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Biexciton in 2D parabolic quantum dot in magnetic fields

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Abstract. We theoretically study biexciton, exciton and charged excitons confined in 2D parabolic quantum dots in a magnetic field by using an unrestricted Hartree-Fock method. The energy and binding energy of exciton and biexciton are presented as a function of magnetic field which show their increase with increasing magnetic field, although small. Our results for the case of strong confinement in InAs/GaAs self-assembled quantum dots show that, while the binding energies of both exciton and negatively charged exciton are positive, the binding energies of the biexciton and positively charged exciton are negative indicating that biexcitons in this system are antibinding.

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

1. Introduction

Exciton and biexcitons in different low-dimensional semiconductor systems have been intensively investigated both theoretically and experimentally in two last decades due to their promising physical properties for future electronics and devices [1–22]. The understanding of the physics of exciton and biexciton together with electron-electron and electron-hole Coulomb interactions which are increased due to lateral confinement is crucial to determine and control the energy structure, hence the electronic, optical, electrical and magnetic properties of the systems.

Most of theoretical approaches used to investigate few-electrons systems such as excitons, charged excitons and biexcitons in different low-dimensional semiconductor structures are method of hyperspherical harmonics [14], variational method [15, 16], diffusion Monte Carlo [17], configuration interaction [18–20] and Hartree-Fock method [21, 22]. The unrestricted Hartree-Fock method seems to be a good approximation for many-electron systems in parabolic quantum dots [23], and spherical quantum dots [24]. In our previous works [21, 22], the unrestricted Hartree-Fock method has been used successfully to study the charging effects, as well as external magnetic field effects on charged magnetoexcitons in parabolic quantum dots. While exciton binding energy is always positive, biexciton binding energy in 2D parabolic quantum dots can



be either positive or negative depending on the parameters of the system such as confinement (dot radius), magnetic field, and other relationship of Coulomb interactions between electrons and holes. However, until now the understanding of these situations remains unclear, even for self-assembled quantum dots which have been studied much so far [1, 9, 14, 18–20].

The aim of the present work is to develop an unrestricted Hartree-Fock method for few-electron and few-hole systems and to provide the detailed calculations of the energy and binding energy of excitonic systems, including exciton, biexciton, positively and negatively charged excitons in InAs/GaAs self-assembled quantum dots. Our numerical results agree very well with previous experimental measurements [19] for the binding energy of the biexciton and charged excitons in small InAs/GaAs self-assembled quantum dots.

2. The model and method

We consider excitons and biexcitons as a system of interacting electrons and holes confined in a 2D quantum dot with parabolic lateral potential in the presence of the perpendicular magnetic field $\vec{B} \parallel z$. In the framework of the effective-mass approximation, the total Hamiltonian of the system of N electrons ($N = 1, 2$) and M holes ($M = 1, 2$) can be written as follows

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

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 with ϵ being the dielectric constant in material. For the exciton and biexciton cases, we have $N=M=1$ and $N=M=2$ respectively. For charged excitons we have $N=1, M=2$ (positively charged) and $N=2, M=1$ (negatively charged).

The Hamiltonians for a single electron (with notations i, e) and single hole (with notations k, h) in a quantum dot with parabolic confinement in a magnetic field are the following:

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

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

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.

The eigenfunction in polar coordinates $\vec{r} = (r, \varphi)$ and the eigenvalue of the single electron and single hole Hamiltonian in the quantum states (n, m) are:

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

$$E_{n,m}^e = \Omega_e(2n + |m| + 1) + \frac{1}{2}m\omega_{ce}, \quad (5)$$

$$\chi_{n,m}^h(r, \varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi} \sqrt{\frac{2n!}{(n+|m|)!}} \alpha_h (\alpha_h r)^{|m|} e^{-(\alpha_h r)^2/2} L_n^{|m|}((\alpha_h r)^2), \quad (6)$$

$$E_{n,m}^h = \Omega_h(2n + |m| + 1) - \frac{1}{2}m\omega_{c_h}, \quad (7)$$

where $L_n^{|m|}(r)$ is generalized Laguerre polynomial, and

$$\Omega_e = (\omega_e^2 + \frac{1}{4}\omega_{c_e}^2)^{1/2}, \quad \alpha_e = \sqrt{m_e^* \Omega_e}, \quad (8)$$

$$\Omega_h = (\omega_h^2 + \frac{1}{4}\omega_{c_h}^2)^{1/2}, \quad \alpha_h = \sqrt{m_h^* \Omega_h}. \quad (9)$$

