

ABSORPTION SPECTRUM OF AN EXCITON IN AN $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ QUANTUM DOT IN THE PRESENCE OF A MAGNETIC FIELD

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We calculate the absorption spectrum of a single exciton, confined in an $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ disk-shaped quantum dot, as a function of the strength of an applied magnetic field. Exciton eigenstates are obtained by numerical diagonalization of the Hamiltonian, within the effective mass approximation. A correction in the expression of the Coulomb interaction matrix elements is verified.

1. Introduction

Many experimental results on the optical and electronic properties of quantum dots have been reported in the last decade. Extreme spatial confinement for electrons and holes, physically implemented in quantum dots, provides an exciting opportunity for controlled manipulation for carrier states and optical, electronic and thermoelectric properties. Quantum dots absorb and emit light in a very narrow spectral range, which can be manipulated by means of a magnetic field, for instance. One application is the design of more efficient and more precisely tunable semiconductor lasers.¹ Also, control of the number of excitons in OD systems opens up interesting possibilities, from exciton condensation, single photonics, to optical quantum logic gates.² In earlier works on magnetoexcitons in quantum dots both the strong³ and the weak⁴ confinement regime were studied, and spatial confinement asymmetry was considered.⁵ Here, a numerical method for obtaining the exciton absorption spectrum in the strong confinement situation is reviewed and applied to $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ self assembled quantum dots. Also, the main steps to calculate the Coulomb interaction matrix element between the electron and the hole in the non-interacting configuration basis are shown, and a correction in the expression for this matrix element is verified.^{6,7}

2. Model

The system is formed by an electron–hole pair with Coulomb interaction, confined in a two-dimensional disk-shaped quantum dot, in the presence of a uniform and constant magnetic field, perpendicular to the plane of the dot. The lateral confinement is represented as an isotropic parabolic potential. In the effective mass approximation, the Hamiltonian of the noninteracting electron–hole pair can be expressed in terms of the Fock–Darwin states⁷ as

$$H_{e-h} = \hbar\omega_+^e \left(N_+^e + \frac{1}{2} \right) + \hbar\omega_-^e \left(N_-^e + \frac{1}{2} \right) + \hbar\omega_+^h \left(N_+^h + \frac{1}{2} \right) + \hbar\omega_-^h \left(N_-^h + \frac{1}{2} \right), \quad (1)$$

where the index e (h) refers to the electron (hole) and $\omega_{\pm} = \sqrt{\omega_o^2 + \frac{1}{4}\omega_c^2} \pm \frac{1}{2}\omega_c$. The confinement and the cyclotron frequencies are ω_o and ω_c respectively and $N_+ = a_+^\dagger a_+$ ($N_- = a_-^\dagger a_-$) is the number operators for right (left) circularly polarized quanta.

Keeping in mind the band structure model of a quantum dot, we assume that electrons and holes are independently bound in the dot due to local inflections of the edges of the valence and conduction bands. The two particle states are the products of electron and hole single particle states: $|n_+^e n_-^e, n_+^h n_-^h\rangle = |n_+^e n_-^e\rangle \otimes |n_+^h n_-^h\rangle$. The projections

of the angular momenta onto the field direction are $l_{ze} = \hbar(n_-^e - n_+^e)$ and $l_{zh} = \hbar(n_+^h - n_-^h)$.

The Hamiltonian for a two-dimensional exciton in a parabolic confinement potential can be written as

$$H = H_{e-h} - \frac{e^2}{\epsilon|\mathbf{r}_e - \mathbf{r}_h|} = H_{e-h} + V_{eh}, \quad (2)$$

where V_{eh} is the electron–hole Coulomb interaction, $\mathbf{r}_{e,h}$ are the electron (hole) positions and ϵ is the dielectric constant. We will consider the strong confinement regime, where the exciton Bohr radius (a_B^{exc}) is larger than the quantum dot radius (R), and therefore the electron–hole interaction energy is smaller than the confinement energy.⁸ This situation can be realized, for instance, in $\text{In}_{0.5}\text{Ga}_{0.5}\text{As}/\text{GaAs}$ self-assembled quantum dots.⁹ We use $a_B^{\text{exc}} = 34$ nm and $R = 18$ nm. The characteristic confinement energy $\hbar\omega_{0,e} + \hbar\omega_{0,h}$ (50 meV) exceeds the characteristic Coulomb energy of the base state (21 meV).

