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Influence of the coupling between center of mass and internal degrees of freedom on the binding energy of magnetotrions

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We present the effects of the center-of-mass dynamics on the negatively charged exciton bound states in the presence of longitudinal magnetic and electric fields. We consider an idealized $GaAs/Al_{0.3}Ga_{0.7}As$ quantum well in the low-field limit and use the configuration interaction method to build up the two-particle basis set. Our results show that the dynamics of the charged exciton center of mass has to be taken into account for a realistic description of the bound states.

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In recent years, there has been an intense discussion about the behavior of positively (X^+) and negatively (X^-) charged excitons in the presence of magnetic field using quantum well (QW) samples. The X^+ photoluminescence spectrum was studied by Shields *et al.*[1] for fields up to 8 T. The high magnetic field limit was investigated by Hayne *et al.*[2] in the case of X^-. Glasberg *et al.*[3] studied the magnetic field influence on the bound states of both charged excitons using the same sample. On the theoretical point of view, the magnetic field influence on the charged exciton bound states has also been investigated.[4–6] Riva *et al.*[5] used the *stochastic variational method* and reached a good agreement with experimental results. Whittaker and Shields[6] studied the high magnetic field limit using a Landau levels basis set for the in-plane (xy) motion.

In a previous work,[7] which we refer as DB from now on, we presented variational calculations of the binding energy of charged excitons (trions) in idealized $GaAs/Al_{0.3}Ga_{0.7}As$ QW's in the absence of magnetic fields. We showed the importance of going beyond the fundamental QW states approximation in order to obtain a quantitative description of the binding energies. This shows that the dynamics of the confined degrees of freedom has to be considered. The aim of this report is to complement the previous analysis with the influence of the trion center-of-mass (CM) dynamics on the negatively charged exciton bound states when a low magnetic field is present. Here, low magnetic field means that the internal degrees of freedom are not strongly affected by the field. As a consequence, we use the same in-plane coordinates, namely, each electron relative to the hole and the CM of the whole system, and relative particle basis set employed in DB (Ref. 7) adding the CM contribution which is no more a free particle. To define low magnetic field in a more quantitative way, we compare the Coulomb interactions energy with the cyclotron one. The neutral exciton binding energy is of the order of 10 meV. On the other hand, the ''second'' electron increases the binding energy of the complex by roughly 1 meV in the absence of external fields. Taking the electronic cyclotron energy as $1.7\times B(T)$ meV for GaAs, one can see that even few Teslas may be considered as a high field for the ''second'' electron. In conclusion, the so-called low magnetic field is actually a delicate limit that has to be carefully treated. Our results show that the trion CM has an important contribution to the binding energy which cannot be properly calculated in the first Landau level approximation even in the low-field limit.

We consider a spin independent Hamiltonian. The trion states can be labeled through the total spin of the two electrons ($S=S_1+S_2$) and the trial wave functions can be separated in singlet and triplet sates. The z component (growth direction) of the total angular momentum is also a good quantum number used to label the trion states in our approximation. The wave function symmetry required by the two electrons indistinguishability leads us to work with a basis set of Slater determinants formed by the single-particle basis wave functions (configuration interaction method). In our case, the one-particle states are nonorthogonal and we solve the *generalized eigenvalue problem*.

As said before, in DB (Ref. 7) we showed the importance of including more than one QW state for electrons and holes in the trion trial wave function. Here, we limit our basis set to the fundamental QW state for electrons. This approximation limits the quantitative validity of our analysis but retains the main physical aspects for the analysis of the influence of the trion CM degree of freedom on its bound states when a magnetic field is present. To include fully the dynamics of all degrees of freedom requires an extremely large basis which is beyond the scope of this work.

