On the Quadron State in Parabolic Quantum Dots

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On the Quadron State in Parabolic Quantum Dots

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Abstract. In this work we consider a quadron – a state of four carriers – two electrons and two holes in quantum dots with parabolic confinement. By using the Hatree-Fock method, the binding energies of the quadron and biexciton have been calculated for a full range of the electron-to-hole oscillator length ratio. The effect of the magnetic field on the binding energy of the quadron and biexciton has been also investigated. The crossing between anti-binding and binding in both the excited quadron and biexciton states for the certain ranges of the electron-to-hole oscillator length ratio has been found .

Keywords: exciton, biexciton, quadron, parabolic quantum dot, Hartree-Fock method, binding energy.

1. Introduction

As a primary elementary excitation in low-dimensional semiconductors, excitonic system have been intensively investigated both theoretically and experimentally in two last decades due to their promising physical properties for future electronic devices and quantum information technologies [1–3]. One of the direct consequences of quantum confinement is that these elementary excitations in semiconductor nano-structures can reach large binding energies. Of particular interest are self-assembled semiconductor quantum dots with parabolic confinement potential [4–12], because this kind of quantum dots demonstrates large biexction binding energies and, on the other hand, it has easily been incorporated in field-effect structures to study the effect of an external magnetic field without breaking the symmetry of the system.

Recently, a new term “quadron” for quasi-particle consisting of four carriers - two electrons and two holes in quantum dots has been introduced by us in [4, 5] to distinguish them from conventional biexcitons. It is interesting to note that the similar idea relating to quadron has been presented almost at the same time, in [6] where the authors show the fundamental differences between usual biexciton and quantum dot “quatuor” - their term for the system of four carriers - two electrons and two holes, instead of our term “quadron”. Both the biexciton and the quadron consist of four interacting carriers - two electrons and two holes, but usual biexciton is traditionally considered as two interacting excitons. In the quantum dots, the picture of a bound biexciton breaks down due to the totally different pair interacting between

four carriers. In our previous works [4, 5] we show that the nontrivial Coulomb effect in a small 2D InAs quantum dot leads rather to a bound quadron than the usual biexciton. However the study in [4, 5] has been limited to the ground state and only for a certain short range of electron-to-hole confinement ratios.

To develop further the investigations in our previous works [4, 5], in this work we consider in more details quadron and biexciton states for a full range of confinement potentials and for excited states. By using the Hatree-Fock method, the binding energies of the quadron and biexciton have been calculated for a full range of electron-to-hole oscillator length ratio. The effect of the magnetic field on the binding energy of the quadron and biexciton has been also investigated.

It is found that in the ground state of 2D InAs quantum dots, where the spins of the electrons are anti-parallel, the biexciton binding energy is negative for all range of the electron-to-hole oscillator length ratio. However, the quadron binding energies is positive within a certain range of electron-to-hole oscillator length ratios. For the excited state we have found an interval of the electron-to-hole oscillator length ratio where the transition from anti-binding to binding states of biexciton occurs, that means inside this interval the biexciton is bound and it is unbound outside it. Such a crossover between binding and anti-binding for the quadron also exits, but the range of crossing is much larger than that for the biexciton. Our results help further clarify the properties of the basic excitations in self-organized semiconductor quantum dots, especially to clarify the results in [11] on sensitive changes of the binding energy within quantum dots ensembles.

2. The model

As in [4, 5] we take the model of the system of interacting electrons and holes confined in a 2D quantum dot with parabolic lateral potential in the presence of the perpendicular magnetic field $\vec{B}\|z$. In the framework of the effective-mass approximation, the total Hamiltonian of the system of N electrons and M holes ($N = M = 2$ for biexciton and quadron) can be written as follows

$$\widehat{H} = \sum_{i=1}^{N} h(\vec{r}_i) + \sum_{k=1}^{M} h'(\vec{r}_k) + \sum_{i=1;i<j}^{N} \frac{e^2}{\epsilon r_{ij}} + \sum_{k=1;k<l}^{M} \frac{e^2}{\epsilon r_{kl}} - \sum_{i=1}^{N}\sum_{k=1}^{M} \frac{e^2}{\epsilon r_{ik}} \ , \tag{1}$$

where first two terms are summations over Hamiltonians of single electrons $h(\vec{r}_i)$ and single holes $h'(\vec{r}_k)$, the third and fourth terms are the total electron-electron and hole-hole Coulomb interactions, respectively, and the last term is the total electron-hole Coulomb interaction, and ϵ is the dielectric constant of the material.

