Excitonic trions in a low magnetic field

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We study the influence of a uniform magnetic field on the excitonic trion and compute the ground-state energy using a 34-term variational wave function in the low-field limit. We show that there appear additional Landau levels which allow one to distinguish the trions from other neutral complexes.

I. INTRODUCTION

Some years ago, Lampert[1] suggested the possible existence of a great variety of excitonic complexes. Among them, the excitonic trions X^- and $X_2{}^+$, which result from the binding of an exciton with a free electron or a free hole, have not been much explored.[2,3] Nevertheless, their stable binding has been proven[4–9] by means of variational calculations for all values of the electron-to-hole effective-mass ratio σ, although their binding energies are low in general. Experimental evidence of these "charged excitons" has been reported only in a few materials.[10–14] This may be due to the difficulty in distinguishing the excitonic trions from other excitonic complexes, because the transitions lines are often expected to appear in the same spectral region.

The aim of the present paper is to show that under the influence of an external magnetic field the excitonic trions exhibit some distinctive properties which cannot be observed in the case of other neutral and mobile quasiparticles (excitons, biexcitons, etc.). Indeed, due to its charge, the momentum of the transverse motion (i.e., in a plane perpendicular to the field) of the center of mass is not a constant of motion and there appear additional Landau energy levels as in the case of free charged particles.[15] However, the influence of the magnetic field on the relative motion results in Zeeman and quadratic diamagnetic shifts which are observed in all complexes.[16,17] To our knowledge, no study of the influence of a magnetic field on the energy of the excitonic trions has been reported up to now.

In the following section we study the constants of motion of the Hamiltonian. We show that after performing a unitary transformation it exhibits an oscillator term which corresponds to the transverse motion of the center of mass. In Sec. III, we outline our method to determine the energy of the ground state. In particular, we show how, in the low-field limit, the relative motion may be separated from the transverse motion of the center of mass. In Sec. IV, we give the details of the variational calculation of the energy using a 34-term trial wave function.

II. HAMILTONIAN

We discuss explicitly the negative excitonic trion X^- (e,e,h) consisting of two electrons (1 and 2) and a hole h, which is quite analogous to the positive excitonic trion $X_2{}^+$ (e,h,h) by interchanging the electrons and the holes. We assume that the effective-mass approximation is valid and that the constant energy surfaces in the reciprocal space are spherical. By using the Lorentz gauge $\mathbf{A}_i=\frac{1}{2}\mathscr{H}\times\mathbf{r}_i=\frac{1}{2}\mathscr{H}(-y_i,x_i,0)$ relating the vector potentials $\mathbf{A}_i$ $(i=e,e,h)$ to a uniform constant magnetic field $\mathscr{H}$ directed along the z axis, and neglecting the spins as well as the electron-hole exchange interaction, the Hamiltonian of the system is given by

$$H=\frac{1}{2m_e^*}\left[p_1^2+2\frac{e}{c}\mathbf{A}_1\cdot\mathbf{p}_1+\frac{e^2}{c^2}A_1^2\right]+[1\to 2]+\frac{1}{2m_h^*}\left[p_h^2-2\frac{e}{c}\mathbf{A}_h\cdot\mathbf{p}_h+\frac{e^2}{c^2}A_h^2\right]+V_c\ . \tag{2.1}$$

m_e^* and m_h^* are the effective masses of the electrons and the hole, and V_C stands for the Coulomb potential

$$V_C=\frac{e^2}{\epsilon}\left[\frac{1}{r_{12}}-\frac{1}{r_{1h}}-\frac{1}{r_{2h}}\right]\ , \tag{2.2}$$

where ϵ is an appropriate dielectric constant taking into account possible polarization effects.

The Hamiltonian (2.1) may be transformed with use of the center-of-mass and relative coordinates:

$$\mathbf{r}=\mathbf{r}_2-\mathbf{r}_1,\quad \mathbf{R}=\tfrac{1}{2}(\mathbf{r}_1+\mathbf{r}_2)-\mathbf{r}_h\ ,$$

$$\mathbf{R}_0=\frac{m_e^*(\mathbf{r}_1+\mathbf{r}_2)+m_h^*\mathbf{r}_h}{2m_e^*+m_h^*}\ , \tag{2.3}$$