Obviously, the trion CM is not sensitive to the internal Coulomb interactions, but as a charged particle it is sensitive to the presence of a magnetic field. As a consequence, it is possible to describe it through Landau levels. The spatial part of the charged exciton trial wave function is given by

$$\Psi=\sum_{i,j,m,n,p,q} c_{i,j,m,n,p,q} N_{i,j,m,n,p,q}\cdot\Lambda_q(\vec{R})\cdot\chi_p(z_h)\cdot\chi_0(z_{e1})\cdot\chi_0(z_{e2})[\,\phi_i^m(\vec{\rho}_1)\phi_j^n(\vec{\rho}_2)\pm\phi_j^n(\vec{\rho}_1)\phi_i^m(\vec{\rho}_2)\,], \tag{1}$$

where $c_{i,j,m,n,p}$ is a linear variational parameter, $N_{i,j,m,n,p}$ is the determinant normalization, $\Lambda_q(\vec{R})$ is the q*th* CM Landau level, $\chi_p(z)$ is the p*th* electron (e) or hole (h) QW solution, $\phi_i^m(\vec{\rho})$ is the relative particle wave function. In Eq. (1) "+" builds up the singlet states while "−" builds up the triplet ones. In the absence of magnetic field, only the singlet state with zero total relative particle angular momentum is a bound state.

The exciton trial wave function is analogous to the trion one. It is interesting to notice that in the exciton case the CM is a neutral particle. Although, even in this case, the CM and relative coordinates are coupled,[8] in the configuration we are considering here, namely, parallel external electric and magnetic fields, the exciton ground-state (Kcm = 0) presents a decoupled wave function for CM and relative coordinates. This is the case we are interested in order to compare with the trion ground state.

We consider external electric and magnetic fields in the z direction. Using the Coulomb gauge, the relative vector potential is given by: $\vec{A}_r=\frac{1}{2}\vec{B}\times\vec{r}$. The CM degrees of freedom can be omitted in the exciton description through a unitary transformation that eliminates the CM vector potential from the Hamiltonian.[9] The transformed Hamiltonian for the neutral exciton is written as

$$H_{ex}=H(z_e)+H(z_h)+H_B+T_{xy}+V_c, \tag{2}$$

where

$$H(z_{e,h})=\frac{1}{2m_{e,hz}}p_{ez,hz}^2+V_{we,wh}Y\left(\frac{L}{2}-|z_{e,h}|\right)\pm|e|Fz_{e,h}, \tag{3}$$

$$H_B=\frac{e^2}{2c^2\mu}\vec{A}_\rho^2+\frac{e}{c}\left(\frac{1}{m_e}-\frac{1}{m_{hxy}}\right)\vec{A}_\rho\cdot\vec{p}, \tag{4}$$

$$T_{xy}=\frac{\vec{p}^2}{2\mu}, \tag{5}$$

$$V_c=-\frac{e^2}{\varepsilon\sqrt{(z_e-z_h)^2+\rho^2}}. \tag{6}$$

Here the QW potential height for electrons (e) and holes (h) is given by $V_{we,wh}$, $Y(z)$ is the step function, L is the QW width, F is the magnitude of the electric field, μ is the exciton in-plane reduced mass, $\vec{p}$ is the relative coordinate linear momentum, $\vec{A}_\rho$ is its vector potential and ε is the GaAs static dielectric constant. The sign "+" is used for electrons and "−" for holes in the electric field component of H($z_{e,h}$).

The relative particle angular momentum conservation leads to the use of only s-like functions in the exciton ground-state basis set. We define the reference value for the exciton binding energy $E_b(X^0)$ as the energy of a noninteracting electron-hole pair in the presence of an external magnetic field. The energy of the fundamental QW states are taken as zero :

$$E_b(X^0)=E(X^0)-\frac{eB\hbar}{2c\mu} \tag{7}$$

In the case of charged excitons, when a longitudinal magnetic field is present, the in-plane conjugate linear momentum, $\vec{\Pi}$, is conserved. In other words, the $\vec{\Pi}$ operator commutates with the Hamiltonian and its eigenvalue is a constant of motion.[10,11] In the case of a trion in a QW, this operator is given by

$$\vec{\Pi}=\vec{P}-\frac{e}{c}\left[\vec{A}_R+\left(1-\frac{m_e}{M}\right)(\vec{A}_{\rho_1}+\vec{A}_{\rho_2})\right], \tag{8}$$

where we used the CM and relative coordinates and $\vec{P}$ is the linear momentum operator of the trion CM.

