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Optical spectra of charged anisotropic quantum boxes

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ABSTRACT

We have developed a numerical scheme for exact diagonalization of the few-particle electron–hole interaction Hamiltonians with a simultaneous resolution of several discrete conserved quantum numbers such as total electron or hole spins, total angular momentum, or parity. The method was applied to a simple model of a two-dimensional rectangular quantum box of arbitrary size and anisotropy, and containing either several electrons or several electrons and a single valence hole. In this model, effects of box size and anisotropy on the photoluminescence spectra are analyzed. Compared to earlier calculations, we were able to include enough single-particle shells in the many-body Hilbert space to observe the transitions between strong and weak spatial quantization regimes.

1. Introduction

Quantum dots [1] are semiconductor nanostructures that confine the motion of conduction band electrons, valence band holes, or electron–hole complexes in a small volume (or area). A small number of confined particles can be controlled for example by applying external electric field. Since typical sizes of quantum dots are ~1–10 nm in all dimensions, motion of a confined particle is quantized and it causes discrete single-particle energy spectra similar to the atomic one. However, the spatial dimension of "artificial atoms", as dots are often called, is sufficiently bigger than that of natural atoms to see inter-particle interaction effects. Hence, the optical properties of quantum dots are a result of competitions between confinement and interaction.

Nowadays one can produce quantum dots of nearly any shape, size and chemical composition—in other words, with any symmetry of confining potential. For that reason we study the effect of size and anisotropy of the confining potential on the dynamics and recombination of confined excitonic complexes. We have concentrated on the studies of how the symmetry of confining potential affects the exciton or trion binding energy, for which the isotropic Coulomb interaction between electrons and holes in the free excitonic complexes is responsible.

The model used in the present calculation was explained in detail in Ref. [2]. In short, to introduce size and anisotropy to the model we use the simple two-dimensional (2D) rectangular geometry [3,4]. If the box has spatial dimensions a and b in x and y directions, one can define the parameter of anisotropy $\beta = b/a$ (aspect ratio) and an average length of the box $d = (ab)^{1/2}$.

Hamiltonian matrices describing electron–hole complexes such as exciton ($X = e{+}h$), trion ($X^- = 2e{+}h$), and double charged state ($X^{2-} = 3e{+}h$) are diagonalized numerically in the configuration interaction (CI) basis, restricted to a few single-particle orbitals $1 \leqslant n,\ m \leqslant n_{\max}$ but including all spin configurations. The calculations are carried out as a function of box size $\rho = d/a_B$ ($a_B = \varepsilon\hbar^2/me^2$ is the Bohr radius) and anisotropy β, for different $4 \leqslant n_{\max} \leqslant 10$. Data shown in Figs. 2–4 were obtained by extrapolation to $n_{\max} = \infty$, and are presented in Rydberg units ($Ry = me^4/2\varepsilon^2\hbar^2$), which allowed us to make the calculations independent of material constants.

2. Results and discussion

In Fig. 1 the examples of exciton ($X = e{+}h$) and negative trion ($X^- = 2e{+}h$) energy spectra for the average box size $\rho = 1$ and two anisotropies $\beta = 1$ and 2 are shown. Parities of the eigenstates (0—even, 1—odd) in both x and y directions are indicated for both complexes, and for the trion also the two-electron spin projections ($S = 0$—singlet, or $S = 1$—triplet) are indicated. The parities of exciton and trion ground states are even–even for all values of (ρ, β). Also, we find that the lowest-energy trion is the singlet state. For an anisotropic box with $\beta \neq 1$ breaking of the $x \leftrightarrow y$ symmetry is clearly seen. With increasing anisotropy β, all spectra shift to higher energies.

We define X and X^- binding energies as $\Delta_X = E_e{+}E_h{-}E_X$ and $\Delta_{X^-} = E_X + E_e - E_{X^-}$, where E_e and E_h are the single-electron or -hole ground state energies. In Fig. 2(a) we show the ratio of trion and exciton binding energies as a function of box size ρ.