giving

$$H=H_0+H_1+H_2\ , \tag{2.4}$$

with

$$H_0=-\frac{\hbar^2}{2\mu}\nabla_r^2-\frac{\hbar^2}{2M}\nabla_R^2-\frac{\hbar^2}{2M_0}\nabla_{R_0}^2+V_C\ ,$$

$$H_1=\frac{\hbar e}{ic}\left[\frac{1}{m_e^*}\mathbf{A}(\mathbf{r})\cdot\nabla_r+\frac{1}{m_e^*}\left[\frac{1-2\sigma^2}{1+2\sigma}\mathbf{A}(\mathbf{R})+(1+\sigma)\mathbf{A}(\mathbf{R}_0)\right]\cdot\nabla_{\mathbf{R}}+\frac{1}{M_0}\left[\frac{2(1+\sigma)}{1+2\sigma}\mathbf{A}(\mathbf{R})+\mathbf{A}(\mathbf{R}_0)\right]\cdot\nabla_{\mathbf{R}_0}\right],$$

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

and

$$\mu=m_e^*/2,\quad M=2m_e^*m_h^*/(2m_e^*+m_h^*)\ ,$$
$$M_0=2m_e^*+m_h^*,\quad \sigma=m_e^*/m_h^*\ . \tag{2.5}$$

Due to the presence of the factor $\mathbf{A}(\mathbf{R}_0)$, the momentum $\mathbf{P}_0=-i\hbar\nabla_{\mathbf{R}_0}$ of the center of mass does not commute with the Hamiltonian. Only its z component P_{0z} is a constant of motion. It is however easy to verify that the operator

$$\mathbf{\Pi}=\mathbf{p}_1+\mathbf{p}_2+\mathbf{p}_h-\frac{e}{c}(\mathbf{A}_1+\mathbf{A}_2-\mathbf{A}_h)$$
$$=\mathbf{P}_0-\frac{e}{c}\left[\frac{2(1+\sigma)}{1+2\sigma}\mathbf{A}(\mathbf{R})+\mathbf{A}(\mathbf{R}_0)\right] \tag{2.6}$$

is a constant of motion. However, its x and y components Π_x and Π_y do not commute with each other, although they do with the z component $\Pi_z=P_{0z}$. This is due to the fact that the number of the electrons and the holes is not the same, unlike what happens in the case of the exciton or the biexciton where the three components of the (2.6) analogous operators may be defined at the same time.

Because the components Π_x,Π_z and the Hamiltonian may be simultaneously diagonalized, we can transform the wave function Ψ by eliminating the coordinates X_0 and Z_0 of the center of mass:

$$\Psi(\mathbf{r},\mathbf{R},\mathbf{R}_0)=U\Phi(\mathbf{r},\mathbf{R},\mathbf{Y}_0)\ , \tag{2.7}$$

where the unitary transformation operator U reads

$$U=\exp i\left[\left[K+\frac{e}{\hbar c}\frac{2(1+\sigma)}{1+2\sigma}\mathbf{A}(\mathbf{R})\right]\cdot\mathbf{R}_0-\frac{e}{\hbar c}\frac{\mathcal{H}}{2}X_0Y_0\right]. \tag{2.8}$$

This transformation is equivalent to a gauge transformation. We remark that the vector $\mathbf{K}(K_x,0,K_z)$, $\hbar K_x$ and $\hbar K_z$ being the eigenvalues of the operators Π_x and Π_z, is not to be confused with the zero-field wave vector $\mathbf{K}_0$ of the center of mass. Only the z component $K_{0z}=K_z$ of the latter may be defined when the magnetic field is nonzero. This results from the fact that the components Π_x and Π_y of the momentum (2.6) do not commute with each other, in contrast with the case of the exciton and the biexciton, where a three-dimentional $\mathbf{K}$ vector may always be defined.[16,17]

The energy of the trion is given by

$$E=\langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle=\langle\Phi|H'|\Phi\rangle/\langle\Phi|\Phi\rangle\ , \tag{2.9}$$

