Dot-ring nanostructure: Rigorous analysis of many-electron effects

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Ustroń, September 8th, 2016

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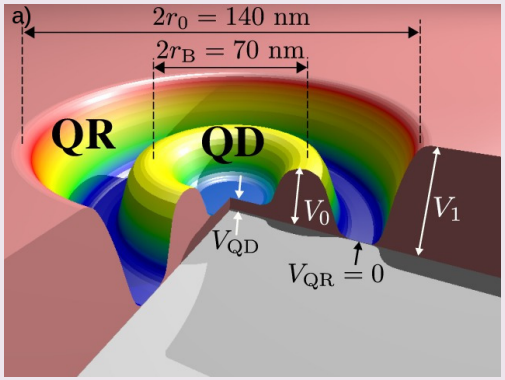
Outline

Solution of Hamiltonian given by potential $V(r)$

$$\hat{H} = \frac{1}{2m^*}\hat{p}^2 + V(r)$$



are single-particle wavefunctions

$$\psi(\vec{r}) = \psi_{||}(x,y)\psi_z(z)$$

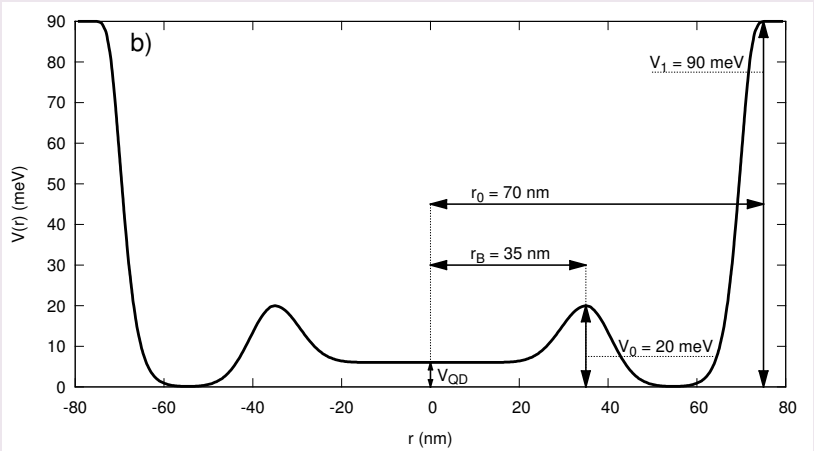
where $\psi_z(z) = \sqrt{\frac{2}{d}}cos(\pi\frac{z}{d})$ is the ground state of the infinite potential well $V_z \to \infty$. Component $\psi_{||}(x,y)$ is given by

$$\psi_{||}(x,y) = \Psi_{nl}(r,\phi) = R_{nl}(r)exp(il\phi)$$

$$n = 0,1,2,... \quad l = 0,\pm1,\pm2,...$$

Input parameters

Potential and dimensions



Material - GaAs

Hence the dielectric constant $\varepsilon = 12.9$ and effective mass $m^* = 0.067 m_e$.

Single-particle wavefunctions and their energies

$$\hat{H} |\psi_{nl}\rangle = \varepsilon_{nl} |\psi_{nl}\rangle$$
$$\langle \psi_{nl} | \psi_{n'l'} \rangle = \delta_{nn'} \delta_{ll'}$$

Many electrons

- Hamiltonian
- $\langle \Psi_N | \hat{H}_N | \Psi_N \rangle \geq E_G$
- $\langle \Psi_N | \hat{O}_N | \Psi_N \rangle = \left\langle \hat{O}_N \right\rangle$

Hamiltonian

We start from second quantization Hamiltonian

$$\mathcal{H} = \sum_{i,\sigma} \epsilon_i \hat{n}_{i\sigma} + \sum_{\sigma, i \neq j} t_{ij} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \sum_{\substack{i,j,k,l \\ \sigma,\sigma'}} V_{ijkl} \hat{c}^{\dagger}_{i\sigma} \hat{c}^{\dagger}_{j\sigma'} \hat{c}_{l\sigma'} \hat{c}_{k\sigma}$$

$$\{\hat{c}^{\dagger}_{i\sigma}, \hat{c}^{\dagger}_{j\bar{\sigma}}\} \equiv \{\hat{c}_{i\sigma}, \hat{c}_{j\bar{\sigma}}\} \equiv 0 \quad \text{oraz} \quad \{\hat{c}^{\dagger}_{i\sigma}, \hat{c}_{j\bar{\sigma}}\} \equiv \delta_{ij}\delta_{\sigma\bar{\sigma}},$$

Microscopic parameters

$$t_{ij} = \left\langle \Psi_i(\mathbf{r}) \middle| \frac{\hat{p}^2}{2m^*} + V(\vec{r}) \middle| \Psi_j(\mathbf{r}) \right\rangle$$

$$V_{ijkl} = \left\langle \Psi_i(\mathbf{r})\Psi_j(\mathbf{r}') \middle| \frac{e^2}{4\pi\varepsilon_0\varepsilon|\mathbf{r}-\mathbf{r}'|} \middle| \Psi_k(\mathbf{r}')\Psi_l(\mathbf{r}) \right\rangle$$

Note

Let M be a number of single-particle states $|\psi_{nl}\rangle$ taken into account with constant number of electrons $N_e \leq 2M$. The trial value of energy

$$E_{N_e}^{(trial)}(M) = \langle \Psi_{N_e,M} | \hat{H}_{N_e,M} | \Psi_{N_e,M} \rangle$$

Choice of basis

Single particle basis $\{ |\psi_{nl}\rangle \}$ is at the same time a set of eigenstates of the single-particle Hamiltonian. Thus

$$t_{ij} = 0.$$

Steps

- calculation of the interaction parameters V_{ijkl} (I quantization picture)
- diagonalisation of the second quantization Hamiltonian (Lanczos, QR) (II quantization picture)

N_e-particle state in second quantization

It is convenient to choose the basis in the Fock space as

$$|\Phi_k\rangle = \prod_{i\in\Omega_{\uparrow k}} \hat{c}^\dagger_{i\uparrow} \prod_{j\in\Omega_{\downarrow k}} \hat{c}^\dagger_{j\uparrow} |0\rangle \,, \langle\Phi_k|\Phi_l\rangle = \delta_{kl}.$$

