Positively charged magneto-excitons in a semiconductor quantum well.

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(January 13, 2022)

A variational calculation of the lower singlet and triplet states of positively charged excitons (trions) confined to a single quantum well and in the presence of a perpendicular magnetic field is presented. We study the dependence of the energy levels and of the binding energy on the well width and on the magnetic field strength. Our results are compared with the available experimental data and show a good qualitative and quantitative agreement. A singlet-triplet crossing is found which for a 200Å wide GaAs is predicted to occur for B = 15 T.

PACS numbers: 71.35.Ji, 78.67
I. INTRODUCTION

In spite of the large number of theoretical and experimental works published in recent years on the subject of charged excitons in quantum wells, only a very small number of them deal with positively charged excitons \( X^+ \). Different authors used the di- usion Monte Carlo technique to calculate the dependence of the binding energy of the positively charged exciton on the well width at zero magnetic field. Stobbe and Moradi reported low magnetic field results for the positively charged exciton spin-singlet state, which was calculated using a determinist-atic variational technique. To our knowledge, this is the only theoretical calculation on the magnetic-field dependence of the \( X^+ \) energy. In the present paper we go beyond the small magnetic field limits and present results for the whole magnetic field range not only for the singlet but also for the triplet state.

Experimental evidence of the positive trion \( X^+ \) in GaAs/AlGaAs quantum wells was found by different groups. These results con firm the existence of both the spin-singlet state and the spin-triplet state at non-zero magnetic field as was also found for \( X^- \). The magnetic-field dependence of the binding energy, on the other hand, can be rather different for the \( X^+ \) as compared to the \( X^- \).

We extended our numerical technique, see Ref. [15], which we used for negatively charged excitons, to describe positively charged excitons in quantum wells under the influence of a magnetic field parallel to the quantum well axis. The present paper is organized as follows. In Sec. II we present the Hamil- lionian of the problem. The dependence of the binding energy on the well width is discussed in Sec. III. In Sec. IV the magnetic-field dependence is investigated and we discuss the dependence of the average distance between different pairs of particles in the system as a function of the magnetic field. We point out the differences and similarities between the \( X^+ \) and the \( X^- \). The behavior of the pair correlation functions is also studied for different magnetic fields. In Sec. V we compare our results with the experimentally measured transition and binding energies. Finally, in Sec. VI we summarize our results and present our conclusions.

II. HAMILTONIAN

In the effective mass approximation the Hamil- lonian describing a positively charged exciton, i.e. \( X^+ \), in an uniform magnetic field \( B \) is:

\[
H = \sum_{i=1}^{N} \left( \frac{\hbar^2}{2m_i} \nabla_i^2 + V(r_i) + \frac{e_i e_j}{r_{ij}} \right)
\]

(1)

where \( \nabla_i \) = \( \frac{1}{\iota} \mathbf{r}_i \), \( m_i \) and \( e_i \) are the masses and charges of the interacting particles and \( e \) is the dielectric constant of the medium the particles are moving in and is taken the same as for the well and barrier material. The confining potential is

\[
V(r_i) = 0 \text{ if } |r_i - W_0| = 2 \text{ and } V(r_i) = V_{\perp} \text{ if } |r_i - W_0| = 2;
\]

(2)

where \( W \) is the quantum well width, and the reference system is taken such that the origin of the coordinate system is at the center of the quantum well. For a GaAs/AlGaAs quantum well the heights of the square well con- nent potentials are \( V_0 = 0.57 \) (1.155x + 0.37x²) eV for the electrons and \( V_h = 0.43 \) (1.155x + 0.37x²) eV for the hole. If we consider the case when the magnetic field is applied along the growth axis of the well, i.e. \( B = (0;0;B) \), the Hamil- tonian becomes:

\[
H = \sum_{i=1}^{N} \left( \frac{\hbar^2}{2m_i} \nabla_i^2 + \frac{e_i e_j}{4\epsilon^2} \left( \mathbf{r}_i \times \mathbf{r}_j \right)^2 + \frac{e_i e_j}{c} \mathbf{L}_i \cdot \mathbf{L}_j + \frac{1}{2} \mathbf{L}_i \cdot \mathbf{L}_j \right) + U(r_i) + X^i \right)
\]

