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Landau levels of two-dimensional negatively charged three-particle Coulomb states

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Abstract. We study the influence of a low external uniform magnetic field on the energy levels of three-particle Coulomb states in a strictly two-dimensional medium. We show that at low magnetic fields, when the coupling between the relative motion and the motion of the centre of mass may be neglected, additional Landau levels appear. We compute the ground state energy corresponding to the relative motion as a function of the strength of the magnetic field for different values of the mass ratio of the negatively and positively charged particles. We compare our results with those we obtained previously in the three-dimensional limit.

1. Introduction

Charged excitons (or excitonic trions) are three-particle excitonic complexes that can result [1] from the binding of an exciton (electron-hole pair) with an electron or a hole in semiconductors (SCs). Two kinds of excitonic trion may be considered: the negative trion X^- (eeh) resulting from the Coulombic interaction between an exciton and an electron and the positive trion X_2^+ (ehh) involving an exciton and a hole. Due to their mobility and charge, they exhibit original properties which may be used to distinguish them from other excitonic complexes.

They have been identified [2–5] in different bulk SCs. However, due to their relative small binding energies, they may be observed only at very low temperature. This situation limits to some extent their practical importance in these materials.

However more favourable conditions of their observation are expected in quasi-two-dimensional (2D) SCs [6, 7] (SC superlattices and quantum wells, surfaces, interfaces). Indeed, the quantum confinement leads to an increase of the binding energy of the excitonic complexes, up to a factor of ten [8], compared to the massive SC, so that they remain stable up to room temperature. Moreover, at low optical excitations, the necessary presence of free charge carriers (electron or holes) involved in transitions to or from excitonic trions states may be realized, for instance, by a previous modulated doping. In fact, the negatively charged exciton X^- has been recently identified [9] in the magneto-absorption spectra of $CdTe/Cd_{1-x}Zn_xTe$ multiple quantum wells.

Very original properties are expected under the influence of a magnetic field. Indeed, in our previous theoretical studies [10, 11] of the action of a magnetic field on excitonic trions in 3D semiconductors, we have shown that the magnetic field gives rise to an increasing of the binding energies as well as to an additional quantization of the energies. Further, the Landau levels associated with the centre of the mass charge lead to an oscillatory magneto-absorption. An enhancement of all these effects is expected in the case of confined SCs.

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In this paper, we report the first theoretical study of the influence of a low magnetic field on the binding energies of excitonic trions in the strictly 2D limit, with a magnetic field perpendicular to the plane. The results of the present work, together with those of our previous 3D calculations [11], are expected to give an estimation of what happens in the case of SC quantum wells.

In the next section, we first study the invariants of the problem and then deduce the specific properties of the Hamiltonian. We show how the centre of mass and relative motions can be separated at low magnetic fields in the adiabatic approximation. In section 3, we present our method for the variational resolution of the Schrödinger equation in the isotropic effective mass model [12]. In section 4, we present the results of our numerical calculations. As expected, the binding energies increase with the intensity of the magnetic field. Moreover, each energy level splits into Landau levels.

2. Theory

Neglecting the spin interactions and choosing a symmetrical Coulomb gauge, the 2D effective mass Hamiltonian reads in the case of the negative trion X^-

$$H = \frac{1}{2m_e^*}\left(\boldsymbol{p}_1 + \frac{e}{c}\boldsymbol{A}_1\right)^2 + \frac{1}{2m_e^*}\left(\boldsymbol{p}_2 + \frac{e}{c}\boldsymbol{A}_2\right)^2 + \frac{1}{2m_h^*}\left(\boldsymbol{p}_h - \frac{e}{c}\boldsymbol{A}_h\right)^2 + V_c \tag{2.1}$$

where the potential vectors $\boldsymbol{A}_i$ of the electrons and the hole are expressed as a function of the uniform magnetic field $\boldsymbol{\mathcal{H}}$:

$$\boldsymbol{A}(\boldsymbol{r}_i) = \tfrac{1}{2}\boldsymbol{\mathcal{H}} \times \boldsymbol{r}_i. \tag{2.2}$$

In the following, we study especially the case corresponding to a magnetic field perpendicular to the plane, $\boldsymbol{\mathcal{H}} \equiv (0,\ 0,\ \mathcal{H})$, where the potential vector (2.2) is written as

$$\boldsymbol{A}(\boldsymbol{r}_i) = \frac{\mathcal{H}}{2}(-y_i,\ x_i,\ 0). \tag{2.3}$$