We calculate the eigenfunctions and eigenvalues of the exciton by numerical diagonalization. The Hamiltonian of the system is divided into two parts, $H = H_{e-h} + V_{eh}$, and the exciton eigenfunctions are expanded in terms of the noninteracting system eigenfunctions. The original problem of finding the eigenfunctions and eigenvalues of H is transformed into a matrix diagonalization problem now, where the diagonal matrix elements (noninteracting Hamiltonian) dominate over the off-diagonal matrix elements (Coulomb contributions). In this case, it is possible to use a rapidly converging procedure where the total infinite matrix is approximated by a finite

one. The results are checked by increasing the size of the finite matrix. The basis functions are chosen such that they are the lowest-energy states of the H_{e-h} Hamiltonian, as usual. The calculations are greatly simplified by the fact that the total angular momentum, L , is a constant of motion and therefore provides a good quantum number. The complexity of numerical calculations can be reduced for optical interband transitions when only states with $L = 0$ are considered. We use the first 15 functions as the basis, since the results do not appreciably change with a larger basis.

Coulomb interaction matrix elements can be calculated in the noninteracting electron–hole pair basis as $\langle N_+^e N_-^e, N_+^h N_-^h | V_{eh} | n_+^e n_-^e, n_+^h n_-^h \rangle$, using the two-dimensional Coulomb interaction in momentum representation

$$V_{eh} = -\frac{e^2}{\epsilon|\mathbf{r}_e - \mathbf{r}_h|} = -\frac{e^2}{2\pi\epsilon} \int \frac{e^{i\mathbf{q}\cdot(\mathbf{r}_e - \mathbf{r}_h)}}{q} d^2q, \quad (3)$$

where $\mathbf{q} = q_x \mathbf{i} + q_y \mathbf{j}$. The electron and hole position operators \mathbf{r} should be expressed in terms of the creation and annihilation operators for right (\hat{a}_+) and left (\hat{a}_-) circularly polarized quanta. So, we find for the electron part

$$\mathbf{q} \cdot \mathbf{r}_e = q_e \hat{a}_+ + q_e^* \hat{a}_+^\dagger + q_e^* \hat{a}_- + q_e \hat{a}_-^\dagger. \quad (4)$$

Here q_e is the complex number $(q_x + iq_y)/2\beta_e$ and $\beta_e = (m\omega_e/\hbar)^{1/2}$.

Using commutation properties, the action of the $e^{i\mathbf{q}\cdot\mathbf{r}_e}$ term over the Fock–Darwin states is evaluated:

$$\begin{aligned} \langle N_+^e N_-^e | e^{i\mathbf{q}\cdot\mathbf{r}_e} | n_+^e n_-^e \rangle &= e(q) \sum_{p_e=0}^{\min(N_+^e, n_+^e)} \frac{i^{2p_e + |N_+^e - n_+^e|} \left(\frac{q}{2\beta_e}\right)^{|2p_e + |N_+^e - n_+^e||} e^{i\theta(n_+^e - N_+^e)} \sqrt{N_+^e! n_+^e!}}{p_e! (\min(N_+^e, n_+^e) - p_e)! (p_e + |N_+^e - n_+^e|)!} \\ &\times e(q) \sum_{k_e=0}^{\min(N_-^e, n_-^e)} \frac{i^{2k_e + |N_-^e - n_-^e|} \left(\frac{q}{2\beta_e}\right)^{|2k_e + |N_-^e - n_-^e||} e^{i\theta(N_-^e - n_-^e)} \sqrt{N_-^e! n_-^e!}}{k_e! (\min(N_-^e, n_-^e) - k_e)! (k_e + |N_-^e - n_-^e|)!}, \end{aligned} \quad (5)$$

where $e(q) = e^{-\frac{1}{2}|\frac{q}{2\beta_e}|^2}$ and $\theta = \arctan(q_y/q_x)$. The hole term is evaluated in an analogous way. Keeping in mind that $N_\pm^{e,h}$ and $n_\pm^{e,h}$ are integer numbers, the evaluation of the angular part of the integral in the complex plane gives

$$\int_0^{2\pi} e^{i\theta(L_{ze} + L_{zh} - l_{ze} - l_{zh})} d\theta = 2\pi \delta_{L_z, l_z}, \quad (6)$$

where $L_z = L_{ze} + L_{zh}$ ($l_z = l_{ze} + l_{zh}$) is the projection of the final (initial) total angular momentum of the pair onto the field direction. This means that the matrix element between the states vanish, unless they possess the same total angular projection in the field direction.