(3)

where \( L_i \) is the component along the \( z \)-axis of the orbital momentum of the \( i \)-th particle. The same considerations made in Ref. [11] for the \( X^- \) hold also in this case and the same functional form for the trial wave function which consists of a linear combination of deformed correlated wave functions is used to solve the Hamil- tonian.

However, here the variational parameters are used which enter in the definition of the deformed gaussian functions can assume also negative values. For our numerical calculation we focus on a GaAs/AlGaAs quantum well with \( x = 0.3 \). The parameters used are \( \alpha = 12.58 \), \( \epsilon = 0.067 \), \( m_0 \), and \( m_\perp = 0.04m_0 \), which result in \( 2R_y = \epsilon^2 m_0 = 11.58 \) eV and \( a_0 = \epsilon^2 m_0 = 99.3 \).

III. ZERO MAGNETIC FIELD TRION ENERGY

First, we study the binding energy of the positively charged excitons which is defined as:

\[
E_B (X^+;B) = E (X) + E_B (W;B) \ E (X^+);
\]

(4)

where \( E (X) \) and \( E (X^+) \) are respectively, the total energy of an exciton and of a positively charged exciton in the quantum well and \( E_B (W;B) \) is the energy of a free hole in the quantum well of width \( W \) in the presence of a magnetic field \( B \) directed along the con- nent direction. The dependence of the binding energy of the positively charged exciton spin-singlet state on the well width is shown in Fig. 1 (solid curve) in the absence of a magnetic field. Our results are also compared with the Monte Carlo calculations of Ref. [16] (dotted curve). The results from the two theories differ by about 0.1 eV at \( W = 200 \) A. One reason for this discrepancy could be attributed to the different choices for the value of the static dielectric constant; we took it equal to 12.58 while in
Ref.[4] was taken equal to 12.5. Notice that while the binding energy is decreasing with increasing well width according to both theories our calculation shows a faster decrease of the positively charged exciton binding energy with increasing well width, this behaviour is particularly strong for the X’ system. The symbols in Fig. 1 represent the experimentally measured values for the spin-singlet state binding energy of the X’ for different quantum well widths and different experiment energies. Notice that these results are in good agreement with the theory of Ref.[4], and agree with ours in the non-inelasticity of the theory, i.e. 0.1 m eV. This error is estimated considering the digit to which we round our result for the total energies, however due to the very good convergence of the calculation we expect the “real error” to be smaller than the estimated one. In general we would expect that the experimental energies are larger than the theoretical calculated ones because: 1) a non zero density of holes leads to a non zero Fermi energy E_F, this has been shown that the experimental data in fact E_F + E_B (X’; B = 0) and 2) quantum well width fluctuations will localize the exciton. Both effects lead to a larger binding energy with respect to the one calculated theoretically for a free translational invariant trion.

In Fig. 1 we also report the dependence of the negatively charged exciton binding energy on the well width (dashed curve). Notice that the X’ binding energy is larger (about 20%) as compared to the X binding energy, both for our theory and for the one of Ref.[3]. Moreover this result is also in good agreement with the experimental results which showed that the energy of the X’ is larger or equal to the one of X. Strobe and Moruzzi found, on the other hand, that for a 300 Å wide quantum well the binding energy of X’ is lower than the one of X, which is opposite to our conclusion and to those of Ref.[4]. It should be stressed that the theoretical value for the trion binding energy depends not only on the obtained value for the trion binding energy but also on the exciton energy. In other words, the latter are both upper bounds to the exact result and consequently the trion binding energy is neither an upper nor a lower bound to the exact value. For example, an overestimate of the exciton energy will lead to an overestimate of the trion binding energy.