For example

$$|\Phi\rangle = \underbrace{|0,1,\ldots,1\rangle}_{\text{spin}\uparrow} \otimes \underbrace{|1,0,\ldots,1\rangle}_{\text{spin}\downarrow} = \hat{c}^\dagger_{2\uparrow}\cdots\hat{c}^\dagger_{N_e\uparrow}\hat{c}^\dagger_{1\downarrow}\cdots\hat{c}^\dagger_{N_e\downarrow}|0\rangle \,,$$

N_e-particle state is given by

$$|\Psi_{N_e}\rangle = \mathcal{N}\sum_k A_k |\Phi_k\rangle$$

Remarks

- for N_e electrons and basis size M the dimensionality of the problem is $\binom{2M}{N_e}$;
- the field operator is constructed from $2M$ wavefunctions;
- for $M = 10$ states and $N_e = 2$ and 3 electrons it gives rather small values of 190, 1140 respectively. For $M = 18$ it increases to 630 and 7140;

Problem

Single-particle basis $\{ |\psi_i\rangle \}$ is complex, thus the parameter integrals have dimensionality of 12.

Solution

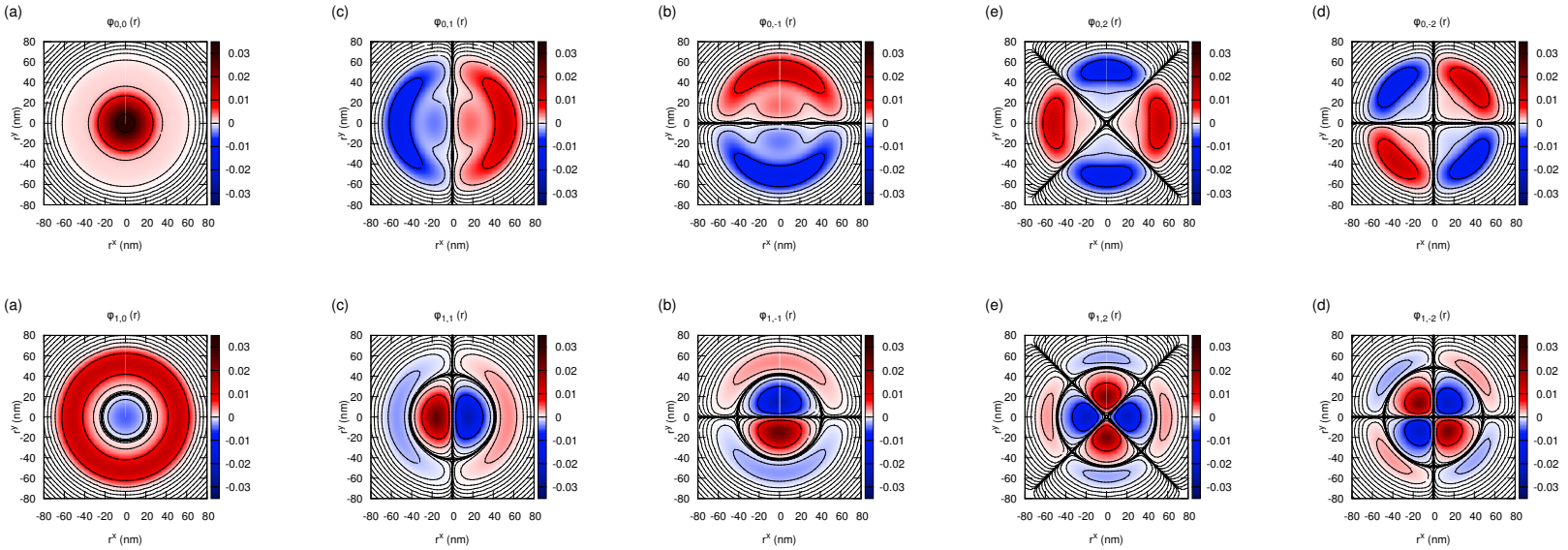
Linear transformation analogical to the spherical harmonics

$$\varphi_{nl}(x,y,z) = \begin{cases} \frac{\psi_{n,l}+\psi_{n,-l}}{\sqrt{2}} & l > 0 \\ \frac{\psi_{n,l}-\psi_{n,-l}}{\sqrt{2}i} & l < 0 \\ \psi_{n,l} & l = 0 \end{cases}$$

Properties of real single-particle basis

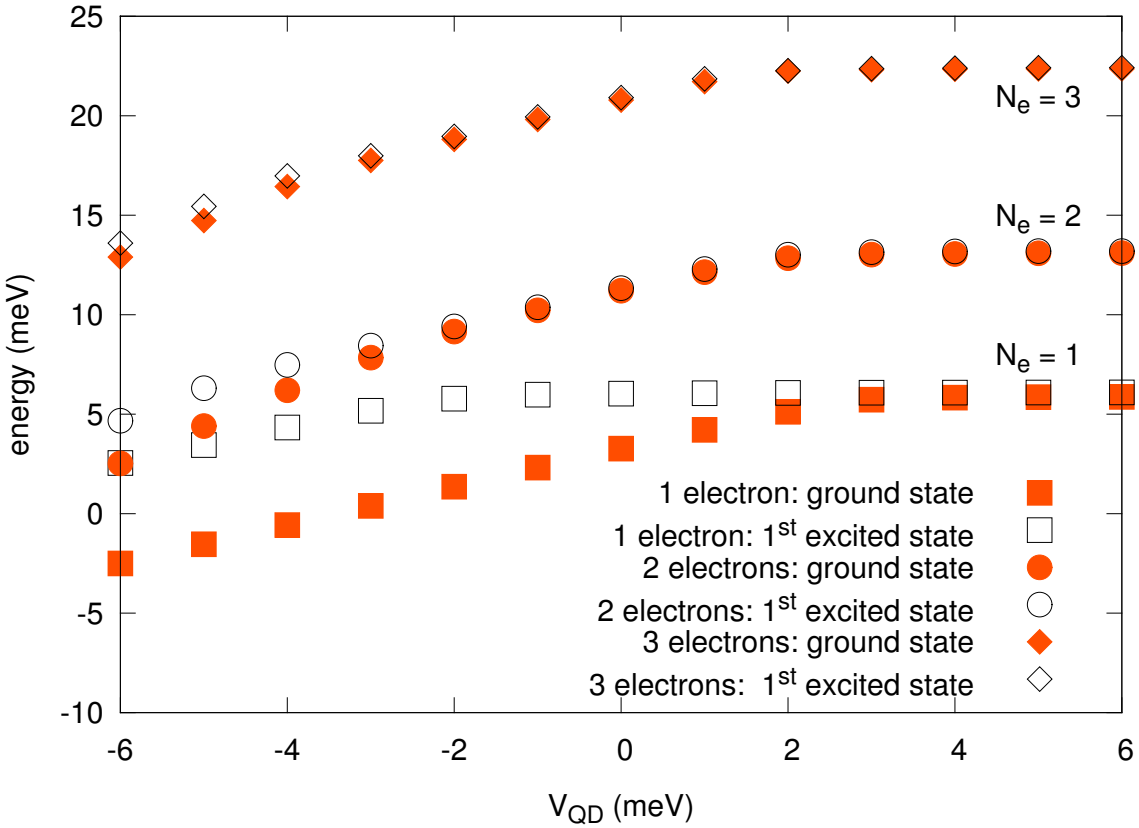
- orthonormal
- consists of the eigenstates of the single-particle Hamiltonian