The interaction between the three particles is modelled by a Coulombic potential which is screened by a quite phenomenological dielectric constant ϵ:

$$V_c = \frac{e^2}{\epsilon}\left(\frac{1}{r_{12}} - \frac{1}{r_{1h}} - \frac{1}{r_{2h}}\right). \tag{2.4}$$

We transform the Hamiltonian (2.1), using the in-plane relative coordinates $\boldsymbol{r}(x,\ y,\ z)$, $\boldsymbol{R}(X,\ Y,\ Z)$ and the in-plane coordinates of the centre of mass $\boldsymbol{R}_0(X_0,\ Y_0,\ Z_0)$:

$$\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2 \qquad \boldsymbol{R} = \frac{\boldsymbol{r}_1 + \boldsymbol{r}_2}{2} - \boldsymbol{r}_h \qquad \boldsymbol{R}_0 = \frac{m_e^*\boldsymbol{r}_1 + m_e^*\boldsymbol{r}_2 + m_h^*\boldsymbol{r}_h}{2m_e^* + m_h^*}. \tag{2.5}$$

Thus, the Hamiltonian can be expressed as the sum of three terms:

$$H = H_0 + H_1 + H_2 \tag{2.6}$$

where

$$H_0 = -\frac{\hbar^2}{2\mu}\Delta_{\boldsymbol{r}} - \frac{\hbar^2}{2M}\Delta_{\boldsymbol{R}} - \frac{\hbar^2}{2M_0}\Delta_{\boldsymbol{R}_0} + V_c \tag{2.7}$$

$$H_1 = -\frac{\mathrm{i}e\hbar}{cm_e^*}\left[\boldsymbol{A}(\boldsymbol{r})\cdot\boldsymbol{\nabla}_{\boldsymbol{r}} + \frac{1-2\sigma^2}{1+2\sigma}\boldsymbol{A}(\boldsymbol{R})\cdot\boldsymbol{\nabla}_{\boldsymbol{R}} + \frac{2\sigma(1+\sigma)}{(1+2\sigma)^2}\boldsymbol{A}(\boldsymbol{R})\cdot\boldsymbol{\nabla}_{\boldsymbol{R}_0} + (1+\sigma)\boldsymbol{A}(\boldsymbol{R}_0)\cdot\boldsymbol{\nabla}_{\boldsymbol{R}} + \frac{\sigma}{1+2\sigma}\boldsymbol{A}(\boldsymbol{R}_0)\cdot\boldsymbol{\nabla}_{\boldsymbol{R}_0}\right] \tag{2.8}$$

$$H_2 = \frac{e^2}{2c^2 m_e^*}\left[\tfrac{1}{2}A^2(\boldsymbol{r}) + 2\frac{1+2\sigma^3}{(1+2\sigma)^2}A^2(\boldsymbol{R}) + (2+\sigma)A^2(\boldsymbol{R}_0) + 4\frac{1-\sigma^2}{1+2\sigma}\boldsymbol{A}(\boldsymbol{R})\cdot\boldsymbol{A}(\boldsymbol{R}_0)\right] \tag{2.9}$$

with

$$\mu = m_e^*/2 \qquad M = (2m_e^* m_h^*)/(2m_e^* + m_h^*) \qquad M_0 = 2m_e^* + m_h^* \qquad \sigma = m_e^*/m_h^*. \tag{2.10}$$

We can easily verify that the centre of mass momentum operator $\boldsymbol{P}_0 = -\mathrm{i}\bar{h}\boldsymbol{\nabla}_{\boldsymbol{R}_0}$ does not commute with the Hamiltonian, because of the occurrence of terms involving $\boldsymbol{A}(\boldsymbol{R}_0)$. Therefore the relative and centre of mass motions can only be separated in the zero-magnetic-field limit. However, we remark that the operator

$$\boldsymbol{\pi} = \boldsymbol{p}_1 + \boldsymbol{p}_2 + \boldsymbol{p}_h - \frac{e}{c}[\boldsymbol{A}(\boldsymbol{r}_1) + \boldsymbol{A}(\boldsymbol{r}_2) - \boldsymbol{A}_h(\boldsymbol{r}_h)] \tag{2.11}$$

$$= -\mathrm{i}\bar{h}\boldsymbol{\nabla}_{\boldsymbol{R}_0} - \frac{e}{c}\left[2\frac{1+\sigma}{1+2\sigma}\boldsymbol{A}(\boldsymbol{R}) + \boldsymbol{A}(\boldsymbol{R}_0)\right] \tag{2.12}$$

commutes with the Hamiltonian although its components π_x and π_y do not commute with each other. Generally speaking, there always exists a common basis of eigenfunctions for π_x and H or π_y and H. In the following, we choose to determine the common basis for H and π_x, where π_x is written as

$$\pi_x = -\mathrm{i}\bar{h}\partial_{X_0} + \frac{e\mathcal{H}}{2c}\left[2\frac{1+\sigma}{1+2\sigma}Y + Y_0\right]. \tag{2.13}$$