Finally, after several mathematical steps the form of the Coulomb interaction matrix element is⁷

$$\begin{aligned}
 \langle N_+^e N_-^e, N_+^h N_-^h | V_{eh} | n_+^e n_-^e, n_+^h n_-^h \rangle &= \frac{-E_o \sqrt{\Omega_{e-h}} \delta_{L_z, l_z} (-1)^{S_e + s_e}}{\sqrt{N_+^e! N_-^e! N_+^h! N_-^h! n_+^e! n_-^e! n_+^h! n_-^h!}} \\
 &\times \sum_{p_e=0}^{\min(N_+^e, n_+^e)} \sum_{k_e=0}^{\min(N_-^e, n_-^e)} \sum_{p_h=0}^{\min(N_+^h, n_+^h)} \sum_{k_h=0}^{\min(N_-^h, n_-^h)} p_e! k_e! p_h! k_h! \\
 &\times \binom{N_+^e}{p_e} \binom{n_+^e}{p_e} \binom{N_-^e}{k_e} \binom{n_-^e}{k_e} \binom{N_+^h}{p_h} \binom{n_+^h}{p_h} \binom{N_-^h}{k_h} \binom{n_-^h}{k_h} \left(-\frac{1}{2}\right)^p \\
 &\times \left(\frac{\Omega_{e-h}}{\Omega_e}\right)^{\frac{S_e + s_e}{2} - p_e - k_e} \left(\frac{\Omega_{e-h}}{\Omega_h}\right)^{\frac{S_h + s_h}{2} - p_h - k_h} \frac{\Gamma(p + \frac{1}{2})}{\sqrt{2\pi}}, \quad (7)
 \end{aligned}$$

where $E_o = R_y \sqrt{2\pi} a_o / l_o$ is the effective energy scale; $R_y = e^2 / 2\epsilon a_o$ is the effective Rydberg; $a_o = \hbar^2 / m_e^2$ is the effective Bohr radius; $l_o = \sqrt{\hbar c / eB}$ is the magnetic length, $\Omega_{e(h)} = \sqrt{1 + 4(\omega_{oe(h)} / \omega_{ce(h)})^2}$, $2\Omega_{e-h}^{-1} = \Omega_e^{-1} + \Omega_h^{-1}$, $p = N_+^e + n_-^e + N_-^h + n_+^h - p_e - k_e - p_h - k_h$, and $s = n_+ + n_-$ ($S = N_+ + N_-$). This result is at variance with Ref. 6, but agrees with Ref. 7, showing that the result of the former reference must be corrected.

3. Absorption Spectrum

The wavelength of light that interacts with the system is much larger than the dot size. Therefore, the Hamiltonian that describes the interaction between the system and the electromagnetic wave can be written in the dipole approximation. In first order of perturbation theory, the probability of creation of an exciton when the system absorbs a photon is determined by the Fermi golden rule. The absorption coefficient is proportional to this quantity and is represented for

$$\alpha(\omega) \propto \sum_f |\langle f | \mathbf{P} | 0 \rangle|^2 \delta(E_f - E_o - \hbar\omega) \quad (8)$$

Here, $|0\rangle$ is the initial state of the system, which corresponds to an empty quantum dot, $|f\rangle$ is a final state corresponding to a single exciton in the dot, and \mathbf{P} is the dipole transition operator.

4. Results

The parameters used correspond to $In_{0.5}Ga_{0.5}As/GaAs$ self-assembled quantum dots⁸ with confining potentials for the electron and the hole of $\hbar\omega_{oe} = 30$ meV and $\hbar\omega_{oh} = 15$ meV respectively.³ All energy

transitions are measured from valence to conduction band gap and the absorption intensities are reported in arbitrary units (arb.units).

Figure 1 shows the absorption spectrum of the noninteracting electron-hole pair as a function of the magnetic field. At zero magnetic field, there are degenerate transitions. As the magnetic field is increased the degeneracies are lifted due to diamagnetic behavior ($n_+^{e,h} \geq n_-^{e,h}$) or paramagnetic behavior ($n_-^{e,h} > n_+^{e,h}$). A major feature of the spectrum is the transition energy crossings, which occur at fields of 11 T and 19 T approximately. See the arrows in Fig. 1. For strong magnetic fields $\omega_c \gg \omega_o$, the well-known Landau levels are present.

In Fig. 2 we can observe the exciton absorption spectrum as a function of the magnetic field.

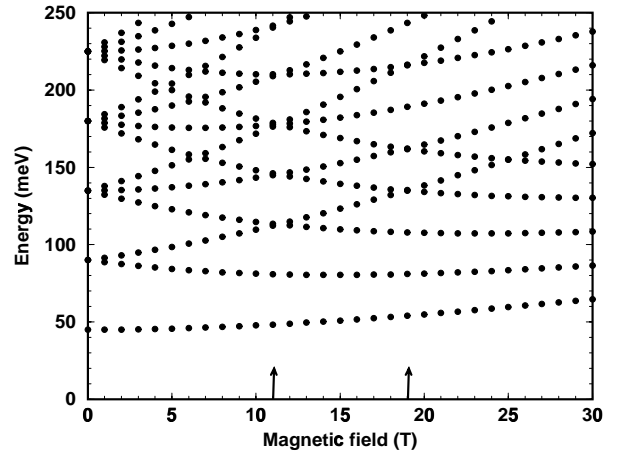


Fig. 1. Absorption spectrum of the electron-hole pair as a function of the magnetic field.