where the transformed Hamiltonian H' reads

$$\begin{aligned}H'=U^{-1}HU=&-\frac{\hbar^2}{2\mu}\nabla_r^2-\frac{\hbar^2}{2M}\nabla_R^2-\frac{\hbar^2}{2M_0}\nabla_{R_0}^2+\frac{\hbar^2}{2M_0}K^2+V_C-\frac{i\hbar e}{m_e^*c}\Bigg[\mathbf{A}(\mathbf{r})\cdot\nabla_r+\frac{1-2\sigma^2}{1+2\sigma}\mathbf{A}(\mathbf{R})\cdot\nabla_{\mathbf{R}}\\&+\frac{4\sigma(1+\sigma)}{(1+2\sigma)^2}\mathbf{A}(\mathbf{R})\cdot\nabla_{\mathbf{R}_0}+\frac{\sigma}{1+2\sigma}[\mathbf{A}(\mathbf{R}_0)-\mathbf{B}(\mathbf{R}_0)]\cdot\nabla_{\mathbf{R}_0}\Bigg]\\&-\frac{i\hbar^2}{m_e^*}\frac{\sigma}{1+2\sigma}\mathbf{K}\cdot\nabla_{\mathbf{R}_0}+\frac{\hbar e}{m_e^*c}\left[\frac{4\sigma(1+\sigma)}{(1+2\sigma)^2}\mathbf{K}\cdot\mathbf{A}(\mathbf{R})+\frac{\sigma}{1+2\sigma}\mathbf{K}\cdot[\mathbf{A}(\mathbf{R}_0)-\mathbf{B}(\mathbf{R}_0)]\right]\\&+\frac{e^2}{m_e^*c^2}\Bigg[\tfrac{1}{4}A^2(\mathbf{r})+\frac{4\sigma(1+\sigma)}{(1+2\sigma)^2}\mathbf{A}(\mathbf{R})\cdot[\mathbf{A}(\mathbf{R}_0)-\mathbf{B}(\mathbf{R}_0)]+\frac{\sigma}{1+2\sigma}\mathbf{A}(\mathbf{R}_0)\cdot[\mathbf{A}(\mathbf{R}_0)-\mathbf{B}(\mathbf{R}_0)]\\&+\frac{1+4\sigma(1+\sigma)(2+\sigma+\sigma^2)}{(1+2\sigma)^3}A^2(\mathbf{R})\Bigg],\end{aligned} \tag{2.10}$$

with

$$\mathbf{B}(\mathbf{R}_0)=\tfrac{1}{2}\mathcal{H}(Y_0,X_0,0)\ . \tag{2.11}$$

Because the function Φ does not depend on the coordinates X_0 and Z_0 of the center of mass, the operators $\mathbf{K}\cdot\nabla_{\mathbf{R}_0}$ and $[\mathbf{A}(\mathbf{R}_0)-\mathbf{B}(\mathbf{R}_0)]\cdot\nabla_{\mathbf{R}_0}$ do not give rise to any contribution.

Finally, the transformed Hamiltonian reads

$$H' = H'_1 + H'_2 + H'_3 + H'_4 + H'_5 \ , \tag{2.12}$$

where the first term, which exhibits no magnetic field dependence, is given by

$$H'_1 = H_0^{\rm rel} + \frac{\hbar^2}{2M_0} K_z^2 \ , \tag{2.13}$$

with

$$H_0^{\rm rel} = -\frac{\hbar^2}{2\mu}\nabla_{\mathbf r}^2 - \frac{\hbar^2}{2M}\nabla_{\mathbf R}^2 + V_C \ . \tag{2.14}$$

The second term

$$H'_2 = -\frac{i\hbar e}{m_e^* c}\left[\mathbf{A}(\mathbf r)\cdot\nabla_{\mathbf r} + \frac{1-2\sigma^2}{1+2\sigma}\mathbf{A}(\mathbf R)\cdot\nabla_{\mathbf R}\right] \tag{2.15}$$

is the orbital Zeeman contribution, which is linear in the magnetic field. The third term

$$H'_3 = \frac{e^2}{m_e^* c^2}\left[\tfrac{1}{4}A^2(\mathbf r) + \lambda(\sigma) A^2(\mathbf R)\right] \ , \tag{2.16}$$

with

$$\lambda(\sigma) = \frac{1+4\sigma(1+\sigma)(2+\sigma+\sigma^2)}{(1+2\sigma)^3} \tag{2.17}$$

the quadratic diamagnetic contribution. The fourth term

$$H'_4 = -\frac{\hbar^2}{2M_0}\frac{\partial^2}{\partial Y_0^2} + \frac{M_0}{2}\left[\frac{e\mathcal{H}}{M_0 c}\right]^2\left[Y_0 - \frac{\hbar c}{e\mathcal{H}}K_x\right]^2 \tag{2.18}$$