IV. MAGNETIC FIELD DEPENDENCE OF THE TRION PROPERTIES

Next, we compare the dependence of the binding energy of the positively charged exciton on the magnetic field with the of the negatively charged exciton for a quantum well of width 100 Å (see Fig. 3). Notice that while for B < 1 T we obtain E_B (X’; B) > E_B (X ; B), which is in agreement with the B = 0 T behaviour as shown in Fig. 1. For B > 1 T the relation between the two energies is reversed and the negatively charged exciton becomes more strongly bound. Moreover the X’ singlet binding energy quickly increases up to about 2.5 m eV for B = 10 T after which it saturates, the X’ binding energy increases slowly from about 1.2 m eV at B = 0 up to about 1.5 m eV for B = 7 T, where it starts to decrease slowly. We found a similar behaviour for the binding energy in the case of a quantum well of width 200 Å (see Fig. 3). For the latter quantum well width we also calculated the spin-triplet state with L = 1 (dashed-dotted line in Fig. 3). The triplet state is unbound at low magnetic field and becomes bound around 1 T. We also noticed that the binding energy of this state increases rather fast with increasing magnetic field and eventually we observe a crossing around B = 15 T. This behaviour is consistent with the one found for the negatively charged exciton where we found that when the hole mass was much larger than the electron one no spin-singlet spin-triplet transition was observed. However, when the hole mass was decreased considerably such singlet-triplet transition occurred. In that case the hole mass was always larger than the electron one, however it is reasonable to assume that decreasing further the hole mass the singlet-triplet transition would still be observed. Here the roles of the hole and the electron are switched and the electron mass is much smaller than the hole one. As a consequence this is then consistent with the fact that we now had a singlet-triplet transition.

The average distance between pairs of particles of the trion in the plane orthogonal to the quantum well axis, i.e. < 2 > 1, is shown in Fig. 4 as function of the magnetic field for quantum well of width 200 Å. Notice that for B = 0 the average distance between the positively charged exciton pairs, i.e. hole-hole and electron-hole ones, are smaller than the correspondent one for the negatively charged exciton. In particular the difference is more pronounced for the pair of particles with the same charge (i.e. hole-hole in case of X’ versus electron-electron in X). Since the attractive and the repulsive contribution to the potential are inversely proportional to the average interparticle distance, the behaviour at B = 0 explains the fact that we find a lower binding energy for the X’ than for the X’ at B = 0. Notice that around 1 T the average distance of the electron-hole pair in X crosses the one of X’, this is the same as magnetic field at which the X’ binding energy becomes larger than the X’ binding energy. For increasing magnetic field the ratio between the average distance between the electron-electron and electron-hole pair in X is rather constant. Looking at the corresponding pairs in X’ we see that the distance between the electron and hole diminishes with increasing magnetic field but less than the one between the two holes. This could explain the slow increase and then the decrease already at low magnetic fields of the X’ binding energy against the fast increase and saturation of the X’ binding energy.

We calculated also the pair correlation function for the positive trion in the cone normal direction, g_{ij}(z) = < (z_j - z_i ) >, and in the orthogonal plane, g_{ij}(z) = <
(j_1 \sim j), both at B = 0 and at B = 4 T (see Fig. 3). Notice that along the z-axis, Figs. 3(a), both the hole-pair and the electron-hole pair correlation function have a peak around the center of the quantum well which is in agreement with the fact that the Coulomb interaction plays a minor role as compared to the confinement due to the presence of the quantum well. Notice also that, as expected, the presence of a magnetic field has only a very small influence on the correlation function in the z-direction. In the -plane, Fig. 3(b), we observe that the electron-hole pair correlation is peaked around zero, i.e., the electron and the hole maximize their interaction by staying as close as possible to each other. The hole-pair correlation function has instead a peak around the average pair inter-particle distance. When a magnetic field is applied the peak of the hole-pair hole correlation function is shifted towards lower . This is consistent with the fact that the average pair inter-particle distance decreases with increasing magnetic field.

