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Rigorous analysis of many-electron effects in nanosystems: Quantum dot - ring nanostructure

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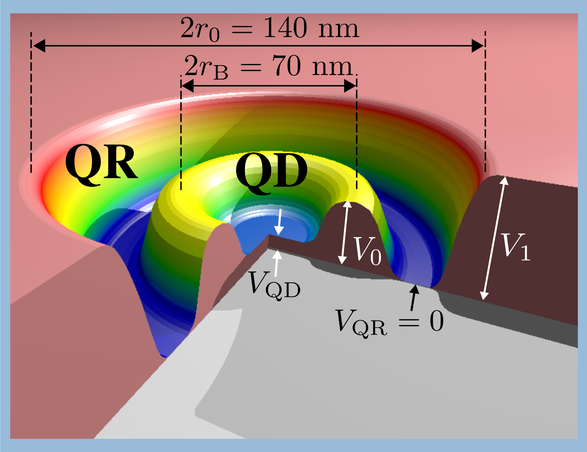
Motivation

Quantum dot (QD) – nanoring (QR) systems (DRN) exhibit an interesting set of features. Namely, there are theoretical predictions, that such a structure will be susceptible to the so-called *wave-function engineering*, allowing to control the transport properties of the system, as well as the optical absorption, with the quantum dot potential depth [1,2]. The natural consequence is to study the system for $N_e > 1$ electrons.

Our aim is to

- calculate the Coulomb-interaction parameters;
- determine the many-electron states;
- describe the energy spectrum and effective degeneracy of ground- and first-excited-states;
- calculate the probability of finding an electron in the quantum dot and the nanoring.

Single-particle problem



Quantum dot - ring nanostructure - shape of the potential

Solution of single-particle problem

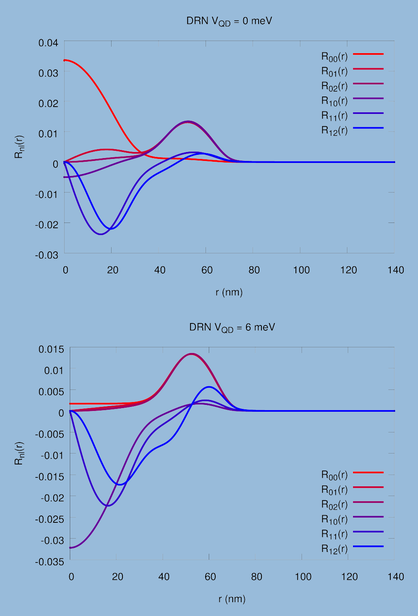
$$\left(\frac{\mathbf{p}^2}{2m^*} + V(\mathbf{r})\right)\psi_{nl}(\mathbf{r}) = \epsilon_{nl}\psi_{nl}(\mathbf{r}),$$

with potential $V(\mathbf{r})$ as shown on the left, are the wavefunctions [1,2]

$$\psi_{nl}(\mathbf{r}) = R_{nl}(r)exp(il\phi).$$

For the degenerate case $\epsilon_{nl} = \epsilon_{n\bar{l}}$ and $R_{nl}(r) = R_{n\bar{l}}(r)$ we can write the real solutions

$$\varphi_{nl}(\mathbf{r}) = \frac{\psi_{n|l|}(\mathbf{r}) + sgn(l)\psi_{n|\bar{l}|}(\mathbf{r})}{\sqrt{2sgn(l)}}.$$



Method

We start the many-electron description with defining the field operators

$$\hat{\Psi}_\sigma(\mathbf{r}) = \sum_{i=1;\sigma=\pm1}^{M} \varphi_{i\sigma}(\mathbf{r})\hat{c}_{i\sigma}; \quad \hat{\Psi}^\dagger_\sigma(\mathbf{r}) \equiv \left(\hat{\Psi}_\sigma(\mathbf{r})\right)^\dagger,$$

where $\{\varphi_{i\sigma}\}$ is an orthonormal basis of single-particle wavefunctions, and $\hat{c}_{i\sigma}$ ($\hat{c}^\dagger_{i\sigma}$) are annihilation (creation) operators of electron with spin σ on i-th orbital.

The Hamiltonian now reads

$$\begin{aligned}\mathcal{H} \equiv &\sum_\sigma \int d^3r \hat{\Psi}^\dagger_\sigma(\mathbf{r})\mathcal{H}_1\hat{\Psi}_\sigma(\mathbf{r}) \\ &+ \frac{1}{2}\sum_{\sigma\sigma'}\iint d^3r d^3r' \hat{\Psi}^\dagger_\sigma(\mathbf{r})\hat{\Psi}^\dagger_{\sigma'}(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\hat{\Psi}_{\sigma'}(\mathbf{r}')\hat{\Psi}_\sigma(\mathbf{r}) \\ = &\sum_{ij}\sum_\sigma t_{ij}\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \frac{1}{2}\sum_{ijkl}\sum_{\sigma,\sigma'} V_{ijkl}\hat{c}^\dagger_{i\sigma}\hat{c}^\dagger_{j\sigma'}\hat{c}_{l\sigma'}\hat{c}_{k\sigma},\end{aligned}$$

where

$$t_{ij} = \int d^3r \varphi^*_i(\mathbf{r})\mathcal{H}_1\varphi_j(\mathbf{r}),$$

$$V_{ijkl} = \iint d^3r d^3r' \varphi^*_i(\mathbf{r})\varphi^*_j(\mathbf{r}')\frac{e^2}{\varepsilon|\mathbf{r}-\mathbf{r}'|}\varphi_l(\mathbf{r}')\varphi_k(\mathbf{r}).$$