is due to the coupling of the xy-plane motion of the center of mass with the magnetic field. It corresponds to an harmonic oscillator with mass M_0 and circular frequency $\omega = e\mathcal{H}/M_0 c$, the motion taking place around the origin $Y_0 = hcK_x/e\mathcal{H}$. The last term

$$H'_5 = \hbar\left[\frac{e\mathcal{H}}{M_0 c}\right]\left[\frac{2+2\sigma}{1+2\sigma}\right]\left[-iX\frac{\partial}{\partial Y_0} + \frac{e\mathcal{H}}{\hbar c}Y\left[Y_0 - \frac{\hbar c}{e\mathcal{H}}K_x\right]\right] \tag{2.19}$$

may be interpreted as a correction to the oscillatory term H'_4 due to the coupling of the relative motion with the xy-plane motion of the center of mass.

It is important to note that no oscillator term, like H'_4, appears in the case of neutral mobile quasiparticles (exciton, biexciton, etc.). In the following section, we will show that it gives rise to additional Landau energy levels, which are expected to allow us to distinguish excitonic trions from other excitonic complexes.

III. GROUND-STATE ENERGY IN THE LOW-FIELD APPROXIMATION

For not too high magnetic fields the xy-plane motion of the center of mass is expected to remain slow in comparison with the relative motion, so that the corrective term H'_5 does not furnish an important contribution to the energy. We therefore try to separate the two motions in the sense of the Born-Oppenheimer approximation by making the ansatz

$$\Phi(\mathbf r, \mathbf R, Y_0) \equiv \Phi_{\rm rel}(\mathbf r, \mathbf R)\Phi_L(Y_0) \ . \tag{3.1}$$

$\Phi_{\rm rel}$ is the fundamental eigenfunction of the Hamiltonian of the relative motion:

$$H^{\rm rel} = H_0 + H'_2 + H'_3 \ , \tag{3.2}$$

whereas Φ_L stands for the eigenstates of the oscillator term H'_4:

$$H'_4 \Phi_L = E_L \Phi_L \ . \tag{3.3}$$

The corresponding energy eigenvalues are the Landau levels:

$$E_L^n = (n + \tfrac{1}{2})\hbar\left[\frac{e\mathcal{H}}{M_0 c}\right], \quad n = 0, 1, 2, \ldots \ , \tag{3.4}$$

and the non-normalized eigenfunction of the fundamental level $n = 0$ is given by

$$\Phi_L = \exp\left[-\frac{e\mathcal{H}}{2\hbar c}\left[Y_0 - \frac{\hbar c}{e\mathcal{H}}K_x\right]^2\right] \ . \tag{3.5}$$

The total energy reads then

$$E = \langle \Phi_{\rm rel} \mid H_0^{\rm rel} + (\hbar^2/2M_0)K_z^2 + H'_2 + H'_3 + E_L^n \mid \Phi_{\rm rel}\rangle / \langle \Phi_{\rm rel} \mid \Phi_{\rm rel}\rangle \ . \tag{3.6}$$

Indeed, the coupling term H'_5 does not rise to any contribution in our approximation because

$$\langle \Phi_{\rm rel} \mid X \mid \Phi_{\rm rel}\rangle = \langle \Phi_{\rm rel} \mid Y \mid \Phi_{\rm rel}\rangle = 0 \tag{3.7}$$

with relative wave functions of spherical or cylindrical symmetry. It may be further verified that

$$\langle \Phi_L \mid \partial/\partial Y_0 \mid \Phi_L\rangle = \langle \Phi_L \mid Y_0 - (\hbar c/e\mathcal{H})K_x \mid \Phi_L\rangle = 0 \tag{3.8}$$

as a consequence of the parity of the functions Φ_L. These results agree with our ansatz (3.1).

