (Bloch picture)
Dimensions in Meso- and Nanoworld

QD is "atom in the cage"

Dimension in this world

\[ D = 3 \] - numbers of confined dimensions
QD not a point: rich picture of eigenvalues statistics and forms (wave-functions)

\[ \frac{l}{a} \ll 1 : \text{QD 3D object} \quad (l \text{ - mean free pass or de Broglie wave length, what is shorter, a size of QD.}) \]

\[ l_B = \frac{1.22}{(\sqrt{E_{k,n}} \text{ (eV)})} = \frac{h}{(3m^*kT)^{1/2}} \]
E kinetic energy of carrier, \( m^* < m \)

\[ \frac{l}{a} \geq 1 : \text{coherence regime, effective } D = 0, \text{ few, even one carrier.} \]

L. Keldysh (1962) first considered \( l \gg a \rightarrow \text{mini-zones} \& \text{negative resistance} \)

Minimal size of QD \( a_{\text{min}} = \pi h / \sqrt{2m^* \Delta E} \approx 4 \text{nm} \) - existence of at least one level
Maximal size: carriers still confined in all 3D. \( a_{\text{max}} = 20 \text{nm}, T = 300 \text{ K} \)
Low T is important.
Quantum Chaos (QCh) - quantum manifestation of classical chaos

Mathematical basis of QCh – RMT

No trajectories —> energy levels, orbits —> wave functions (scars)

Level repulsion Wigner-Dyson type, scars, etc.

Regular, non-chaotic systems —> Poisson distribution of Nearest Neighbor Level Statistics (NNS)

Level Statistics (NNS)

Model of calculation energy levels of QD (on the example of Si/SiO₂; Ga As /AlₓGa₁₋ₓAs; InAs/GaAs. (I. Filikhin, SM, B.Vlahovic, Physica E42, 1979, 2010))
Statistics of electron level in Si QDs

The nearest neighbor spacing statistics

There are hundred levels

Energy levels

\[ E_i \quad i = 0, 1, \ldots, N \]

Spherical Si/SiO\(_2\) DQ (D=17 nm) N=245, M=9

Neighbor spacing

\[ \Delta E_i = E_i - E_{i-1} \quad i = 1, \ldots, N \]

Distribution function:

\[
R_j = N_j / H_{\Delta E} / N \quad j = 1, \ldots, M
\]

\[
H_{\Delta E} = ((\Delta E)_1 - (\Delta E)_N) / M
\]

\[
\sum N_j = N \quad \int R(\Delta E) d\Delta E = 1
\]

Spline smoothing for the distribution function:

\[
\sum_{i=1}^{M} (R_i - R(\Delta E_i))^2 + \int R(\Delta E)'^2 d(\Delta E) / \lambda.
\]

For \( \lambda \to \infty \) an interpolating spline
For \( \lambda \to 0 \) a linear least squares approximation

\( D > 10 \text{ nm}! \)
Symmetry and QC h in QD

Semi classical and classical considerations (earlier, Baranger et al., 1992 -1993 ) connect the transport properties of QD and their Symmetry L - R and Up -Down reflection symmetry, Inversion symmetry (preserving the loop orientation, in the case of magnetic field) connected with the transport phenomena (R. Whitney et al., 2009)

Quantum case:
Brody distribution imitating the Wigner- Dyson dstr.

\[ R(s) = (1 + \beta)bs^\beta \exp(-bs^{1+\beta}), \]

\[ b = (\Gamma[(2 + \beta)/(1 + \beta)])/D)^{1+\beta}, \quad s = \frac{\Delta E}{D} \]
Symmetry and QC h in QD

Poisson-like distribution

\[ R(s) = (1 + \beta)bs^\beta \exp(-bs^{1+\beta}), \]

\[ b = (\Gamma((2 + \beta)/(1 + \beta))/(D)^{1+\beta}) \]


Brody distribution

Distribution functions for electron neighboring levels in Si/SiO2 QD for different shapes:
- a) ellipsoidal shape,
- b) ellipsoidal like shape with cut.

QD shape has rotation symmetry
Symmetry and QC in QD

Violation of QD shape Up-Down symmetry

QD shape has rotation symmetry
Symmetry and QC h in QD

Distribution functions for electron neighboring levels in Si/SiO2 QD for spherical-like shape with cut. In inset the geometry of this QD are shown in 3D, the QD diameter is 17 nm. The Brody parameter beta=1.0
Symmetry and QC $h$ in QD

Fig. 8. Distribution functions for electron neighboring levels in Si/SiO$_2$ QD for different elliptical-like shapes. In insets the QD cross-sections are shown. The Brody parameter $\beta$ for distribution of “shape 1” is equal to 0.95 in Eq. (3).
Symmetry and QC $h$ in QD

**What is the type of the statistics?**

2D InAs/GaAs QDs (quantum wells); shapes and squares of wave functions for $i^{th}$ level

**Conclusion:** Single QD with RL or Up-Down mirror symmetry obey Poisson NNS (level attraction) Violation of both these symmetries lead to the QC $h$ (level repulsion)
**Disappearance of Quantum Chaos in the Tunnel Coupled Chaotic QD**


Coulomb effects are weak for thin barrier between QD (tunneling), dots size is **large enough** (G. Bryant, 1993; D. Bimberg et al., 2001).

Select only s-levels, no spin-orbit coupling: Selection of levels with the same quantum numbers is requisite for the correct study of NNS and other types of the level statistics and fluctuations.
Large inter-dot distance: electron levels degenerate, i.e. it can be found either in one or other isolated dot.

Smaller distance: wave function delocalizes extend to the whole DQD. Symmetrically arranged QD \(\rightarrow\) Poisson distribution, even separate QD are chaotic. Gradual transition to the regular behavior intermediate behavior between Poisson and Brody distributions, with beta close to 1.

**QD shape has rotation symmetry**

**Electron wave function**

**Distribution function**
"Butterfly double QD"


Technology issue: What is easier: try to achieve a perfect shape of SQD or not paying the attention to the chaotic shape, arrange their more or less symmetric mutual location.
Conclusions

• We found that the PL spectra of neutral exciton recombination energy of Si/SiO₂ spherical QDs can be well described by our model. The effect of non-parabolicity is important for the small size QDs.

• We found that the deformations of shape of QD strongly affect the statistical properties of QD energy levels, and it may have technological implications.

• In particular, the deviation of the shapes from the discrete symmetry leads to the non-Poisson statistics, which may be a sign of the quantum chaos. This, particularly, will influence the conductance and other transport properties of the QD.

• In system of the tunnel coupled double chaotics QD the quantum chaos is absent. Technological aspects of it.

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