The x and y components of $\vec{\Pi}$ do not commutate but the trion Hamiltonian eigenstates are also their eigenstates. As a consequence, we can choose to write the trion eigenstates in terms of the $\vec{\Pi}_x$ eigenfunction. Using q_x as the eigenvalue of $\vec{\Pi}_x$ and writing $\vec{q}=(q_x,0,0)$, the $\vec{\Pi}_x$ eigenstate is given by

$$f=\exp\left\{\frac{i}{\hbar}\left[\vec{q}+\frac{e}{c}\left(1-\frac{m_e}{M}\right)(\vec{A}_{\rho1}+\vec{A}_{\rho2})\right]\vec{R}\right.$$
$$\left.-\frac{ie}{2c\hbar}B.Y_{CM}.X_{CM}\right\}, \tag{9}$$

and Λ_q depends only on Y_{CM} [Eq. (1)].

After applying this transformation, the trion Hamiltonian is written as

$$H_{ce}=\sum_{i=1,2}\{H(z_{ei})+H(ex_i)\}+H(z_h)+\frac{1}{m_{hxy}}\vec{p}_1\cdot\vec{p}_2$$
$$+\frac{e^2}{\varepsilon}\frac{1}{\sqrt{|\vec{\rho}_1-\vec{\rho}_2|^2+(z_{e1}-z_{e2})^2}}+H_B, \tag{10}$$

where $H(z_{ei})$ and $H(z_h)$ are the z dependent Hamiltonians for the two electrons and the hole [Eq. (3)], $H(ex_i)$ is the in-plane exciton Hamiltonian for the relative particles plus the respective Coulomb attraction [Eqs. (5) and (6)], the term proportional to $\vec{p}_1\cdot\vec{p}_2$ is a consequence of our choice of coordinates and represents the hole mobility,[12] the next term is the Coulomb repulsion and

$$H_B=\frac{1}{2M}\left[\vec{P}+\frac{e}{c}(\vec{A}_R-\vec{C})\right]^2+\frac{2e^2}{c^2M}\left(1-\frac{m_e}{M}\right)(\vec{A}_R-\vec{C})\cdot(\vec{A}_{\rho1}+\vec{A}_{\rho2})+\frac{2e}{cM}\left(1-\frac{m_e}{M}\right)(\vec{A}_{\rho1}+\vec{A}_{\rho2})\cdot\vec{P}+\frac{e}{c}\left(\frac{1}{m_e}-\frac{m_e}{M\mu}\right)$$
$$\times(\vec{A}_{\rho1}\cdot\vec{p}_1+\vec{A}_{\rho2}\cdot\vec{p}_2)-\frac{em_e}{cM\mu}(\vec{A}_{\rho1}\cdot\vec{p}_2+\vec{A}_{\rho2}\cdot\vec{p}_1)+\frac{e^2}{2c^2M^2}\left(\frac{m_e^2}{m_{hxy}}+\frac{m_{hxy}^2}{m_e}+2m_e+2m_{hxy}\right)(\vec{A}_{\rho1}^2+\vec{A}_{\rho2}^2)$$
$$+\frac{e^2}{c^2M^2}\left(\frac{m_e^2}{m_{hxy}}-2m_e-2m_{hxy}\right)(\vec{A}_{\rho1}\cdot\vec{A}_{\rho2})+\frac{3e^2}{2c^2M}\left(1-\frac{m_e}{M}\right)^2(\vec{A}_{\rho1}+\vec{A}_{\rho2})^2 \tag{11}$$

is the magnetic field dependent part of the trion Hamiltonian where $\vec{C}=(B/2)(Y_{CM},X_{CM},0)$ and q_x was taken as zero (ground state). Note that the first term in the right side of Eq. (11) allows us to express the CM trion states in terms of Landau levels.

In the fundamental CM Landau level approximation, the CM and internal degrees of freedom are uncoupled. The coupling between two different CM Landau levels occurs when the basis states simultaneously satisfy the following conditions: (i) the Landau levels have distinct parities. (ii) the respective total relative particle angular momenta [$m+n$ in Eq. (1)] differs by ± 1.

The negative trion binding energy [$\mathrm{E}_b(X^-)$] is defined as the difference between the binding energy of an exciton [Eq. (7)] and the energy of the charged complex taken the noninteracting two electrons and one-hole system in the fundamental QW states as zero :

$$E_b(X^-)=E(X^-)-\frac{eB\hbar}{2c}\left(\frac{2}{m_e}+\frac{1}{m_{hxy}}\right)-E_b(X^0). \quad (12)$$

In the absence of magnetic field, we obtain the convergence for the trion binding energy in the fundamental QW solutions approximation when *s*-, *p*- and *d*-like one-particle states are included in the basis set.[7] All results shown here include these states and two QW solutions for heavy holes in the trial wave function.