Some years ago, we studied the binding of the ground state of the negative trion X^- in the zero-field limit.[4] In that case, the Schrödinger equation can be separated into an equation for the translational motion of the center of mass and a second equation for the relative motion. Because the zero-field ground state is invariant with respect to the rotations of the system, the wave function depends only on the three mutual distances r_{12}, r_{1h}, and r_{2h}:

$$\Phi_{\rm rel}^0(\mathbf r, \mathbf R) = \Phi(r_{12}, r_{1h}, r_{2h}) \ . \tag{3.9}$$

For an accurate calculation of the zero-field ground-state energy, we used the coordinates

$$s = r_{1h} + r_{2h}, \quad t = r_{1h} - r_{2h}, \quad u = r_{12} \ , \qquad s \geq 0, \quad -s \leq t < s, \quad |t| \leq u \leq s \ , \tag{3.10}$$

and the following 34-term trial wave function:

$$\Phi(s,t,u)=\phi(ks,kt,ku)\ ,$$
$$\Phi(s,t,u)=\sum_{m,n,p} c_{mnp}\,|\,mnp\,\rangle\ , \quad (3.11)$$
$$|\,mnp\,\rangle=\exp\left[-\frac{s}{2}\right]s^m t^n u^p\ ,$$

where m,n,p are positive integers or zero, with $m+n+p\le 5$ and even values of n due to the symmetry of ϕ by interchanging the two electrons. The scaling factor k and the linear parameters were determined using the variation method.

For the present study, we choose the same wave function in the low-field approximation

$$\Phi_{\rm rel}(\mathbf{r},\mathbf{R})\simeq\Phi^0_{\rm rel}(\mathbf{r},\mathbf{R})\ , \quad (3.12)$$

although its spherical symmetry does not reflect all the properties of the Hamiltonian at higher values of the magnetic field. In particular, this function does not depend on the angles defining the triangle $(12h)$ in the space. Therefore the linear orbital-Zeeman term H'_2 does not give any contribution in Eq. (3.6), although a nonzero term may result from the use of a better adapted wave function. Nevertheless, this function is expected to give acceptable results in the low-field limit by varying the parameters k and c_{mnp} in our 34-term basis (3.11). Within these approximations, the total energy reads then

$$E=E_{\rm rel}+E^n_L+\frac{\hbar^2}{2M_0}K_z^2\ , \quad (3.13)$$

where the relative energy $E_{\rm rel}$, the scaling factor k, and the parameters c_{mnp} are determined by the variation condition

$$\bar{E}_{\rm rel}=\langle\Phi^0_{\rm rel}\,|\,H^{\rm rel}_0+H'_3\,|\,\Phi^0_{\rm rel}\rangle/\langle\Phi^0_{\rm rel}\,|\,\Phi^0_{\rm rel}\rangle=min\ . \quad (3.14)$$

The zero-field relative Hamiltonian $H^{\rm rel}_0$ (2.14) and the remaining quadratic diamagnetic term H'_3 (2.16) may be simplified by using the usual atomic units $\epsilon\hbar^2/m_e^*e^2$ for length, $m_e^*e^4/\epsilon^2\hbar^2=2R_Y$ for energy and the effective magnetic field parameter $\gamma=\hbar\omega_c/2R_Y$, $\omega_c=e\mathscr{H}/m_e^*c$ being the effective electron cyclotron frequency:

$$H^{\rm rel}_0=T+V_c\ , \quad (3.15)$$

$$T=-\tfrac{1}{2}(\nabla_1^2+\nabla_2^2)-\frac{\sigma}{2}\nabla_h^2,\quad V_C=\frac{1}{r_{12}}-\frac{1}{r_{1h}}-\frac{1}{r_{2h}}\ ,$$

$$H'_3=\frac{\gamma^2}{4}\left[\frac{\rho_r^2}{4}+\lambda(\sigma)\rho_R^2\right]\ ,$$
$$\rho_r^2=x^2+y^2,\quad \rho_R^2=X^2+Y^2\ . \quad (3.16)$$

IV. NUMERICAL RESULTS AND DISCUSSION

In order to fulfill the condition (3.14), we rewrite the relative energy mean value

$$E_{\rm rel}=k^2\frac{M}{N}-k\frac{L}{N}+\frac{1}{k^2}\frac{P}{N} \quad (4.1)$$

in terms of the quadratic forms

$$M=\underline{c}^\dagger\underline{T}\,\underline{c},\quad L=-\underline{c}^\dagger\underline{V}\,\underline{c},\quad P=\underline{c}^\dagger\underline{D}\,\underline{c},\quad N=\underline{c}^\dagger\underline{S}\,\underline{c}\ . \quad (4.2)$$

where $\underline{c}$ denotes the column matrix of the linear coefficients c_{mnp}. The matrices $\underline{T}$, $\underline{V}$, $\underline{D}$, and $\underline{S}$ are defined with respect to the basis functions $|\,mnp\,\rangle$ given by (3.11):

$$T^{m'n'p'}_{mnp}=\langle m'n'p'\,|\,T\,|\,mnp\,\rangle\ ,$$
$$V^{m'n'p'}_{nmp}=\langle m'n'p'\,|\,V_c\,|\,mnp\,\rangle\ ,$$
$$D^{m'n'p'}_{mnp}=\langle m'n'p'\,|\,H'_3\,|\,mnp\,\rangle\ , \quad (4.3)$$
$$S^{m'n'p'}_{mnp}=\langle m'n'p'\,|\,I\,|\,mnp\,\rangle\ .$$