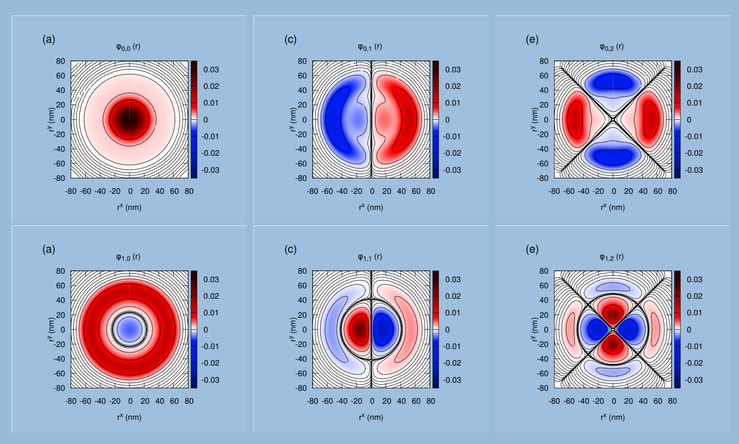
Hamiltonian is diagonalized for set, *rich enough*, finite basis of single-particle wavefunctions, setting microscopic parameters t_{ij}, V_{ijkl} (see *Microscopic parameters*).

As we selected the single-particle basis (see *Single-particle basis*) to be the lowest-energy eigenstates of single-particle Hamiltonian, we have

$$t_{ij} = \epsilon_i\delta_{ij},$$

where ϵ_i is a single-particle energy, and δ_{ij} Kronecker delta.

Single-particle basis



Selected singe-particle wavefunctions in real number basis $\{\varphi_i\}$ for the quantum-dot potential depth $V_{\mathrm{QD}} = 0$.

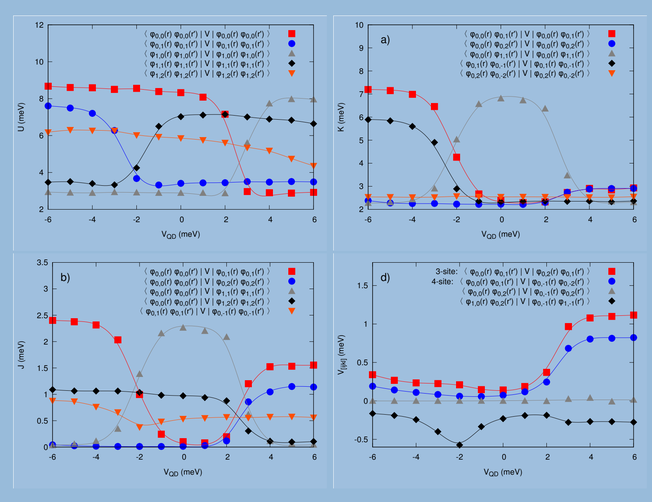
Quantum Metallization Tools

QMT Quantum Metallization Tools

https://bitbucket.org/azja/qmt

Calculation where carried out using the QMT library, suitable for similar problem solutions [3].

Microscopic parameters



Evolution of selected microscopic parameters vs V_{QD}: Hubbard on-site repulsion $U_i \equiv V_{iiii}$, interstate repulsion $K_{ij} \equiv V_{ijij}$, exchange integral $J_{ij} \equiv V_{ijji}$, and multistate parameters $V_{[ijkl]}$.

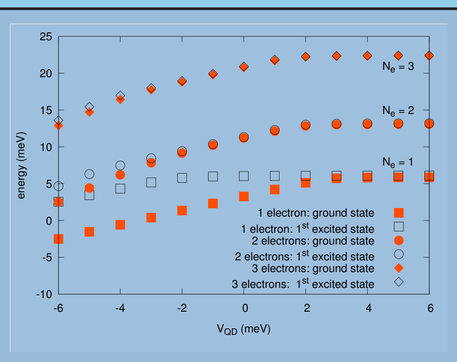
All integrals (10 000 for $M = 10$ single-particle wavefunctions) are calculated by means of the Monte Carlo method with CUBA library [4], and accuracy of 0.005 meV. Rapid changes of parameter values for $V_{\mathrm{QD}} = -2meV$ and $V_{\mathrm{QD}} = 3meV$ are related to the energy-level crossing and their repulsion.