As a consequence, it is possible to transform the effective Hamiltonian into an expression which does not contain the coordinate X_0 of the centre of mass. Because the operators π_x and H commute, the envelope wave function $\phi_{X^-}(\boldsymbol{r},\ \boldsymbol{R},\ \boldsymbol{R}_0)$ is the solution of the equation

$$\pi_x\phi_{X^-}(\boldsymbol{r},\ \boldsymbol{R},\ \boldsymbol{R}_0) = \bar{h}K_x\phi_{X^-}(\boldsymbol{r},\ \boldsymbol{R},\ \boldsymbol{R}_0). \tag{2.14}$$

Its resolution leads to

$$\phi_{X^-}(\boldsymbol{r},\ \boldsymbol{R},\ \boldsymbol{R}_0) = U\Phi_{X^-}(\boldsymbol{r},\ \boldsymbol{R},\ Y_0) \tag{2.15}$$

where the unitary operator U is expressed as

$$U = \exp\mathrm{i}\left[\left\{\boldsymbol{K} + \frac{2e}{c\bar{h}}\frac{1+\sigma}{1+2\sigma}\boldsymbol{A}(\boldsymbol{R})\right\}\cdot\boldsymbol{R}_0 - \frac{e\mathcal{H}}{2c\bar{h}}X_0Y_0\right]. \tag{2.16}$$

In (2.16) we have introduced the vector $\boldsymbol{K} \equiv (K_x,\ 0)$, which must not be confused with the wave vector $\boldsymbol{K}_0$ of the centre of mass without magnetic field. The operator U corresponds to a canonical transformation which conserves the norm and the scalar product. The energy of the trion can then be expressed in terms of the transformed Hamiltonian H' and the transformed function Φ_{X^-}:

$$E = \frac{\langle\Phi_{X^-}(\boldsymbol{r},\ \boldsymbol{R},\ Y_0)|H'|\Phi_{X^-}(\boldsymbol{r},\ \boldsymbol{R},\ Y_0)\rangle}{\langle\Phi_{X^-}(\boldsymbol{r},\ \boldsymbol{R},\ Y_0)|\Phi_{X^-}(\boldsymbol{r},\ \boldsymbol{R},\ Y_0)\rangle}. \tag{2.17}$$

The transformed Hamiltonian H' reads

$$H' = U^{-1}HU = -\frac{\bar{h}^2}{2\mu}\Delta_{\boldsymbol{r}} - \frac{\bar{h}^2}{2M}\Delta_{\boldsymbol{R}} - \frac{\bar{h}^2}{2M_0}\Delta_{\boldsymbol{R}_0} + \frac{\bar{h}^2}{2M_0}K_x^2 + V_c - \frac{\mathrm{i}e\bar{h}}{cm_e^*} \times\left[\boldsymbol{A}(\boldsymbol{r})\cdot\boldsymbol{\nabla}_{\boldsymbol{r}} + \frac{1-2\sigma^2}{1+2\sigma}\boldsymbol{A}(\boldsymbol{R})\cdot\boldsymbol{\nabla}_{\boldsymbol{R}} + \frac{4\sigma(1+\sigma)}{(1+2\sigma)^2}\boldsymbol{A}(\boldsymbol{R})\cdot\boldsymbol{\nabla}_{\boldsymbol{R}_0}\right.$$