Starting real single-particle basis



The single-particle basis for $V_{QD} = 0$ and quantum numbers $n = 0, 1,\ l = 0, \pm 1, \pm 2$.

Results



Ground- and first-excited-state energies versus different V_{QD} values for 1, 2 and 3 electrons.

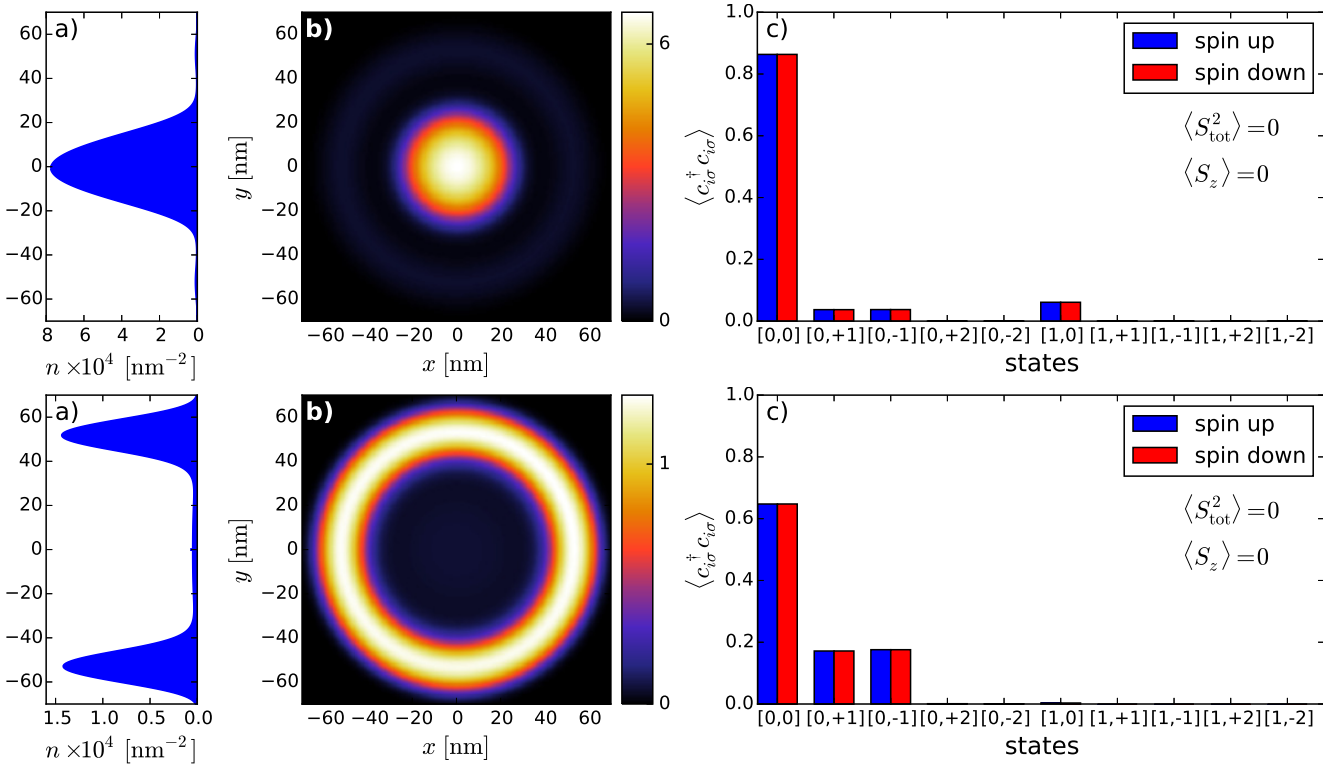
Degeneracy

The degrees of degeneracy for different QD potentials, with $N_e = 2, 3$.

	2 electrons				3 electrons			
	ground state		first-excited state		ground state		first-excited state	
V_{QD} (meV)	deg.	S_{tot}	deg.	S_{tot}	deg.	S_{tot}	deg.	S_{tot}
-6	1	0	3×2	1	2×3	1/2	2×2	1/2
-5	1	0	3×2	1	2×3	1/2	2×2	1/2
-4	1	0	3	1	2×3	1/2	4×2	3/2
-3	1	0	3	1	2×3	1/2	4×2	3/2
-2	1	0	3	1	2×3	1/2	4×2	3/2
-1	1	0	3	1	2×3	1/2	4×2	3/2
0	1	0	3	1	2×3	1/2	4×2	3/2
1	1	0	3	1	2×3	1/2	4×2	3/2
2	1	0	3×2	1	4	3/2	2×2	1/2
3	1	0	3×2	1	4	3/2	2×2	1/2
4	1	0	3×2	1	4	3/2	2×2	1/2
5	1	0	3×2	1	4	3/2	2×2	1/2
6	1	0	3×2	1	4	3/2	2×2	1/2