Degeneracy

State multiplicity for different QD potential, for $N_e = 2, 3$.

	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

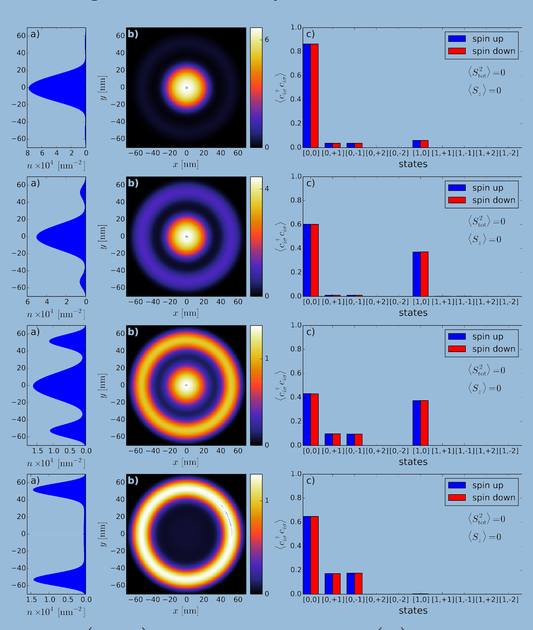
Results: 2 and 3 electrons



Ground- and first-excited states energies for $N_e = 1$, 2, and 3.

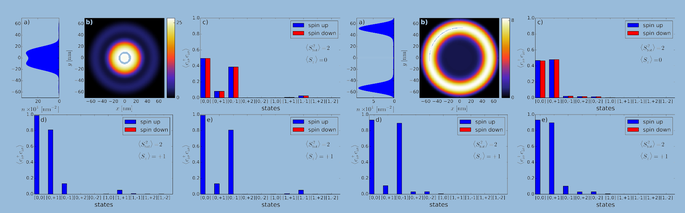
2 electrons

We observe evolution of many-particle state from the dot-located electrons for low values of V_{QD}, to the ring-located electrons for larger values of V_{QD}.



Density profiles $\big($a), b)$\big)$ and state occupancies $\big($c)$\big)$ for $V_{\mathrm{QD}} = -4meV$, $-2meV$, $2meV$, $4meV$

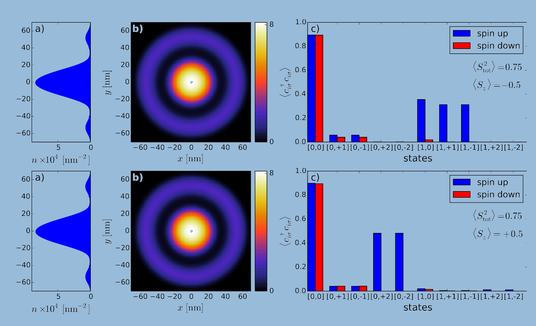
Similar behavior takes place for the first-excited state.



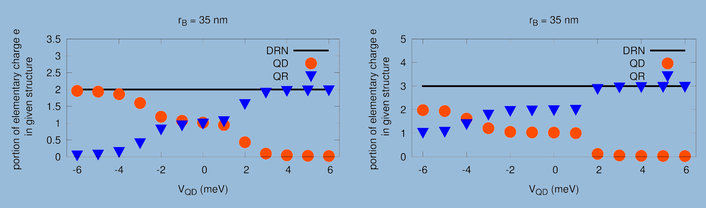
Density profiles $\big($a), b)$\big)$ and state occupancies $\big($c)$\big)$ for $V_{\mathrm{QD}} = -6meV$, $4meV$

3 electrons

For the case of three electrons we observe an evolution from superposed state, where two electrons are in the dot, whereas third one in the ring, to the ring-located all electrons.



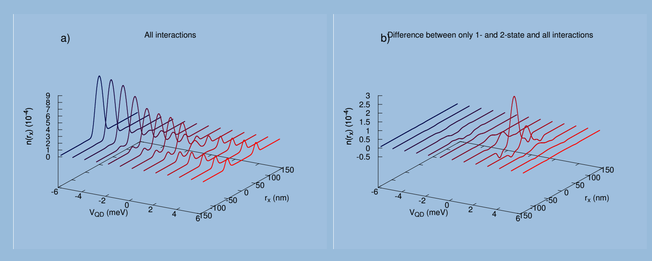
Density profiles $\big($a), b)$\big)$ and state occupancies $\big($c)$\big)$ for $V_{\mathrm{QD}} = -6meV$



Portion of elementary charge in quantum dot (QD) and nanoring (QR) versus dot potential V_{QD} for 2 (left) i 3 (right) electrons.

Role of many-state parameters

In our approach we are able to include and neglect selected interaction channels to study their relative importance.



Evolution of electron density profile versus the QD potential V_{QD} (left) and the difference in the density profiles for the three- and four-state interaction parameters neglected (right).

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Narodowe Centrum Nauki

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