$$+\frac{\sigma}{1+2\sigma}(\boldsymbol{A}(\boldsymbol{R}_0)-\boldsymbol{B}(\boldsymbol{R}_0))\cdot\boldsymbol{\nabla}_{\boldsymbol{R}_0}\Bigg]-\frac{\mathrm{i}\overline{h}^2}{m_e^*}\frac{\sigma}{1+2\sigma}\boldsymbol{K}\cdot\boldsymbol{\nabla}_{\boldsymbol{R}_0}+\frac{e\overline{h}}{cm_e^*}$$
$$\times\left[\frac{4\sigma(1+\sigma)}{(1+2\sigma)^2}\boldsymbol{K}\cdot\boldsymbol{A}(\boldsymbol{R})+\frac{\sigma}{1+2\sigma}\boldsymbol{K}\cdot(\boldsymbol{A}(\boldsymbol{R}_0)-\boldsymbol{B}(\boldsymbol{R}_0))\right]+e^2/c^2m_e^*$$
$$\times\left[\tfrac{1}{4}A^2(\boldsymbol{r})+\frac{4\sigma(1+\sigma)}{(1+2\sigma)^2}\boldsymbol{A}(\boldsymbol{R})\cdot[\boldsymbol{A}(\boldsymbol{R}_0)-\boldsymbol{B}(\boldsymbol{R}_0)]\right.$$
$$\left.+\frac{\sigma}{1+2\sigma}\boldsymbol{A}(\boldsymbol{R}_0)\cdot[\boldsymbol{A}(\boldsymbol{R}_0)-\boldsymbol{B}(\boldsymbol{R}_0)]+\lambda(\sigma)A^2(\boldsymbol{R})\right] \tag{2.18}$$

with

$$\boldsymbol{B}(\boldsymbol{R}_0)=(\mathcal{H}/2)(Y_0,\ X_0,\ 0) \tag{2.19}$$

and

$$\lambda(\sigma)=\frac{1+4\sigma(1+\sigma)(2+\sigma+\sigma^2)}{(1+2\sigma)^3}. \tag{2.20}$$

Because the function $\Phi_{X^-}=U^{-1}\phi_{X^-}$ is independent of the coordinate X_0 of the centre of mass, the acting of the operators $\boldsymbol{K}\cdot\boldsymbol{\nabla}_{\boldsymbol{R}_0}$ and $[\boldsymbol{A}(\boldsymbol{R}_0)-\boldsymbol{B}(\boldsymbol{R}_0)]\cdot\boldsymbol{\nabla}_{\boldsymbol{R}_0}$ on Φ_{X^-} does not make any contribution. Finally, the transformed Hamiltonian can be written as the sum of five terms:

$$H'=H_1'+H_2'+H_3'+H_4'+H_5'. \tag{2.21}$$

The first one corresponds to the relative movement without magnetic field:

$$H_1'=H_0^{rel}=-\frac{\overline{h}^2}{2\mu}\Delta_{\boldsymbol{r}}-\frac{\overline{h}^2}{2M}\Delta_{\boldsymbol{R}}+V_c. \tag{2.22}$$

The second one is the contribution due to the linear Zeeman effect:

$$H_2'=-\frac{\mathrm{i}\overline{h}e}{cm_e^*}\left[\boldsymbol{A}(\boldsymbol{r})\cdot\boldsymbol{\nabla}_{\boldsymbol{r}}+\frac{1-2\sigma^2}{1+2\sigma}\boldsymbol{A}(\boldsymbol{R})\cdot\boldsymbol{\nabla}_{\boldsymbol{R}}\right]. \tag{2.23}$$

The contribution H_3' represents the quadratic diamagnetic effect:

$$H_3'=\frac{e^2}{c^2m_e^*}[\tfrac{1}{4}A^2(\boldsymbol{r})+\lambda(\sigma)A^2(\boldsymbol{R})]. \tag{2.24}$$

The fourth term H_4' describes the action of the magnetic field on the motion of the charged centre of mass:

$$H_4'=-(\overline{h}^2/2M_0)\partial_{Y_0^2}^2+(M_0\omega_c^2/2)(Y_0-(\overline{h}c/e\mathcal{H})K_x)^2. \tag{2.25}$$

H_4' is analogous to the Hamiltonian of a harmonic oscillator of mass M_0 and circular frequency $\omega_c=e\mathcal{H}/M_0c$ which oscillates around the point $Y_0^0=(\overline{h}c/e\mathcal{H})K_x$. Its contribution leads in the two cases to a splitting of the energy levels into Landau levels. Finally the fifth term

$$H_5'=2\overline{h}\omega_c\frac{1+\sigma}{1+2\sigma}\left[-\mathrm{i}X\partial_{Y_0}+\frac{M_0\omega_c}{\overline{h}}Y\left(Y_0-\frac{\overline{h}c}{e\mathcal{H}}K_x\right)\right] \tag{2.26}$$

is the coupling between the relative and centre of mass motions.