Many-body wave functions: 2 electrons

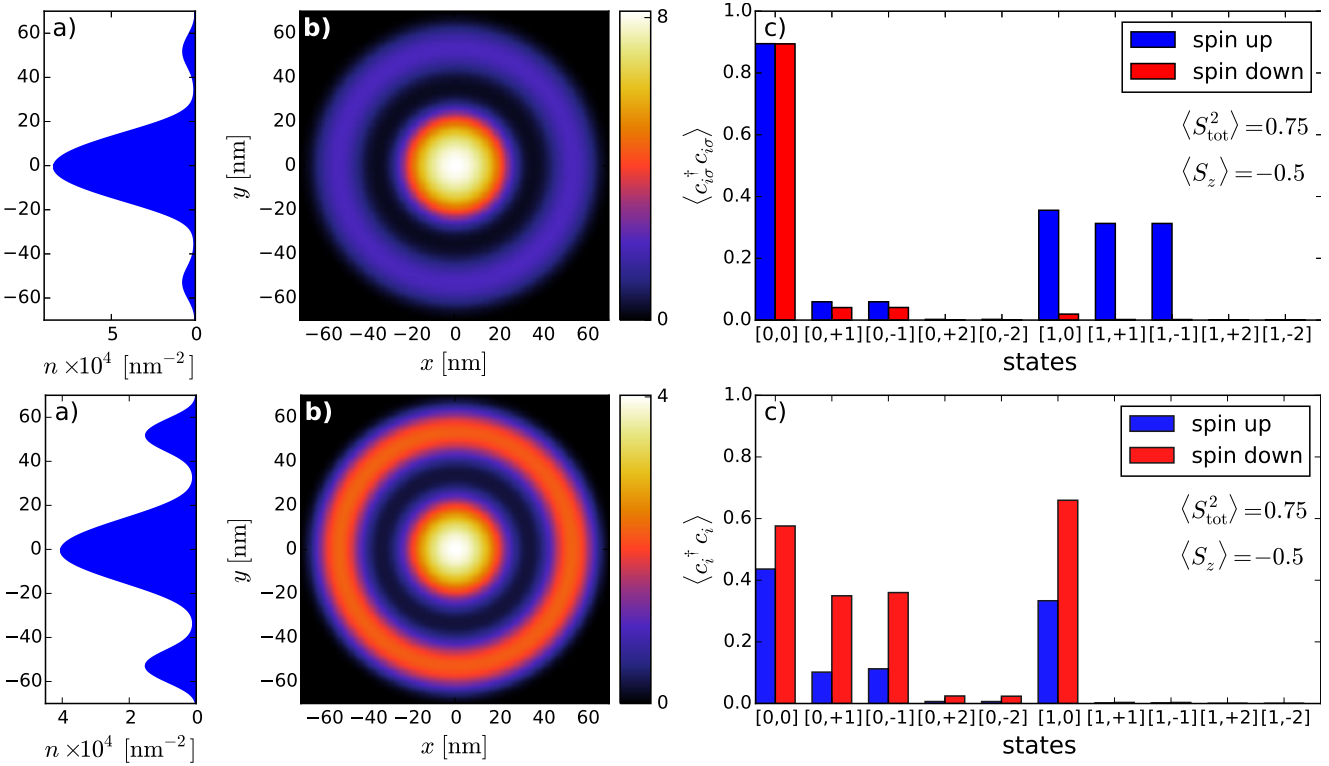
$V_{QD} = -4meV$



$V_{QD} = 4meV$

Many-body wave functions: 3 electrons

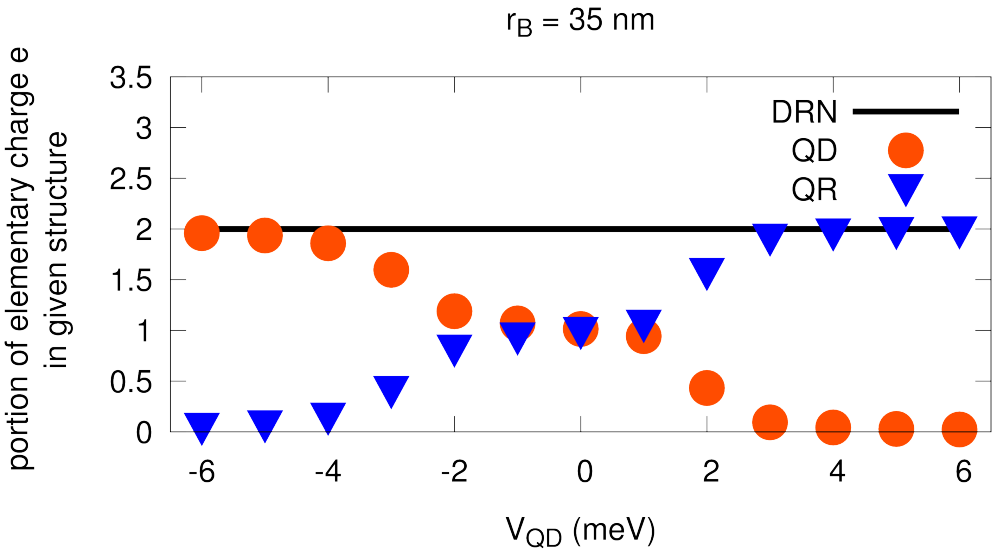
$V_{QD} = -6meV$



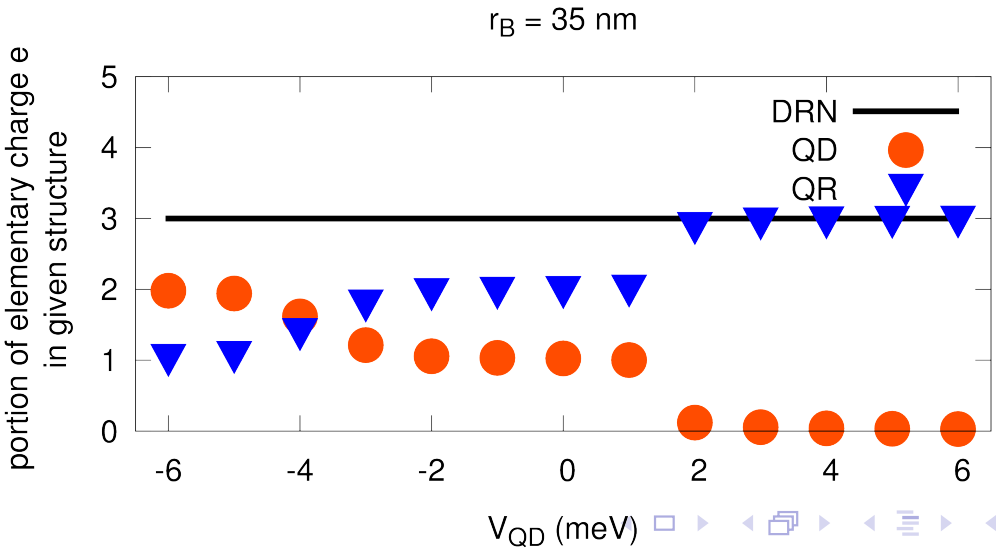
$V_{QD} = 1meV$

Portions of elementary charge

$N_e = 2$



$N_e = 3$

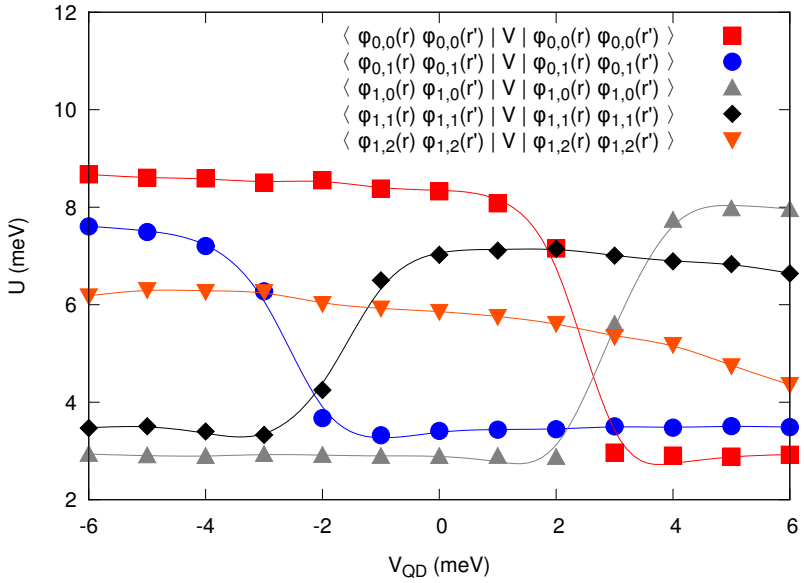


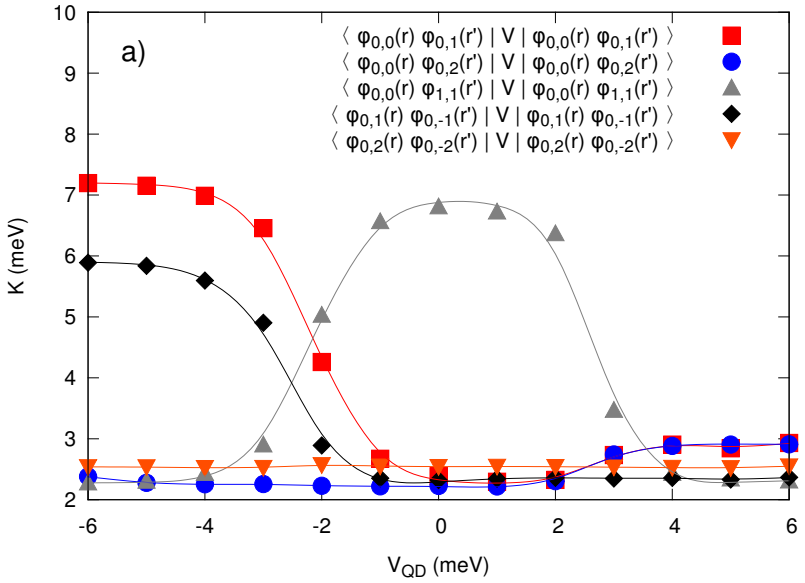
Microscopic parameters

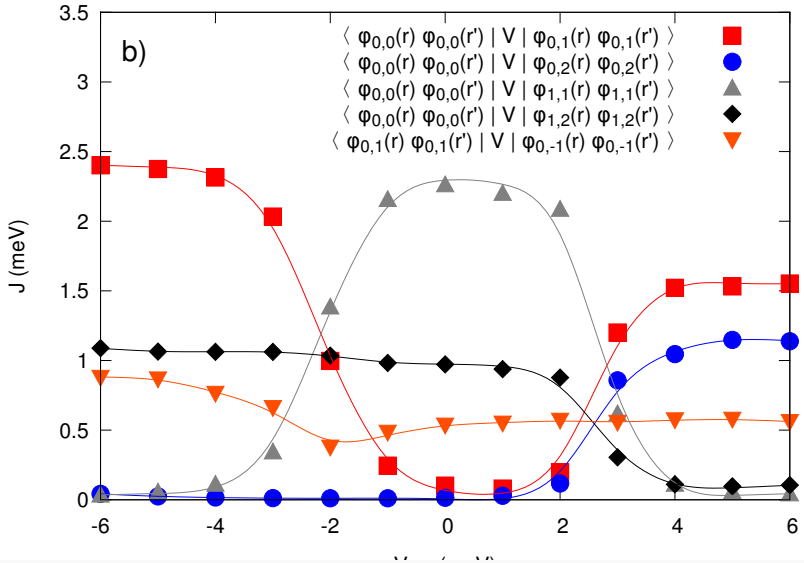
Hubbard-like form of the Hamiltonian

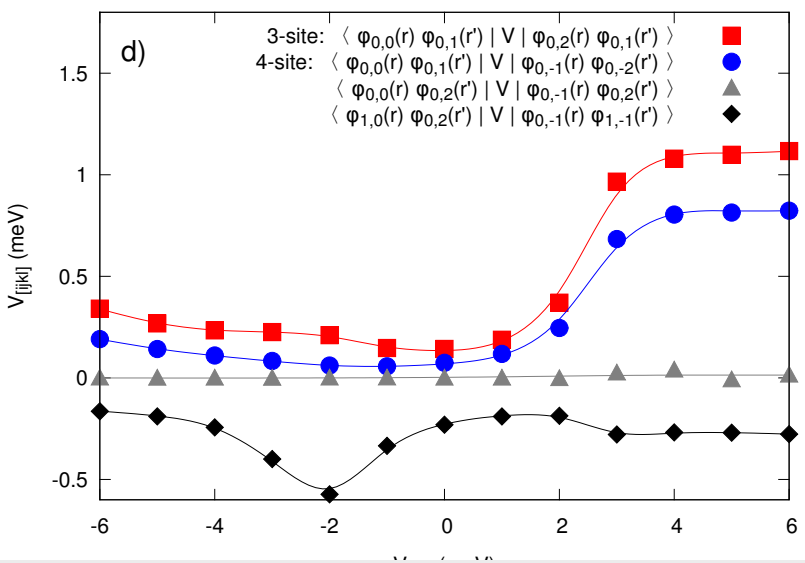
$$\hat{\mathcal{H}} = \sum_{i,\sigma} \epsilon_i \hat{n}_{i\sigma} + \sum_i U_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \tag{1}$$
$$- \sum_{i\neq j} J_{ij} \vec{S}_i \cdot \vec{S}_j + \frac{1}{2}\sum_{i\neq j}\left(K_{ij} - \frac{1}{2}J_{ij}\right)\hat{n}_i\hat{n}_j$$
$$+ \sum_{i\neq j} J_{ij}\hat{c}^\dagger_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{j\downarrow}\hat{c}_{j\uparrow} + \sum_{\sigma, i\neq j} C_{ij}\hat{n}_{i\sigma}\left(\hat{c}^\dagger_{i\bar{\sigma}}\hat{c}_{j\bar{\sigma}} + \hat{c}^\dagger_{j\bar{\sigma}}\hat{c}_{i\bar{\sigma}}\right)$$
$$+ \frac{1}{2}\sum_{[ijkl],\sigma,\sigma'} V_{ijkl}\hat{c}^\dagger_{i\sigma}\hat{c}^\dagger_{j\sigma'}\hat{c}_{l\sigma'}\hat{c}_{k\sigma},$$