In the framework of the unrestricted Hartree-Fock approximation, 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:

$$\Psi(\xi_1, \dots, \xi_N, \xi'_1, \dots, \xi'_M) = |\psi_1(\xi_1) \dots \psi_N(\xi_N)| \cdot |\psi'_1(\xi'_1) \dots \psi'_M(\xi'_M)|, \quad (10)$$

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 [22], 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 $\chi_{nm}^e(\vec{r})$ and $\chi_{nm}^h(\vec{r})$ defined by (4) and (6), respectively:

$$\phi_i^{\alpha,\beta}(\vec{r}) = \sum_{\nu} C_{i\nu}^{\alpha,\beta} \chi_{\nu}^e(\vec{r}), \quad (11)$$

$$\phi'_k{}^{\alpha,\beta}(\vec{r}) = \sum_{\mu} C'_{k\mu}{}^{\alpha,\beta} \chi_{\mu}^h(\vec{r}), \quad (12)$$

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

Note that in such a basis, the Coulomb interaction matrix elements in Hartree-Fock Roothaan equations can be calculated analytically (see *e.g.* [10]). We solve the unrestricted Hartree-Fock Roothaan equations self-consistently. Once wave functions are known, the total energy of the system can be calculated according to the following formula

$$E = \frac{1}{2} \sum_{\mu,\nu} \left\{ \delta_{\mu\nu} P_{\mu\nu}^T [\Omega_e(2n + |m| + 1) + m\omega_{c_e}] + P_{\mu\nu}^{\alpha} F_{\nu\mu}^{\alpha} + P_{\mu\nu}^{\beta} F_{\nu\mu}^{\beta} \right\} \\ + \frac{1}{2} \sum_{\mu,\nu} \left\{ \delta_{\mu\nu} P'_{\mu\nu}{}^T [\Omega_h(2n + |m| + 1) - m\omega_{c_h}] + P'_{\mu\nu}{}^{\alpha} F'_{\nu\mu}{}^{\alpha} + P'_{\mu\nu}{}^{\beta} F'_{\nu\mu}{}^{\beta} \right\}, \quad (13)$$

where

$$P_{\mu\nu}^T = P_{\mu\nu}^{\alpha} + P_{\mu\nu}^{\beta}, \quad P'_{\mu\nu}{}^T = P'_{\mu\nu}{}^{\alpha} + P'_{\mu\nu}{}^{\beta}, \\ P_{\mu\nu}^{\alpha} = P_{\nu\mu}^{\alpha} = \sum_{i=1}^{N_{\alpha}} C_{\mu i}^{\alpha} C_{\nu i}^{\alpha*}, \quad P_{\mu\nu}^{\beta} = P_{\nu\mu}^{\beta} = \sum_{i=1}^{N_{\beta}} C_{\mu i}^{\beta} C_{\nu i}^{\beta*}, \\ P'_{\mu\nu}{}^{\alpha} = P'_{\nu\mu}{}^{\alpha} = \sum_{k=1}^{M_{\alpha}} C'_{\mu k}{}^{\alpha} C'_{\nu k}{}^{\alpha*}, \quad P'_{\mu\nu}{}^{\beta} = P'_{\nu\mu}{}^{\beta} = \sum_{k=1}^{M_{\beta}} C'_{\mu k}{}^{\beta} C'_{\nu k}{}^{\beta*},$$

with $N_\alpha(M_\alpha)$ and $N_\beta(M_\beta)$ being the number of up-spin and down-spin electrons (holes), respectively, $N_\alpha + N_\beta = N$, $M_\alpha + M_\beta = M$, and

$$\begin{aligned}
F_{\mu\nu}^{\alpha,\beta} &= \delta_{\mu\nu}[\Omega_e(2n + |m| + 1) + m\omega_{c_e}] + \sum_{\lambda,\sigma} P_{\lambda\sigma}^T \langle \chi_\mu^e(1)\chi_\sigma^e(2) | \frac{e^2}{\epsilon r_{12}} | \chi_\nu^e(1)\chi_\lambda^e(2) \rangle \\
&\quad - \sum_{\lambda,\sigma} P_{\lambda\sigma}^{\alpha,\beta} \langle \chi_\mu^e(1)\chi_\sigma^e(2) | \frac{e^2}{\epsilon r_{12}} | \chi_\lambda^e(1)\chi_\nu^e(2) \rangle \\
&\quad - \sum_{\lambda,\sigma} P_{\lambda\sigma}^{\prime T} \langle \chi_\mu^e(1)\chi_\sigma^h(2) | \frac{e^2}{\epsilon r_{12}} | \chi_\nu^e(1)\chi_\lambda^h(2) \rangle,
\end{aligned} \tag{14}$$