All these matrix elements may be expressed in terms of the integrals (m,n,p), which are defined for even values of n by

$$(m,n,p)=\int_0^\infty ds\,e^{-s}s^m\int_{-s}^{s}dt\,t^n\int_{|t|}^{s}du\,u^p=\frac{2(m+n+p+2)!}{(n+1)(n+p+2)!}\ , \quad (4.4)$$

$$\begin{aligned}T^{m'n'p'}_{mnp}=\pi^2[&m(m-1)(m'+m-2,n'+n+2,p'+p+1)-m(m'+m-1,n'+n+2,p'+p+1)\\&-(m-n)(m+n+2p+3)(m'+m,n'+n,p'+p+1)+p(2m+p+1)(m'+m,n'+n+2,p'+p+1)\\&+\tfrac{1}{4}(m'+m,n'+n+2,p'+p+1)+(m+p+2)(m'+m+1,n'+n,p'+p+1)\\&-p(m'+m+1,n'+n+2,p'+p-1)-n(n-1)(m'+m+2,n'+n-2,p'+p+1)\\&-p(2n+p+1)(m'+m+2,n'+n,p'+p-1)-\tfrac{1}{4}(m'+m+2,n'+n,p'+p+1)]\\+\sigma\pi^2[&2m(m-1)(m'+m-2,n'+n,p'+p+3)-2m(m'+m-1,n'+n,p'+p+3)\\&-2n(n-1)(m'+m,n'+n-2,p'+p+3)-2(m-n)(m+n+1)(m'+m,n'+n,p'+p+1)\\&+\tfrac{1}{2}(m'+m,n'+n,p'+p+3)+2(m+1)(m'+m+1,n'+n,p'+p+1)\\&-\tfrac{1}{2}(m'+m+2,n'+n,p'+p+1)]\ ,\end{aligned} \quad (4.5)$$

$$V_{mnp}^{m'n'p'}=\pi^2[-(m'+m,n'+n+2,p'+p)-4(m'+m+1,n'+n,p'+p+1)+(m'+m+2,n'+n,p'+p)] , \quad (4.6)$$

$$D_{mnp}^{m'n'p'}=\gamma^2\frac{\pi^2}{24}\{[(m+m'+2,n+n',p+p'+3)-(m+m',n+n'+2,p+p'+3)]$$
$$+\lambda(\sigma)[(m+m'+4,n+n',p+p'+1)-(m+m',n+n'+4,p+p'+1)$$
$$-(m+m'+2,n+n',p+p'+3)+(m+m',n+n'+2,p+p'+3)]\} , \quad (4.7)$$

$$s_{nmp}^{m'n'p'}=-\pi^2[(m'+m,n'+n+2,p+p'+1)] . \quad (4.8)$$

The extremun condition (3.14) reads now

$$\frac{\partial \overline{E}_{\rm rel}}{\partial k}=0, \quad \frac{\partial \overline{E}_{\rm rel}}{\partial c_{nmp}}=0 , \quad (4.9)$$

whatever the indices m,n,p. The first equation leads to the relations

$$k^4-Lk^3/2M-P/M=0 , \quad (4.10)$$

$$\overline{E}_{\rm rel}=-k^2M/N+3P/k^2N , \quad (4.11)$$

whereas the last equations are equivalent to the system

$$(k^2\underline{T}+k\underline{V}+\underline{D}/k^2-E_{\rm rel}\underline{S})\underline{c}=\underline{0} . \quad (4.12)$$

The eigenvalue $E_{\rm rel}$ and the eigenvector $\underline{c}$ are determined using the 34-term basis (3.11), each term being normalized to unity. The scaling factor k is obtained by a converging iterative method, using the generalized virial theorem (4.10) and (4.11). In a first step, and for fixed values of σ and γ, we use the k values previously obtained,[4] and determine the quadratic forms (4.2) with the set of parameters c_{mnp} relative to the lowest eigenvalue of Eq. (4.12). Next, we solve numerically Eq. (4.10) and compute the energy values (4.11) corresponding to each root. The k value giving rise to the lowest energy is then used in a second step to solve again Eq. (4.12), and so on until the desired accuracy on the energy is obtained.