Microscopic parameters - values

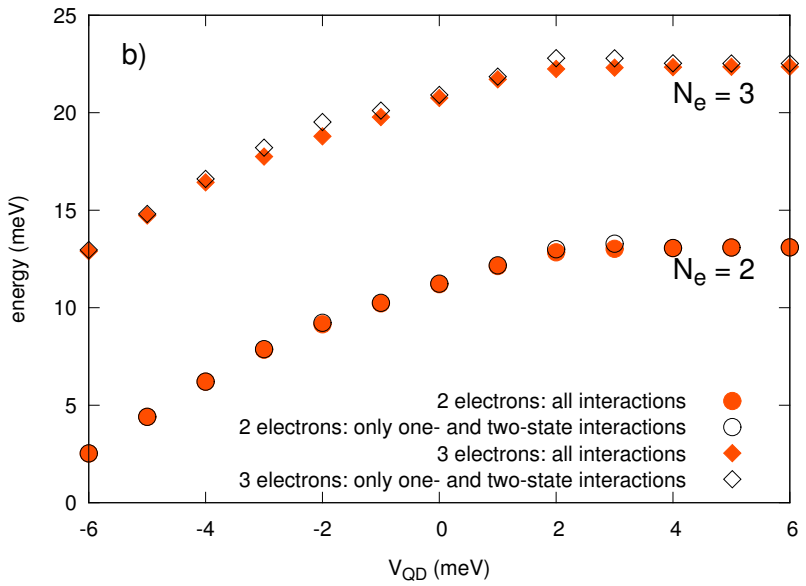


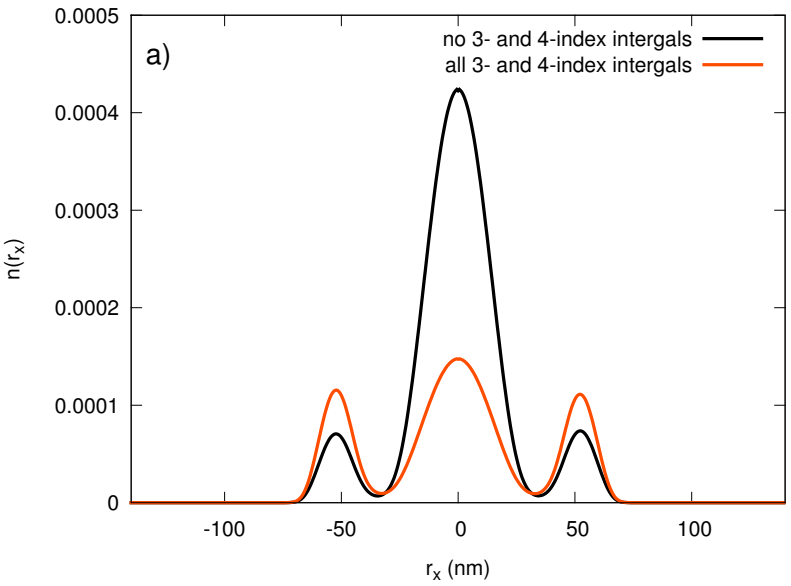






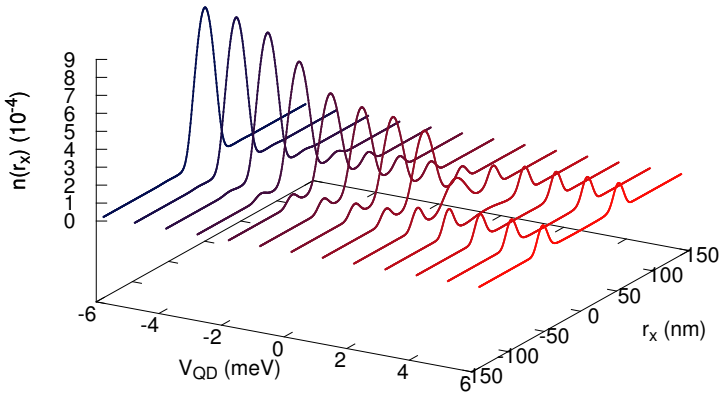
Influence of 3- and 4-state interaction

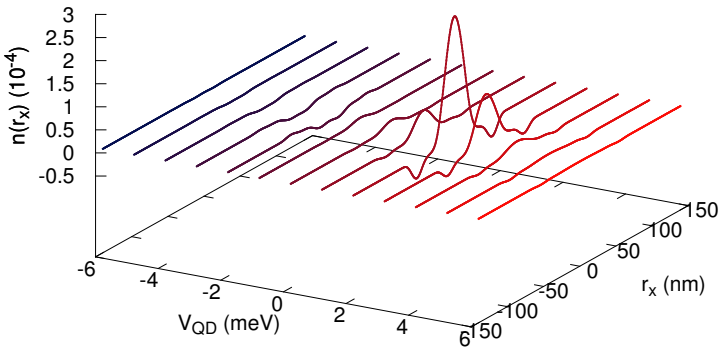




a) All interactions

b) Difference between only 1- and 2-state and all interactions





Conclusions

Many-electron effects in dot-ring nanostructure - important points

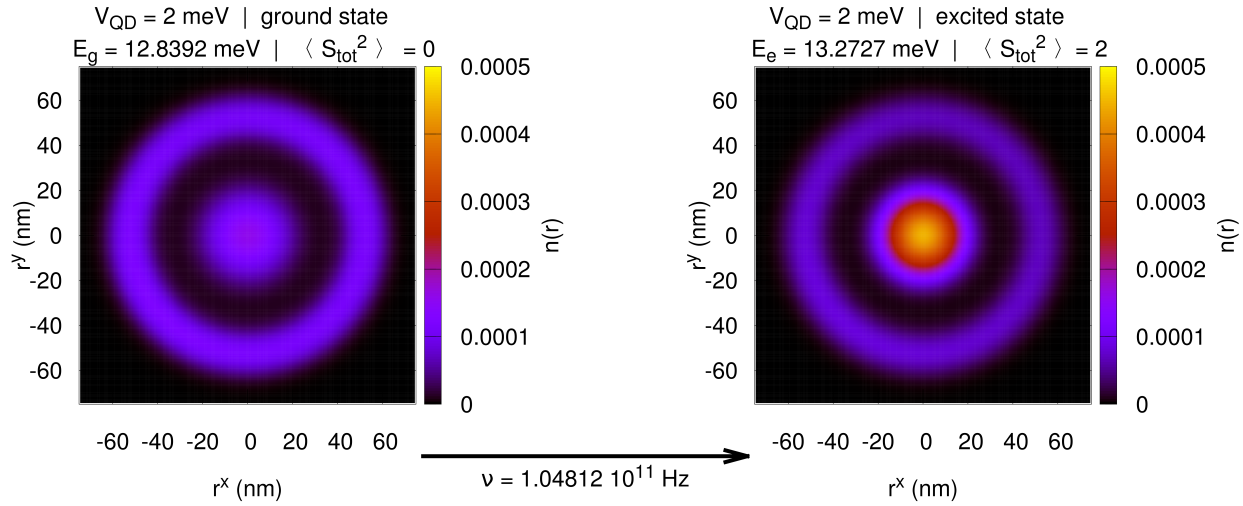
- the existence of the Coulomb blockade confirmed
- the wavefunction engineering for few-electron systems
- the degeneracy of the ground and first-excited states
- the importance of 3- and 4-state interaction terms
- the possibility of excitations changing the distribution of the charge in the system

Reference

A. Biborski, APK, A. Gorczyca-Goraj, E. Zipper, M. M. Maśka & J. Spałek, Scientific Reports **6**, 29887 (2016)

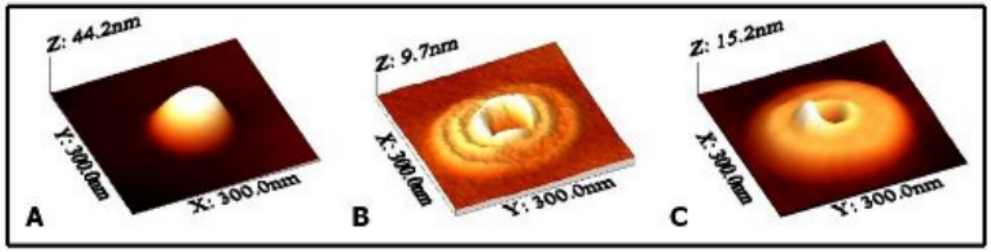
Thank you!

Possible excitation $N_e = 2$



Change in the overall electronic density for two electrons in DRN, for $V_{\mathrm{QD}} = 2$ meV, after absorption of a photon of frequency $\nu = 1.05\ 10^{11}\ Hz$. Note that this excitation is allowed as the change of respective angular orbital and spin momenta are $\Delta L_{tot} = 0$ and $\Delta S_{tot} = 1$.

Dot-Ring Nanostructure = Quantum Dot + Nano-Ring