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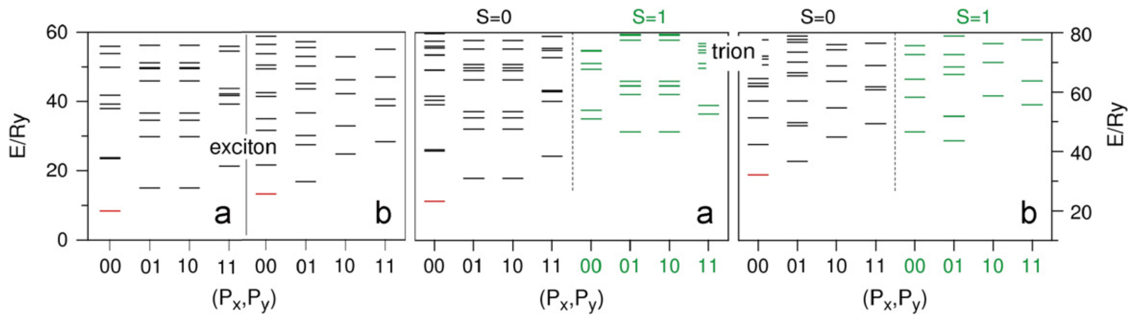

Fig. 1. Exciton (left) and trion (middle, right) energy spectra in an isotropic $\beta = 1$ (a) and anisotropic $\beta = 2$ (b) quantum box.

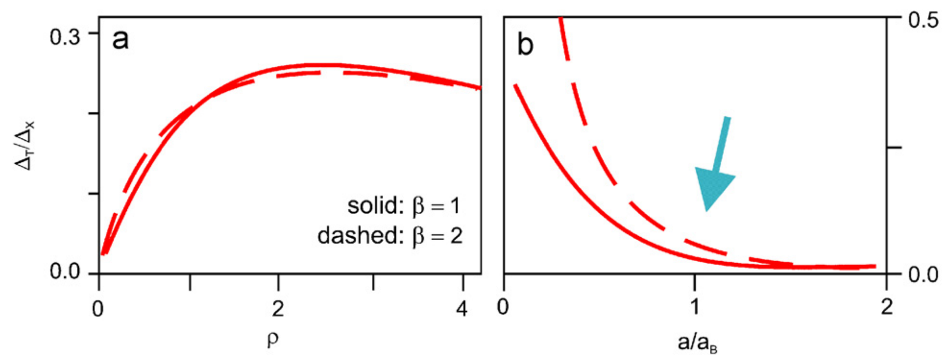

Fig. 2. (a) Trion to exciton binding energy ratio plotted as a function of the box size ρ. (b) Relative difference in the trion binding energies due to the box anisotropy $\delta\Delta/\Delta$ (see the text) plotted as a function of the shorter box side a/a_B.

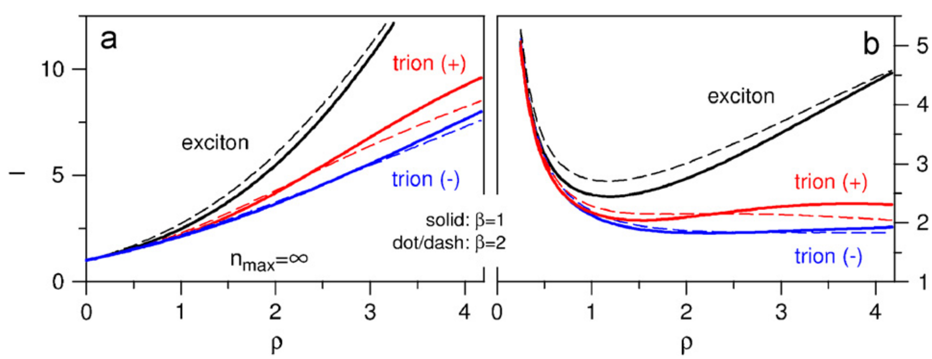

Fig. 3. Exciton and trion PL oscillator strengths I plotted as a function of the box size ρ.