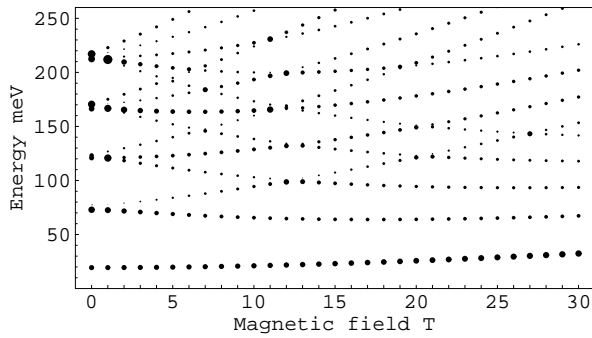


Fig. 2. Absorption spectrum of an exciton as a function of the magnetic field.

This shows the difference of intensity among the transitions, which it is proportional to the size of the circles. The main effects of Coulomb interaction are to decrease the transition energies and to lift the degeneracies at zero magnetic field. The new level crossings occur at fields around 12 T and 20 T, approximately one tesla above the values obtained in the noninteracting case. However, the exciton spectrum resembles the spectrum of an electron–hole pair, as expected in the strong confinement regime, where Coulomb interaction is a small effect.

Figure 3, top panel, corresponds to the absorption spectrum of the electron–hole pair at zero field. The linear increase in the absorption intensity as a function of energy is entirely due to level degeneracies. In order to take into account effects such as interaction among quantum dots, variations in their shape or size, and other disorder effects, we use a phenomenological inhomogeneous Gaussian broadening.

The bottom panel of Fig. 3 shows the absorption spectrum of the exciton at zero magnetic field as a function of energy. Coulomb interaction modifies the intensity of the peaks. In particular the figure shows the appearance of selection rules for optical transitions. Despite the approximate conservation of the total intensity of each shell, giving by the appropriate areas, the intensity of particular transitions is strongly enhanced or forbidden. Notice, for example, that the fifth shell has contribution from only two of the five possible transitions. Our numerical results predict a transfer of intensity from the stronger peak to the lower one. This result deserves further research. The differences in the relative intensity of energy transitions are proportional to the size of the

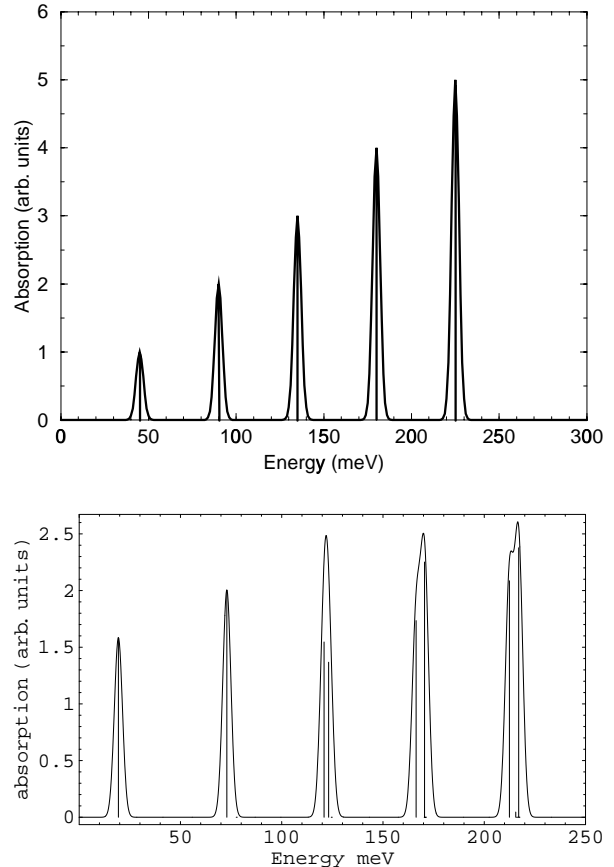


Fig. 3. Absorption spectrum of the e - h pair (top panel) and the exciton (bottom panel) at $B = 0$ T.

filled circles in Fig. 2. Also, we observe the shift of the spectrum toward lower energies.

We compare our results with experimental measures from the photoluminescence spectrum at zero magnetic field of self-assembled quantum dots.⁹ Our energy differences between nearest neighbor levels are in agreement with the experimental report. We expect that the deviations between the results can be explained as many-body effects not considered in this work.

5. Conclusions

We have corroborated a correction in the expression for Coulomb interaction matrix elements. Moreover we have shown that Coulomb interaction produces three main effects: the shift of the absorption spectrum toward low energies, the lift of degeneracy at zero magnetic field, and the appearance of selection rules for optical transitions. The theoretical energy

difference between optical transitions is in agreement with experimental results for zero magnetic field.

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