V. COMPARISON WITH EXPERIMENT

In Fig. 3, we compare the binding energy of the X+ and the X singlet state for a 200 Å wide quantum well with the experimental results obtained by G. Lasberg et al. [5] and the very recent results by Yuza et al. [6] (open triangles). When comparing the experimental results with our theoretical results we notice that for B = 0 the experimental and theoretical results for the negatively charged exciton binding energy differ by about 0.3 m eV, which may be due to a non-zero density of states and/or to localization induced by quantum well width fluctuations. In the range 1 T < B < 7 T there is very good agreement between theory and experiment. For B > 8 T the experimental binding energy saturates, while this occurs at higher fields for our theoretical result. The agreement of the X+ singlet energy with the very recent experimental results of the same group is on the other hand remarkable. Not only theoretical but also experimental results improve with time.

For the X+ spin-singlet state binding energy, the agreement is rather good over the whole magnetic field range at which experimental results are available. However, at low magnetic fields the theoretical binding energy underestimate the experimental value. It has been argued that this effect can be attributed to localization effects due to quantum well width fluctuations. Notice that localization effects are less important on the positively charged exciton than on the negatively charged exciton, which is consistent with the larger mass of the holes and which leads to a less extended trion (see Fig. 4). For the X+ spin-triplet state a comparison with the experimental data by G. Lasberg et al. [5] shows a good agreement for magnetic fields up to about 3 T. Beyond 3 T the experimental energy saturates while the theory still predicts an increasing binding energy with increasing magnetic field.

VI. CONCLUSION

The present work is the first theoretical work in which a detailed comparison is made between experimental and theoretical singlet and triplet binding energies of the positively charged exciton. The theoretical results explain the different magnetic field dependence of the X and X+ ground state binding energy, which was observed experimentally. Namely, the X+ singlet has a very weak magnetic field dependence while the X singlet binding energy increases rapidly in the low magnetic field region and saturates at higher fields. We find good qualitative and quantitative agreement with the available experimental results. The X+ triplet binding energy on the other hand increases with magnetic field and we predict for a quantum well of width 200 Å a singlet-triplet crossing at B ≈ 15 T. The experimental results of Ref. [3] show a saturated triplet binding energy for B > 3 T, which we do not find in our theoretical results.

VII. ACKNOWLEDGMENT

Part of this work is supported by the Flemish Science Foundation (FWO-Vl), the ‘Inteniversity Poles of Attraction’ program – Belgian State, Prime M. Inter’s O ce –Federale on for Scienti c, Technical and Cultural Affairs’ and the Flemish-Hungarian cultural exchange program. K. Varga was supported by the U.S. Department of Energy, Nuclear Physics Division, under contract No. W-31-109-ENG-39 and OTKA grant No. T029003 (Hungary). We thank Go Yuza for providing us with his experimental data for the 200 Å wide quantum well before publication.

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FIG. 1. Dependence of the binding energy of the positively and negatively charged exciton on the well width at zero magnetic field. The symbols represent experimental data for the X' from Ref. 18 (full circles), Ref. 14 (open circle) and Ref. 16 (triangle).

FIG. 2. The binding energy of a negatively and a positively charged exciton in a 100 Å wide quantum well as a function of the applied magnetic field.

FIG. 3. The binding energy of a negatively and positively charged exciton in a 200 Å wide quantum well. The open and full circles as well as the diamonds are the experimental data from Ref. 19, the triangles are experimental data from Ref. 24. The bars represent the nominal error of our calculation.

FIG. 4. The average pair distance in a positively and in a negatively charged exciton in a 200 Å wide quantum well as a function of the magnetic field.