We expect that for big boxes this ratio should converge to results obtained by Suris and Sergeev [5] for the quantum well with analogous $\mu_e/\mu_h = 0.2$ effective masses ratio. It can be easily noticed that the influence of anisotropy on Δ_{X^-}/Δ_X is low.

If we define relative difference in the binding energies due to the box anisotropy as $\delta\Delta/\Delta = [\Delta(\beta) - \Delta(1)]/\Delta(1)$, this value decreases with increasing average box size for both exciton and trion complexes. However, a more interesting question is how this difference for the case of a trion depends on the length of the shorter box side a/a_B (a_B is the free-trion Bohr radius). This dependence is shown in Fig. 2(b). A rapid drop of those curves to zero beyond a critical length of the box side ($a = a_B$) for all box anisotropies can be observed. Therefore, two size/shape regimes can be distinguished: (i) $a > a_B$, when trion motion is not restraint—trion behaves like a simple particle bouncing off the walls (the shape and symmetry of the confining potential has little influence); (ii) $a < a_B$, when trion center of mass is quantized and configuration of electrons and hole forming the trion is changed compared to the free-trion regime. In this case, anisotropy causes strong effect.

In Fig. 3, we plot the PL oscillator strengths ($I_X = |\langle \mathrm{vac}|\hat{\varepsilon}\cdot\bar{p}|e+h\rangle|^2$ for exciton and $I_{X^-} = |\langle e|\hat{\varepsilon}\cdot\bar{p}|2e+h\rangle|^2$ for trion) as a function of the average box size ρ. For small boxes, $\rho = 0$, oscillator strengths of both exciton and trion complexes equal unity, and they increase with growth of the box, due to emerging electron–hole correlations. Oscillator strengths shown as functions of the box size ρ look quite different (I_X—quadratic and I_X—linear function of ρ). It is the result of a different type of final state left behind after the recombination of an electron–hole pair.

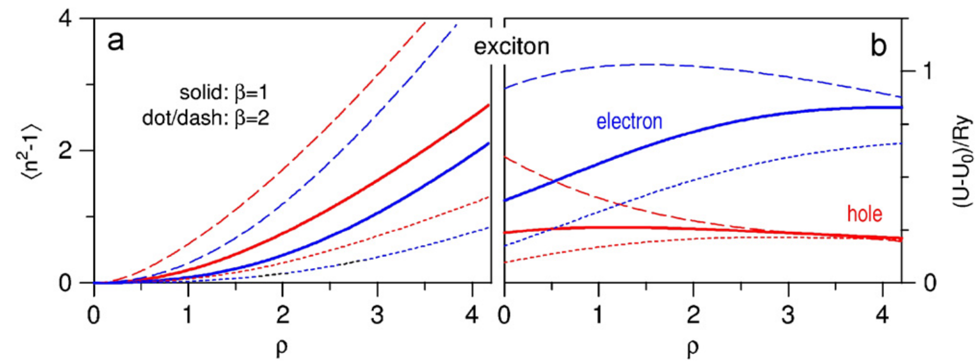

Fig. 4. (a) Comparison of average single-particle *e* and *h* excitations in the *X* and *Y* directions calculated for the exciton ground state plotted as a function of box size. (b) Electron and hole excitation energy in exciton. U_0 is the single-particle energy corresponding to $n = 1$.

Anisotropy affects *I* only for intermediate box sizes, and the effect is rather insignificant.

In Fig. 4(a) we show the average single-particle electron and hole excitations in both *X* and *Y* directions calculated for the exciton ground state (quantum numbers *n* and *m* are distinguished by dotted and dashed lines for $\beta = 2$) plotted as a function of box size. In anisotropic case breaking of the $X \leftrightarrow Y$ symmetry (just like in Fig. 1) is evident. Excitations in *Y* direction are easy because of the closely spaced single-particle levels. In Fig. 4(b) we plot electron and hole excitation energies in the exciton counted from U_0 (the single-particle ground state energy with $n = 1$).

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