The Hamiltonians for a single electron and single hole in a quantum dot with parabolic confinement in a magnetic field are the following (the terms describing the spin Zeeman splitting due to interaction of the spin with the magnetic field have been omitted because of its smallness):

$$h(\vec{r}_i) = -\frac{\nabla_i^2}{2m_e^*} + \frac{m_e^*}{2}(\omega_e^2 + \frac{1}{4}\omega_{ce}^2)r_i^2 + \frac{1}{2}\omega_{ce}\hat{L}_{zi} \ , \tag{2}$$

$$h'(\vec{r}_k) = -\frac{\nabla_k^2}{2m_h^*} + \frac{m_h^*}{2}(\omega_h^2 + \frac{1}{4}\omega_{ch}^2)r_k^2 + \frac{1}{2}\omega_{ch}\hat{L}_{zk} \ , \tag{3}$$

where m_e^* (m_h^*) and ω_e (ω_h) are the effective mass and the confinement potential of the electron (hole), respectively; $\omega_{ce} = eB/m_e^*$ ($\omega_{ch} = eB/m_h^*$) and $\hat{L}_{zi}$ ($\hat{L}_{zk}$) are the cyclotron frequency for the electron (hole) and the z-components of orbital angular momentum operators of the electron (hole), respectively.

In the following we write down the eigenfunction in polar coordinates $\vec{r} = (r, \varphi)$ and the eigenvalue of the single electron in the quantum states (n, m) (analogously for the hole, where the index e is replaced by index h):

$$\chi^e_{n,m}(r,\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi} \sqrt{\frac{2n!}{(n+|m|)!}} \alpha_e (\alpha_e r)^{|m|} e^{-(\alpha_e r)^2/2} L_n^{|m|}((\alpha_e r)^2) \ , \tag{4}$$

$$E^e_{n,m} = \Omega_e(2n + |m| + 1) + \frac{1}{2} m\omega_{c_e} \ , \tag{5}$$

where $L_n^{|m|}(r)$ is generalized Laguerre polynomial, and $\Omega_e = (\omega_e^2 + \frac{1}{4}\omega_{c_e}^2)^{1/2}$, $\alpha_e = \sqrt{m_e^* \Omega_e}$.

The total wave function of the system of N electrons and M holes can be found in the form of direct product of the Slater determinants for electrons and for holes:

$$\Psi(\xi_1, ..., \xi_N, \xi'_1, ..., \xi'_M) = |\psi_1(\xi_1)...\psi_N(\xi_N)|.|\psi'_1(\xi'_1)...\psi'_M(\xi'_M)| \ , \tag{6}$$

where the electron and hole orbitals $\psi_i(\xi), \psi'_k(\xi)$ in the Slater determinants are spin dependent: $\psi_i(\xi) = \phi_i^\alpha(\vec{r})\sigma(\alpha)$ or $\phi_i^\beta(\vec{r})\sigma(\beta)$ for up- or down-spin electrons, and $\psi'_k(\xi) = {\phi'_k}^\alpha(\vec{r})\sigma(\alpha)$ or ${\phi'_k}^\beta(\vec{r})\sigma(\beta)$ for up- or down-spin holes.

In the Hartree-Fock-Roothaan formulation [4, 5, 12], the spatial parts of electron and hole orbitals $\phi_i^{\alpha,\beta}(\vec{r})$ and ${\phi'_k}^{\alpha,\beta}(\vec{r})$ are found in the form of expansions in the basis functions - the single electron and single hole wavefunctions:

$$\phi_i^{\alpha,\beta}(\vec{r}) = \sum_\nu C_{i\nu}^{\alpha,\beta} \chi^e_\nu(\vec{r}) \ , \ {\phi'_k}^{\alpha,\beta}(\vec{r}) = \sum_\mu {C'_{k\mu}}^{\alpha,\beta} \chi^h_\mu(\vec{r}) \ ,$$

where indexes ν, μ run over all single electron or hole states with quantum numbers (n, m).