3. Binding energy in the low-field approximation

3.1. The adiabatic approximation

In the last section, we have seen that due to the occurrence of the coupling term H_5' (2.26), the relative and centre of mass motions remain coupled. However, they may be separated when the expression (2.26) for H_5'

$$H_5' = (\mathcal{H}/M_0)(a + b\mathcal{H}) \tag{3.1}$$

takes lower values than the other terms of the Hamiltonian (2.21). This situation happens for low enough magnitudes of the magnetic field and because the dependence of H_5' on the mass M_0 is greater than those of the individual particles. In this case, we can still separate the two motions by using an adiabatic approximation based on the fact that the motion of the centre of mass is much slower than the relative motion. In these conditions, we can write the envelope wave function $\Phi_{X^-}(\boldsymbol{r},\ \boldsymbol{R},\ Y_0)$ as

$$\Phi_{X^-}(\boldsymbol{r},\ \boldsymbol{R},\ Y_0) \simeq \phi_{rel}\Phi_{CM} \tag{3.2}$$

where ϕ_{rel} describes the relative motion within the plane and satisfies the following equation:

$$H^{rel}\phi_{rel} = E_{rel}\phi_{rel} \tag{3.3}$$

where the relative Hamiltonian H^{rel} is given by

$$H^{rel} = H_0^{rel} + H_2' + H_3'. \tag{3.4}$$

The wave function Φ_{CM} describing the oscillatory motion of the centre of mass satisfies the equation

$$H_4'\Phi_{CM} = E_{CM}\Phi_{CM}. \tag{3.5}$$

Its resolution gives rise to Landau levels, leading to a splitting of the energies of the charged excitons. We will see later that these energies increase considerably with the magnitude of the magnetic field as well as with the ratio of the effective masses. The eigenvalue and eigenfunction of the equation (3.5) are written respectively as

$$\begin{aligned} E_{CM} &= E_L^N = \bar{h}\omega_c(N + \tfrac{1}{2}) \\ \Phi_{CM}^0 &= \mathcal{A}\exp[-(e\mathcal{H}/2\bar{h}c)(Y_0 - (\bar{h}c/e\mathcal{H})K_x)^2] \end{aligned} \tag{3.6}$$

where Φ_{CM}^0 represents the eigenfunction of the fundamental level.

Finally, the total energy of the trion X^- in a magnetic field is written as

$$E = \langle\phi_{rel}|H_0^{rel} + H_2' + H_3' + E_{CM}|\phi_{rel}\rangle/\langle\phi_{rel}|\phi_{rel}\rangle \tag{3.7}$$

and will be determined by a variational calculation.

3.2. Variational calculation of the binding energy

In order to compare our results with those obtained with a zero magnetic field, we will use the same Hylleraas variational wave function [13] containing 22 terms, but, in our case, the linear as well as the non-linear variational parameters depend on the magnitude of the magnetic field. Let us recall that this function depends only on the distances r_{1h}, r_{2h} and r_{12} between the three particles. In these conditions we can write

$$\phi_{rel}(\boldsymbol{r},\ \boldsymbol{R}) = \phi(r_{1h},\ r_{2h},\ r_{12}) \tag{3.8}$$

or using elliptical coordinates $(s,\ t,\ u)$ defined by

$$s = r_{1h} + r_{2h} \qquad t = r_{1h} - r_{2h} \qquad u = r_{12}$$
$$s \geqslant 0 \qquad -u \leqslant t \leqslant +u \qquad 0 \leqslant u \leqslant s$$
$$\phi(s,\ u,\ t) = \psi(ks,\ ku,\ kt)$$
$$\psi(s,\ u,\ t) = \sum_{lmn} c_{lmn}|lmn\rangle$$

where

$$|lmn\rangle = \exp(-s/2)s^l u^m t^n. \tag{3.9}$$

l, m and n are zero or positive integers; the parameters c_{lmn} and the scaling factor k are determined by the variational method and depend on the magnitude of the magnetic field. The Zeeman term H_2', which occurs for a perpendicular magnetic field, does not give any contribution to the total energy (3.7), because the selected wave function does not depend on the angles defining the orientation of the trion (eeh) in the plane. In the following, we use the atomic units for the length $\epsilon\hbar^2/m_e^*e^2$ and the energy $m_e^*e^4/\epsilon^2\hbar^2 = 2$ Ryd. Taking into account the approximations described above, the average total energy of the trion X^- is written as

$$E = E_{rel} + E_{CM} \tag{3.10}$$

with

$$E_{rel} = \langle\phi_{rel}|H_0^{rel} + H_3'|\phi_{rel}\rangle/\langle\phi_{rel}|\phi_{rel}\rangle. \tag{3.11}$$