In Fig. 1, we show the binding energy of the negative trion as a function of longitudinal magnetic field for a 100 Å QW. Our results (lines) are compared with calculations performed by Riva *et al.*[5] (solid symbols) and Whittaker and Shields[6] (open symbols) for singlet (squares) and triplet (triangles) bound states. Only the singlet state with total relative particle angular momentum equal to zero ($S0$) and the triplet state with total relative particle angular momentum equal to -1 ($T-1$) are bound states in our calculations and for the parameters we considered here.[7] Results for trial wave functions with one and two CM Landau levels are presented. One can see the importance of including more than one Landau level in the trion basis. In the case of the $S0$ state (dashed and full lines), the inclusion of the second CM Landau level (full line) significatively increases the trion binding energy for magnetic fields higher than 2 T. At the same time, the T-1 state (dotted line) becomes a bound state only when the second CM Landau level is considered. The inclusion of the third Landau level gives rise to a binding-energy increase of less than 2% (not shown). We can then infer that two CM Landau levels are sufficient to obtain a good accuracy in the low magnetic field limit.

The main magnetic field effect on the internal degrees of freedom is the shrinkage of the relative particle orbitals, which strengthens the Coulomb interactions. At very low fields, the Coulomb attraction dominates and the trion binding-energy increases for singlet and triplet states. On the other hand, after 1.5 T (dashed line) or 3 T (full line) the repulsion becomes relevant for the $S0$ state and its binding-energy starts to decrease. The same effect can be notice in T-1. In this case and for the magnetic field range considered here, these contributions tend to cancel each other and the binding-energy increase becomes less pronounced for fields higher than 2.5 T. It is important to stress that these results were obtained in the fundamental QW states approximation for electrons. This lack of flexibility in the basis set is more severe an approximation for higher magnetic field values. For instance, the maximum in the $S0$ binding energy is not reproduced by more flexible approaches[5] which obtain higher energies (see Fig. 1). One can then understand this maximum as a breakdown in our fundamental QW sates approximation for electrons as could be expected from our previous results.[7]

Despite of this, the comparison of our results with other theoretical models shows a good agreement for the triplet state while for the singlet one they diverge from the results of Riva *et al.*[5] at high-fields presenting a better agreement with Whittaker and Shields[6] (see Fig. 1). The discrepancy among the different theoretical results may also indicate the intrinsic difficulties of calculations that involve difference between two variational results and the consequent care one should take before concluding about the quality of the model.

Figure 2 shows the $S0$ (a) and T-1 (b) binding energies as a function of electric field for a constant magnetic field (1 T) and three QW widths : 100 Å (full line), 200 Å (dashed line), and 300 Å (dotted line). As one can see, the binding energy of the T-1 state increases with the electric field for a 100 Å QW. This occurs because the electric field tends to diminish the effective structural confinement weakening the triplet *intrinsic repulsion* while this behavior is not observed in the singlet case. When a 300 Å QW is considered, the structural confinement is not so important. The electric field strengths the Coulomb repulsion and weakens the attraction giving rise to a binding-energy decrease in both symmetries. The 200 Å QW presents an intermediate behavior in the triplet case. The triplet *intrinsic repulsion* is a consequence of its spatial sym-

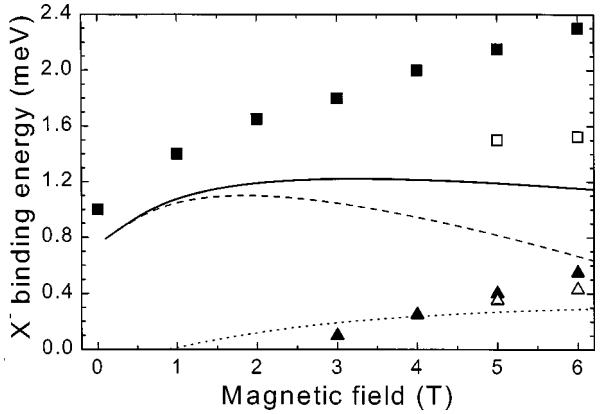

FIG. 1. X^- binding energy as a function of longitudinal magnetic field for the singlet ($S0$) and triplet (T-1) bound sates. Results for $S0$ with one (dashed line) and two (full line) CM Landau levels and for T-1 with two CM Landau levels (dotted line) are shown. In all cases, two QW states for holes were included in the basis set. For comparison, data from Riva *et al.* (Ref. 5) (solid symbols) and Whittaker and Shields (Ref. 6) (open symbols) are also presented for the singlet (squares) and triplet (triangles) bound states. The QW width is 100 Å.