The Coulomb interaction matrix elements in Hartree-Fock Roothaan equations with such basis functions can be calculated analytically (see *e.g.* [14]). Solving the unrestricted Hartree-Fock Roothaan equations self-consistently, one can obtain the total energy of the system which can be calculated by the following formula:

$$\begin{aligned} E &= \frac{1}{2}\sum_{\mu,\nu}\Big\{\delta_{\mu\nu}P^T_{\mu\nu}[\Omega_e(2n+|m|+1) + m\omega_{c_e}] + P^\alpha_{\mu\nu}F^\alpha_{\nu\mu} + P^\beta_{\mu\nu}F^\beta_{\nu\mu}\Big\} \\ &+ \frac{1}{2}\sum_{\mu,\nu}\Big\{\delta_{\mu\nu}{P'_{\mu\nu}}^T[\Omega_h(2n+|m|+1) - m\omega_{c_h}] + {P'_{\mu\nu}}^\alpha {F'_{\nu\mu}}^\alpha + {P'_{\mu\nu}}^\beta {F'_{\nu\mu}}^\beta\Big\}, \end{aligned} \tag{7}$$

where the explicit expressions for $P^T_{\mu\nu}, {P'_{\mu\nu}}^T, P^\alpha_{\mu\nu}, P^\beta_{\mu\nu}, {P'_{\mu\nu}}^\alpha, {P'_{\mu\nu}}^\beta$ and $F^{\alpha,\beta}_{\mu\nu}, {F'_{\mu\nu}}^{\alpha,\beta}$ are given in [4].

3. The numerical results and discussions

In this section we present the numerical results using the parameters appropriate for InAs/GaAs self-assembled quantum dots [4, 5, 12]: $m_e^* = 0.067m_o$, $m_h^* = 0.25m_o$, $\omega_e = 49$ meV, $\omega_h = 25$ meV, $\epsilon_s = 12.53$. The adopted units of length and energy are $a_B^* = \epsilon_s/m_e^* e^2 = 9.9$ nm, $2Ry^* = m_e^* e^4/\epsilon_s^2 = 11.61$ meV. The oscillator lengths for electrons and holes in the absence of magnetic fields $l_{e,h} = (m^*_{e,h}\omega_{e,h})^{-1/2}$ are 4.8 nm and 3.5 nm, respectively. These values are much smaller than the effective excitonic Bohr radius which is about 13 nm, that means that electrons and a hole in small InAs/GaAs dots are strongly confined.

The binding energies of the biexciton and the quadron in the ground state have been shown in Figure 1. One can see that for all range of the electron-to-hole oscillator length ratio l_e/l_h, the biexciton binding energy is always negative, indicating that biexciton is anti-binding. As for

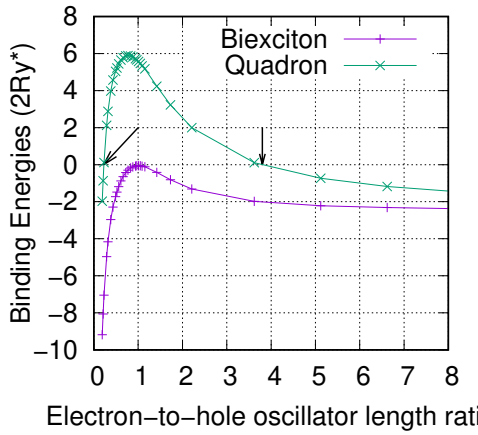

Figure 1. (color online) The binding energies of biexciton and quadron in the ground state as function of electron-to-hole oscillator length ratio.

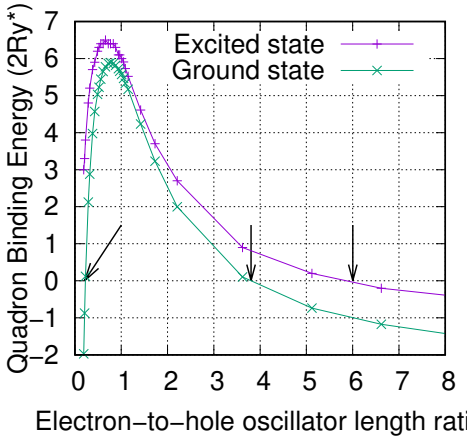

Figure 2. (color online) The comparison of the quadron binding energies in the ground and excited state as function of electron-to-hole oscillator length ratio.

the quadron, its binding energy is positive within the interval of $l_e/l_h \in [0.23 : 3.62]$, the ends of which are marked by arrows, indicating the quadron is bound. It becomes unbound when crossing outward this interval of the electron-to-hole oscillator length ratio. In [4, 5] we have analized the agreement between our rerults and the experimental data for the binding energy of the biexciton and charged excitons. Here we only note that for InAs/GaAs self-assembled quantum dot, the electron-to-hole oscillator length ratio $l_e/l_h = 1.3$ corresponds to the value of the biexciton binding energy $-0.45\ (2Ry^*) \approx -5.1$ meV, which agrees well with the experimental data interval [-1 meV : -6 meV] in [10].