E_{CM} is the energy of the centre of mass; H_0^{rel} is the Hamiltonian of the relative motion without a magnetic field. The diamagnetic term H_3' is written as

$$H_3' = H_{dia} = (\gamma^2/4)[\tfrac{1}{4}\rho_r^2 + \lambda(\sigma)\rho_R^2] \tag{3.12}$$

where

$$\rho_r = x^2 + y^2 \qquad \rho_R = X^2 + Y^2 \tag{3.13}$$

with

$$\gamma = \hbar\omega_c/2 \text{ Ryd} \qquad \omega_e = e\mathcal{H}/(m_e^*c). \tag{3.14}$$

From the relations (3.13), it can be easily verified that

$$H_{dia}(s,\ u,\ t) = (\gamma^2/16)[u^2 + \lambda(\sigma)\{s^2 + t^2 - u^2\}] = (1/k^2)H_{dia}(ks,\ ku,\ kt). \tag{3.15}$$

The average value of the relative energy (3.11) can be expressed as a function of the matrix elements of $H_3' = H_{dia}$, H_0^{rel} and the norm in a basis of vectors $|lmn\rangle$ by

$$E_{rel} = (k^2M - kL + P/k^2)/N \tag{3.16}$$

where M, L, P and N are quadratic forms associated with the kinetic energy, the potential energy, the diamagnetic energy and the normation factor which no longer depend on the scaling factor k. They are given by

$$M = \boldsymbol{c}^\dagger\mathbf{T}\boldsymbol{c} \qquad L = -\boldsymbol{c}^\dagger\mathbf{V}\boldsymbol{c} \qquad P = \boldsymbol{c}^\dagger\mathbf{D}\boldsymbol{c} \qquad N = \boldsymbol{c}^\dagger\mathbf{S}\boldsymbol{c}. \tag{3.17}$$

$\boldsymbol{c}^\dagger$ denotes the transposed column matrix of the c_{lmn} coefficients. The matrices $\mathbf{T}$, $\mathbf{V}$ and $\mathbf{D}$ correspond to the representation of the kinetic energy, potential energy and diamagnetic energy operators defined in a basis of vectors $|lmn\rangle$ and $\mathbf{S}$ denotes the normation matrix. The different matrix elements are given in the appendix. Within the variational principle, the coefficients k and c_{lmn} must satisfy the conditions

$$\partial E_{rel}/\partial k = 0 \qquad \partial E_{rel}/\partial c_{lmn} = 0. \tag{3.18}$$

The first equation leads to

$$k^4 - k^3 L/2M - P/M = 0. \tag{3.19}$$

Therefore

$$E_{rel} = -k^2 M/N + 3P/k^2 N. \tag{3.20}$$

The second equation leads to a system of linear equations involving the c_{lmn} coefficients:

$$(k^2\mathbf{T} + k\mathbf{V} + \mathbf{D}/k^2 - E_{rel}\mathbf{S})\boldsymbol{c} = 0. \tag{3.21}$$

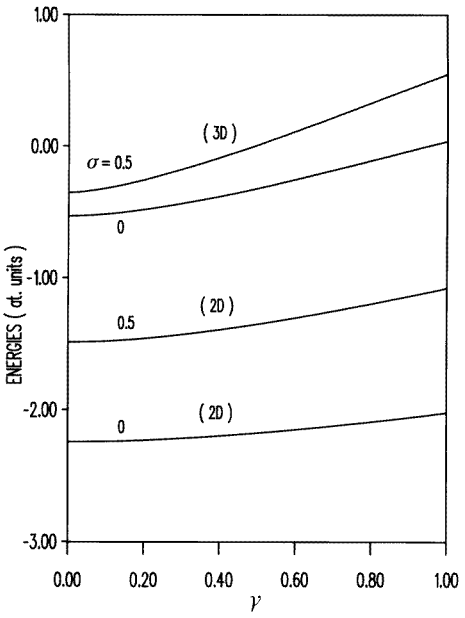

Figure 1. The variation of the relative energy of the fundamental state of the negative trion X^- as a function of the effective magnetic field γ in the 2D and 3D cases for two values of the electron to hole effective mass ratio σ.