$$\begin{aligned}
F_{\mu\nu}^{\prime\alpha,\beta} &= \delta_{\mu\nu}[\Omega_h(2n + |m| + 1) + m\omega_{c_h}] + \sum_{\lambda,\sigma} P_{\lambda\sigma}^{\prime T} \langle \chi_\mu^h(1)\chi_\sigma^h(2) | \frac{e^2}{\epsilon r_{12}} | \chi_\nu^h(1)\chi_\lambda^h(2) \rangle \\
&\quad - \sum_{\lambda,\sigma} P_{\lambda\sigma}^{\prime\alpha,\beta} \langle \chi_\mu^h(1)\chi_\sigma^h(2) | \frac{e^2}{\epsilon r_{12}} | \chi_\lambda^h(1)\chi_\nu^h(2) \rangle \\
&\quad - \sum_{\lambda,\sigma} P_{\lambda\sigma}^T \langle \chi_\mu^h(1)\chi_\sigma^e(2) | \frac{e^2}{\epsilon r_{12}} | \chi_\nu^h(1)\chi_\lambda^e(2) \rangle.
\end{aligned} \tag{15}$$

3. The numerical results and discussions

Using the formula (13), numerical calculations have been done to study the energy of exciton (E_X), biexciton (E_{XX}) and charged excitons (E_{X+} , E_{X-}) in dependence of magnetic field. Then the binding energy of the systems is found as defined by $E_{XX}^b = 2 * E_X - E_{XX}$ for biexciton, $E_X^b = E^e + E^h - E_X$ for exciton, $E_{X+}^b = E^h + E_X - E_{X+}$ for positively charged exciton, $E_{X-}^b = E^e + E_X - E_{X-}$ for negatively charged exciton.

The effective Bohr radius $a_B^* = \hbar^2 \epsilon / m_e^* e^2$ has been adopted as an unit of length and two times of the effective Rydberg $2Ry^* = m_e^* e^4 / \hbar^2 \epsilon^2$ as an unit of energy. For numerical calculations for InAs/GaAs self-assembled quantum dots, same parameters as in [21, 22] have been used, namely: $m_e^* = 0.067m_o$, $m_h^* = 0.25m_o$, $\omega_e = 49$ meV, $\omega_h = 25$ meV, $\epsilon_s = 12.53$. The corresponding units of length and energy are $a_B^* = 9.9$ nm, $2Ry^* = 11.61$ meV. The oscillator lengths for electrons and holes in the absence of magnetic fields $L_{e,h} = \sqrt{\hbar / (m_{e,h}^* \omega_{e,h})}$ 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 dependence of the exciton energy and binding energy on the magnetic field has been studied. In Fig.1 the energy and binding energy of the exciton as function of magnetic fields are presented. One can see that the magnetic field increases both energy and binding energy of the exciton as expected, mainly because the magnetic field gives additional confinement on the electron and hole increasing their total energies. The result for biexciton energy has been shown in Fig. 2, where for comparison purpose the exciton energy multiplied by 2 has also been plotted. For all variation range of magnetic field the biexciton energy is always larger than two times of exciton energy (the actual calculations are for very large fields, but Fig. 2 has been shown only up to 8 T since the qualitative behaviour remains the same). These results indicate that the biexciton binding energy is negative ($E_{XX}^b = 2 * E_X - E_{XX}$), and at the same time, biexciton is antibinding and unstable in such a system.

The negative biexciton binding energy is shown in Fig. 3 together with the binding energy of the charged excitons. For all variation range of magnetic field, the binding energies of the biexciton and the positively charged exciton are negative, whereas the binding energy of the negatively charged exciton is always positive. The increase of binding energies of the biexciton

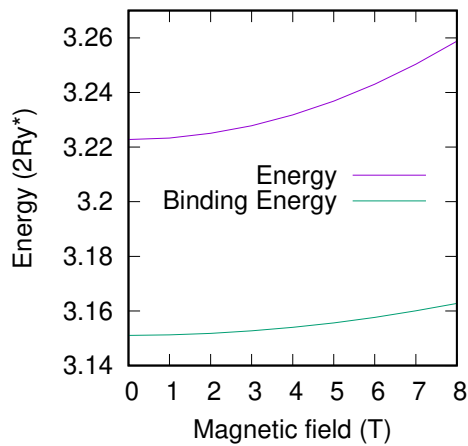


Figure 1. (color online) The energy and binding energy of exciton as function of magnetic fields.