In Figure 2 the quadron binding energies in the ground and excited states as function of electron-to-hole oscillator length ratio are compared. The quadron binding energy in the excited states is always larger than that of the ground state due to the contribution from the exchange interaction between the carriers with parallel spin in the excited state. Again, here we observe

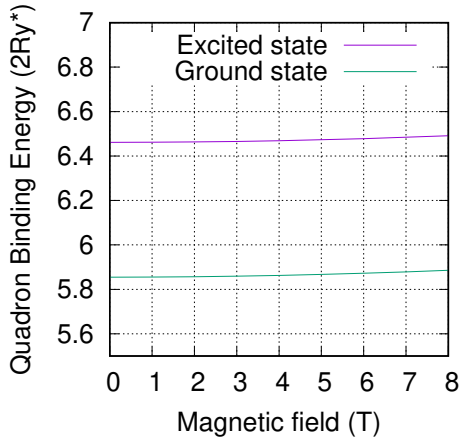

Figure 3. (color online) The quadron binding energy in the ground and excited state as function of magnetic fields.

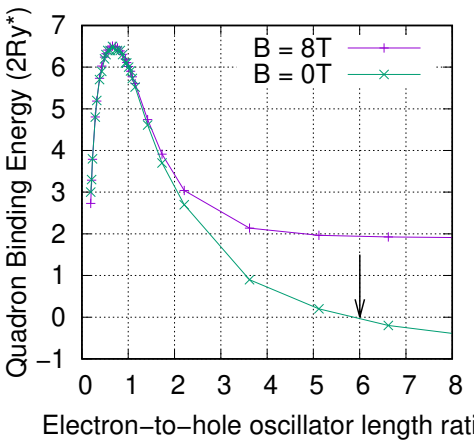

Figure 4. (color online) The comparison of the quadron binding energy in the excited state between the cases B=0T and B=8T.

the transition from binding to anti-binding state of the quadron for the regions of too large or too small values of the electron-to-hole oscillator length ratio. The ends of these interval are marked by arrows. Note that the situation for the biexciton in the excited state is similar as for the quadron in the excited state and not shown here. It is interesting to note that our new results can help to understand and clarify sensitive changes in the binding energy of a biexciton in natural ensembles of InAs / GaAs quantum dots with randomly fluctuating parameters [11].

Figure 3 and Figure 4 show the effect of the magnetic field on the quadron state. In Figure 3 the quadron binding energy in the ground and excited state as function of magnetic fields are presented. One can see that the binding energies increase with magnetic field due to additional confinement on the electron and hole caused by the magnetic field. However, this increase is small, about 0.03 $(2Ry^*) \approx 0.35$ meV at $B = 8$T. In Figure 4 the quadron binding energies in the excited state as function of the electron-to-hole oscillator length ratio are compared in two cases, without magnetic field and in the presence of magnetic field $B = 8$T. The magnetic field shows almost no effect at small values of ratio, but the effect is enhanced at large ratios of the oscillator strengths between the electron and the hole.

4. Conclusion

In conclusion, the quadron state in 2D parabolic quantum dots has been investigated by unrestricted Hartree-Fock method. The biexciton and quadron binding energies have been calculated for a full range of electron-to-hole oscillator length ratios. It is found that in the ground state of 2D InAs quantum dots, where the spins of the electrons are anti-parallel, the biexciton binding energy is negative for all range. However, the quadron binding energies is positive within a certain range of electron-to-hole oscillator length ratios. For the excited state with parallel spins of the carriers, it is shown that both the biexciton and quadron binding energies are larger than those in the ground state. The transition from anti-binding to binding state and vice versa of the biexciton and quadron have been found. The magnetic field dependence of the binding energy has been investigated and it is shown that magnetic fields increase the binding energies of biexciton and quadron but the effect is rather small. However, the impact of the magnetic field is enhanced at large ratios of the oscillator strengths between the electron and the hole. Our results help further clarify the properties of the basic excitations in semiconductor quantum dots and serve as a suggestion for experimental findings related to quadrons in quantum dots.

Acknowledgments

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