4. Results and discussion

The resolution of the system given by (3.21) allows us to determine the energies E_{rel} as well as the variational parameters c_{lmn} and k. Our 22-term wave function, (3.9), is defined by the condition $l+m+n \leqslant 4$. We start our calculations using the values of the scale factor k obtained without magnetic field [8]. For fixed values of k, γ and σ, we diagonalize the system given by (3.21) and use the c_{lmn} coefficients to determine the quadratic forms L, M, N and P corresponding to the fundamental eigenvalue of (3.21). Then we determine numerically the real roots of the fourth-order equation for k, (3.19). These roots are then used to solve (3.20). The value of k which gives rise to the lowest relative energy E_{rel} is used as initial value for a next iteration and so on until the desired accuracy for the energy is reached. In figure 1, we show the variations with γ of the fundamental relative energy for some values of the effective mass ratio σ. A maximum number of 50 iterations has been necessary to obtain an accuracy of five significant digits. Now we can compare the present

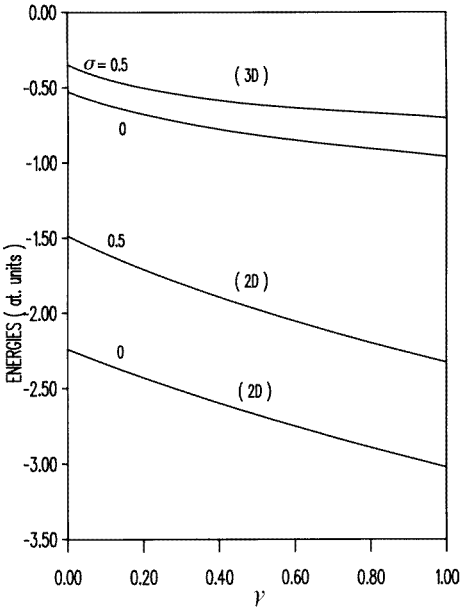

Figure 2. Variations of the difference between the relative energy E_{rel} and the Landau fundamental energy of the three non-interacting particles as a function of the effective magnetic field γ.

2D values to our previously obtained 3D values [8] using the same 22-term wave function. We remark that the values of the 2D relative energies are lower than the 3D energies because of the dimensional confinement. In all cases the relative energy increases with the magnetic field:

$$E_{rel}(\mathrm{2D}) < E_{rel}(\mathrm{3D}). \tag{4.1}$$

In order to point out the influence of the dimensional and magnetic confinements on the Coulombic interaction energy, it is necessary to subtract the energy of the three non-interacting particles under the action of a magnetic field from the relative energy. For this purpose, we have represented in figure 2 the variations with γ of the difference between the relative energy E_{rel} and the Landau fundamental energy of the three non-interacting particles under the action of the magnetic field. We note that the dimensional and magnetic confinements increase the effect of the Coulombic interaction. For a fixed value of γ, it appears that $E_{2D} < E_{3D}$. On the other hand, in all cases, the Coulombic interaction increases with the magnetic field. We remark also that our results can be useful in atomic physics. Indeed, if we consider the limit case in which σ tends to zero, the trion X^- becomes analogous to a hydrogen ion H^-, while the trion X_2^+ reduces to an ionized hydrogen molecule H_2^+. Therefore the behaviour of the H^- ion under the action of a magnetic field may be deduced from figure 1. In order to study the influence of the magnetic field and of the confinement on the motion of the centre of mass, we have represented in figure 3 the variations with γ of the total energy (3.11) of the trion X^-, for $\sigma = 0.1$. This figure shows how the zero-field energy levels split into Landau levels under the influence of a magnetic field.

The present study has been limited to the case of a low magnetic field. However, some interesting behaviours may be expected in the high-field limit. Indeed, the similar problem

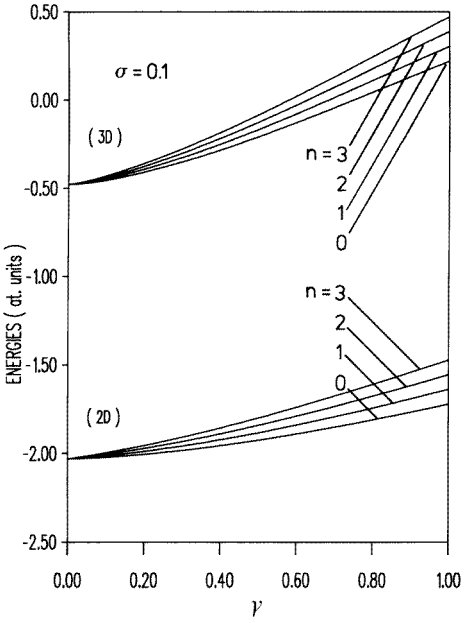

Figure 3. Variations of the total energy of the trion X^- with the effective magnetic field, for $\sigma = 0.1$ in the 2D and 3D cases, showing the splitting into Landau levels.