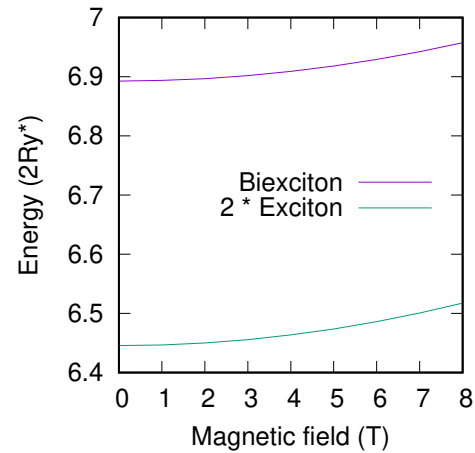


Figure 2. (color online) The energy of biexciton and exciton (multiplied by 2) as function of magnetic fields.

and charged excitons are very small, almost un-noticeable. Our results agree very well with the experimental measurement for the binding energy of the biexciton and charged excitons in small InAs/GaAs self-assembled quantum dots [19]. Thus, from our calculation the binding energy of the negatively charged exciton almost remain fixed at about $0.58 (2Ry^*) \approx 6.8$ meV, which compares well with the experimental value 6.2 ± 0.4 meV. The results for biexciton and positively charged exciton binding energies are $-0.45 (2Ry^*) \approx -5.1$ meV and $-0.62 (2Ry^*) \approx -7.2$ meV, respectively, which are just in the range of experimental data for different dots, namely from -1 to -6 meV for biexciton, and from -7 to -12 meV for positively charged exciton [19].

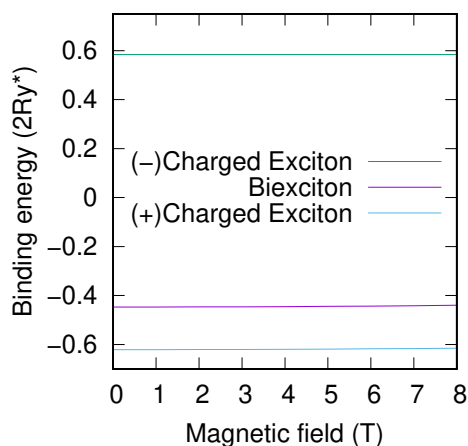


Figure 3. (color online) The binding energies of biexciton and (+/-) charged excitons as function of magnetic fields.

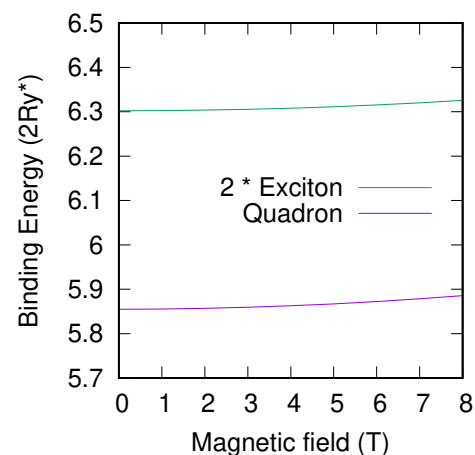


Figure 4. (color online) The binding energies of exciton (multiplied by 2) and quadron as function of magnetic fields.

Fig.4 displays the variation of binding energies of a single exciton (multiplied by 2) and quadron - the four-particle system with two electrons and two holes ($2e+2h$). It is interesting to note while biexciton as two interacting excitons is antibinding, the four-particle system with two electrons and two holes is binding as a whole. To our knowledge, this has been never noted

so far in the literature. It is possible that in small InAs/GaAs self-assembled quantum dots a bound quadron would rather be formed instead of a bound biexciton. Since $E_{XX} = E_{2e+2h}$ in our calculation approach, we have established a relation between the binding energies of the biexciton, quadron and exciton by an equality: $E_{XX}^b = E_{2e+2h}^b - 2 * E_X^b$, and it has been exactly checked during our numerical calculation for all variation range of magnetic field.

4. Conclusion

The excitonic systems, including exciton, biexciton, and charged excitons, are investigated by unrestricted Hartree-Fock method. It is found that in small InAs/GaAs self-assembled quantum dots while the exciton and negatively charged exciton always have positive binding energy, the binding energy of biexciton and positively charged exciton are negative. These results show that biexciton and positively charged exciton are antibinding and unstable. The magnetic field dependence of the energy and binding energy has been investigated and found to be very weak. Our results agree very well with the experimental data for the binding energy of the biexciton and charged excitons in small InAs/GaAs self-assembled quantum dots.

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