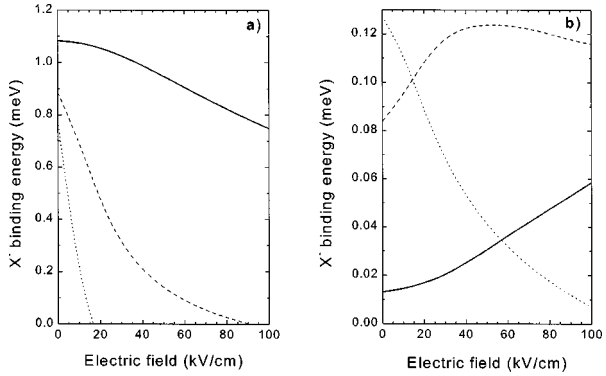

FIG. 2. Binding energy of the $S0$ (a) and T-1 (b) states as a function of electric field for a constant magnetic field (1 T) and three QW widths: 100 Å (full line), 200 Å (dashed line), and 300 Å (dotted line). Two Landau levels and two QW states for holes were included in the basis set.

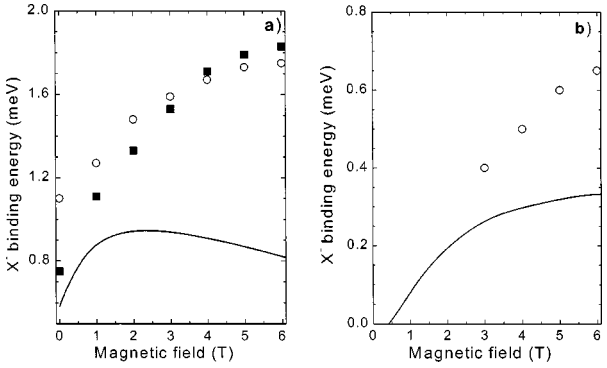

FIG. 3. Binding energy of the $S0$ (a) and T-1 (b) states as a function of the magnetic field for a 200 Å QW. The full lines correspond to our results. For comparison, data from Glasberg *et al.* (Ref. 3) (circles) and from Riva *et al.* (Ref. 13) (squares) are also shown.

metry [Eq. (1)] which prevents the relative particles coordinates from assuming the same value. As a consequence, Fig. 2(b) shows lower binding energies for thinner QW's in the absence of electric field. In Fig. 2(a) we observe that the trion is unbound for some values of the electric field. This result, however, has to be understood as a limitation of our basis set, Eq. (1), which is not able to fully include the X^- continuum.

Figure 3 shows the $S0$ (a) and T-1 (b) binding energies as a function of magnetic field for a 200 Å QW comparing our results (full line) with the experiments of Glasberg *et al.*[3] (circles) and calculations of Riva *et al.*[13] (squares). As one can see, our theoretical values for the trion binding energy are always lower than the other ones. Moreover, a qualitative disagreement can be seen in both singlet (a) and triplet (b) cases. This discrepancy has several origins. As mentioned above, one of them is the lack of flexibility of our basis set which does not include excited QW states for electrons.[6] In DB (Ref. 7) we showed that the inclusion of the second QW state for electrons in the trion basis set is responsible for a gain in the binding energy of the order of 40%. We believe that such a gain may give rise to a better qualitative agreement when a magnetic field is considered. Another source of discrepancy is the ideal QW interfaces consideration. We showed[14] that the interface defects are responsible for a considerable increase in the trion binding energy. This effect should take place even in the presence of a magnetic field. A more quantitative comparison with experimental results requires the inclusion of all these effects.

In conclusion, we variationally calculated the negative trion binding energy in $GaAs/Al_{0.3}Ga_{0.7}As$ QW's in the presence of longitudinal electric and magnetic fields. In agreement with experiments, our results showed only one singlet ($S0$) and one triplet (T-1) bound states. The importance of including more than one CM Landau level in the basis set was shown, what means that the coupling between internal and CM degrees of freedom is relevant even in the low magnetic field limit.

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