Laboratory for Nanostructure Epitaxy and Spintronics on Silicon, Italy
http://lness.como.polimi.it/dante.php

Physical implementation

- gate over the 2d-electron gas
- semiconductor nanostructure fabrication (GaAs) (droplet epitaxy)

Values of microscopic parameters

All Hubbard intrastate repulsion amplitudes $U_i \equiv V_{iiii}$ (in meV) for different QD potentials.

V_{QD} (meV)	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6
$U_{(0\ 0)}$	8.67	8.60	8.59	8.51	8.55	8.38	8.33	8.08	7.15	2.97	2.90	2.88	2.92
$U_{(0\ 1)}$	7.61	7.49	7.20	6.27	3.67	3.32	3.41	3.44	3.45	3.50	3.48	3.51	3.49
$U_{(0\ \bar{1})}$	7.63	7.47	7.14	6.21	3.63	3.29	3.39	3.47	3.43	3.49	3.49	3.51	3.53
$U_{(0\ 2)}$	3.19	3.23	3.28	3.29	3.28	3.29	3.28	3.32	3.28	3.30	3.27	3.27	3.26
$U_{(0\ \bar{2})}$	3.26	3.24	3.25	3.27	3.31	3.26	3.27	3.30	3.26	3.32	3.26	3.29	3.26
$U_{(1\ 0)}$	2.94	2.90	2.89	2.93	2.91	2.89	2.89	2.89	2.87	5.60	7.74	7.97	7.96
$U_{(1\ 1)}$	3.47	3.51	3.40	3.33	4.25	6.50	7.02	7.11	7.15	7.01	6.89	6.83	6.64
$U_{(1\ \bar{1})}$	3.46	3.46	3.42	3.28	4.27	6.50	6.97	7.12	7.08	7.02	6.88	6.83	6.66
$U_{(1\ 2)}$	6.18	6.31	6.27	6.26	6.02	5.93	5.86	5.76	5.61	5.35	5.18	4.74	4.36
$U_{(1\ \bar{2})}$	6.20	6.29	6.30	6.25	6.15	6.04	5.93	5.82	5.63	5.29	5.09	4.75	4.40

Values of microscopic parameters

Selected values of the interstate Coulomb repulsion amplitudes $K_{ij} \equiv V_{ijij}$ (in meV) for different QD potentials.