of three electrons in two dimensions has been discussed [14] in a strong magnetic field. In this case, it has been found that the interelectronic spacing has characteristic values not depending on the form of the interaction, which change discontinuously as pressure is applied, and that the system has characteristic excitation energies proportional to $1/\mathcal{H}$. Finally, we remark that the present 2D results together with those previously obtained [11] in the 3D case may be used in order to estimate what happens in SC quantum wells. Indeed, the 2D limit corresponds to a quantum well with zero well width and infinite conduction and valence band offsets. Therefore, we expect that in the case of a finite well width and finite band offsets the Coulomb correlation energies lie between the 2D and 3D limits.

Acknowledgments

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Appendix. Expression of the matrix elements

All the matrix elements T_i^j, V_i^j, D_i^j and S_i^j with $i \equiv (lmn)$ and $j \equiv (l'm'n')$, can be expressed in terms of the integrals $J_{lmn}^{l'm'n'}$, defined by

$$J_i^j(\lambda,\ \mu,\ \nu) = 2\pi \int_0^\infty \exp(-ks)s^{l+l'+\lambda}\,\mathrm{d}s \int_0^s \frac{u^{m+m'+\mu}}{\sqrt{s^2-u^2}}\,\mathrm{d}u \int_0^u \frac{t^{n+n'+\nu}}{\sqrt{u^2-t^2}}\,\mathrm{d}t \tag{A.1}$$

$$= \frac{2\pi(l+l'+\lambda+m+m'+\mu+n+n'+\nu)!}{k^{l+l'+\lambda+m+m'+\mu+n+n'+\nu+1}} I_{m+m'+\mu+n+n'+\nu} I_{n+n'+\nu} \tag{A.2}$$

where

$$I_{2n} = \frac{\pi(2n!)}{(n!)^2 2^{2n+1}} \qquad I_{2n+1} = \frac{(n!)^2 2^{2n}}{(2n+1)!}. \tag{A.3}$$

We obtain

$$\begin{aligned} T_i^j = \frac{k^2}{4}[J_i^j(0,\,1,\,2) - J_i^j(2,\,1,\,0)] + k(l+m+1)J_i^j(1,\,1,\,0) - klJ_i^j(-1,\,1,\,2) \\ + l(l-1)J_i^j(-2,\,1,\,2) + (n-1)(n+l+2m+1)J_i^j(0,\,1,\,0) \\ - n(n-1)J_i^j(2,\,1,\,-2) + m(m+2l)J_i^j(0,\,-1,\,2) \\ - m(m+2n)J_i^j(2,\,-1,\,0) - mkJ_i^j(1,\,-1,\,2) \\ + \sigma\frac{k^2}{2}[J_i^j(0,\,3,\,0) - (2,\,1,\,0)] + \sigma k(2l+1)J_i^j(1,\,1,\,0) \\ - 2\sigma klJ_i^j(-1,\,3,\,0) + 2\sigma l(l-1)J_i^j(-2,\,3,\,0) + 2\sigma(n^2-l^2)J_i^j(0,\,1,\,0) \\ - 2\sigma n(n-1)J_i^j(0,\,3,\,-2) \end{aligned} \tag{A.4}$$

$$V_i^j = J_i^j(2,\,0,\,0)J_i^j(0,\,0,\,2) - 4J_i^j(1,\,1,\,0) \tag{A.5}$$

$$\begin{aligned} D_i^j = \frac{\gamma^2}{16}[J_i^j(2,\,3,\,0) - J_i^j(0,\,3,\,2) + \lambda(\sigma)\{J_i^j(4,\,1,\,0) - J_i^j(0,\,1,\,4) \\ + J_i^j(0,\,3,\,2) - J_i^j(2,\,3,\,0)\}] \end{aligned} \tag{A.6}$$

$$S_i^j = J_i^j(2,\,1,\,0) - J_i^j(0,\,1,\,2). \tag{A.7}$$

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