V_{QD} (meV)	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6
$K_{(0\ 0),(0\ 1)}$	7.20	7.15	6.99	6.46	4.26	2.67	2.38	2.29	2.32	2.73	2.90	2.84	2.93
$K_{(0\ 0),(0\ 2)}$	2.38	2.28	2.25	2.26	2.23	2.22	2.23	2.22	2.30	2.74	2.88	2.91	2.91
$K_{(0\ 0),(1\ 0)}$	2.28	2.27	2.27	2.27	2.27	2.27	2.29	2.38	2.88	3.53	2.45	2.29	2.26
$K_{(0\ 0),(1\ 1)}$	2.28	2.31	2.43	2.90	5.03	6.57	6.81	6.72	6.37	3.47	2.44	2.34	2.31
$K_{(0\ 0),(1\ 2)}$	6.17	6.15	6.11	6.11	6.03	5.92	5.87	5.66	5.35	3.17	2.50	2.44	2.46
$K_{(0\ 1),(0\ \bar{1})}$	5.89	5.84	5.60	4.90	2.89	2.35	2.32	2.34	2.36	2.35	2.36	2.33	2.37
$K_{(0\ 2),(0\ \bar{2})}$	2.54	2.54	2.53	2.53	2.57	2.55	2.54	2.55	2.54	2.53	2.53	2.52	2.55
$K_{(1\ 1),(1\ \bar{1})}$	2.33	2.32	2.35	2.37	3.41	5.11	5.47	5.51	5.47	5.47	5.35	5.29	5.14

Values of microscopic parameters

Selected values of the interstate exchange integral $J_{ij} \equiv V_{ijji}$ (in meV) for different QD potentials.

V_{QD} (meV)	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6
$J_{(0\ 0),(0\ 1)}$	2.40	2.37	2.31	2.03	1.00	0.24	0.10	0.08	0.20	1.20	1.52	1.53	1.55
$J_{(0\ 0),(0\ 2)}$	0.04	0.02	0.02	0.01	0.01	0.01	0.01	0.03	0.12	0.86	1.05	1.15	1.14
$J_{(0\ 0),(1\ 0)}$	0.04	0.03	0.03	0.03	0.04	0.05	0.08	0.17	0.62	1.28	0.25	0.09	0.05
$J_{(0\ 0),(1\ 1)}$	0.04	0.06	0.11	0.35	1.39	2.16	2.26	2.20	2.09	0.62	0.11	0.06	0.04
$J_{(0\ 0),(1\ 2)}$	1.09	1.06	1.06	1.06	1.04	0.98	0.97	0.94	0.88	0.30	0.11	0.10	0.10
$J_{(0\ 1),(0\ \bar{1})}$	0.88	0.87	0.76	0.66	0.38	0.48	0.53	0.55	0.57	0.56	0.57	0.58	0.56
$J_{(0\ 2),(0\ \bar{2})}$	0.34	0.36	0.37	0.36	0.39	0.37	0.35	0.40	0.36	0.38	0.38	0.39	0.39
$J_{(1\ 1),(1\ \bar{1})}$	0.57	0.57	0.53	0.47	0.43	0.71	0.80	0.79	0.80	0.79	0.77	0.77	0.73

Values of microscopic parameters

Selected correlated interstate hopping parameter values $C_{ij} \equiv V_{ijjj}$ (in meV) for different QD potentials.

V_{QD} (meV)	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6
$C_{(0\ 0),(0\ 1)}$	0.05	-0.03	0.01	-0.06	-0.01	-0.01	0.01	0	0	-0.02	0	-0.01	0.03
$C_{(0\ 0),(0\ 2)}$	0	0.01	0	0	0	0	0	0	-0.01	0.02	0.02	0.01	0.01
$C_{(0\ 0),(1\ 0)}$	-0.38	-0.37	-0.37	-0.39	-0.44	-0.51	-0.65	-0.94	-1.65	-0.47	0.09	0.08	0.06
$C_{(0\ 0),(1\ 1)}$	0	-0.01	0	0	-0.05	0.02	-0.02	0	0.03	0	0	0	0
$C_{(0\ 0),(1\ 2)}$	0.03	0	-0.03	0.02	-0.03	-0.01	-0.01	0.02	0	-0.02	0	0.01	-0.01
$C_{(0\ 1),(0\ \bar{1})}$	0.03	0.01	0.01	-0.01	-0.01	-0.02	0	0	-0.01	0	-0.01	0	-0.01
$C_{(0\ 2),(0\ \bar{2})}$	-0.03	0.03	-0.01	0	0	0.02	-0.01	-0.01	0	0.03	-0.01	-0.02	-0.01
$C_{(1\ 1),(1\ \bar{1})}$	0	0.02	0	0	0.01	-0.03	-0.02	0.04	0	0.02	-0.02	0	-0.01

Values of microscopic parameters

Selected three- and four-state parameters $V_{[ijkl]}$ (in meV) for different QD potentials.

V_{QD} (meV)	-6	-5	-4	-3	-2	-1	0	1	2	3	4	5	6
$V_{(0\ 0),(0\ 1),(0\ 1),(0\ 2)}$	0.34	0.27	0.23	0.23	0.21	0.15	0.14	0.19	0.37	0.97	1.08	1.10	1.12
$V_{(0\ 0),(0\ 1),(0\ \bar{2}),(0\ \bar{1})}$	0.19	0.14	0.11	0.08	0.06	0.06	0.07	0.12	0.25	0.68	0.80	0.81	0.82
$V_{(0\ 0),(0\ \bar{1}),(0\ 1),(0\ \bar{2})}$	0.35	0.27	0.23	0.23	0.21	0.15	0.15	0.19	0.37	0.95	1.06	1.11	1.09
$V_{(0\ 0),(0\ 2),(0\ 2),(0\ \bar{1})}$	0	0	0	0	0	0	0	0	0	0.03	0.04	-0.01	0.01
$V_{(0\ 1),(0\ 1),(1\ 0),(0\ 0)}$	0.04	0.03	0.04	0.09	0.18	0.18	0.20	0.26	0.48	0.67	0.29	0.18	0.12
$V_{(1\ 0),(0\ 2),(1\ \bar{1}),(0\ \bar{1})}$	-0.16	-0.19	-0.24	-0.40	-0.57	-0.33	-0.23	-0.19	-0.19	-0.28	-0.27	-0.27	-0.28

Influence of DRN size