In Fig. 1 we have reported the relative energies $E_{\rm rel}$ obtained for the negative excitonic trion X^-. The corresponding values for the positive trion X_2^+ may be deduced from this curve. Indeed, the symmetry properties of the Hamiltonian show that, in our units, the energies of the two complexes are related by the relation

$$E_{X_2^+}(\sigma,\gamma')=\sigma^{-1}E_{X^-}(\sigma,\gamma) , \quad (4.13)$$

where the effective fields γ and γ' are assumed to have the same numerical value. γ' is defined in the same manner as γ by replacing the electron mass by the hole mass. In particular, for a given magnetic field, $\gamma=\gamma'/\sigma^2$.

Figure 2 shows how the scaling factor k increases with

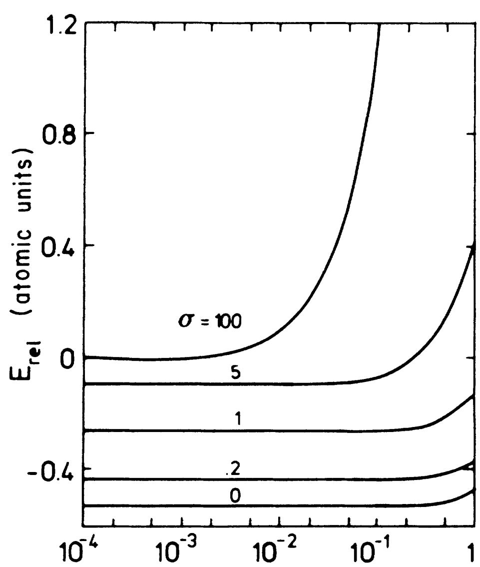

FIG. 1. Variations of the relative energy $E_{\rm rel}$, as defined in (3.13) vs the effective magnetic field γ.

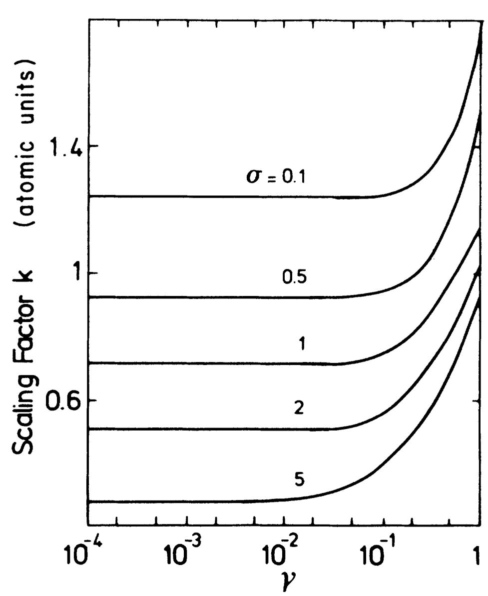

FIG. 2. Variations of the scaling factor k vs the effective magnetic field γ.

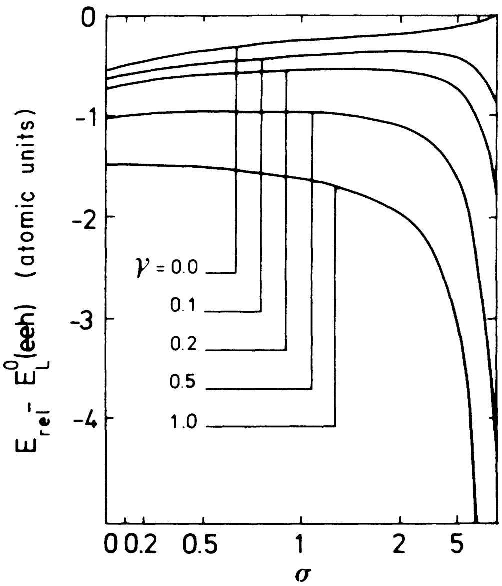

FIG. 3. Variations of the relative energy $E_{\rm rel}$ defined with respect to the sum of the fundamental Landau levels $E_L^0(e,e,h)$ of the three noninteracting particles.

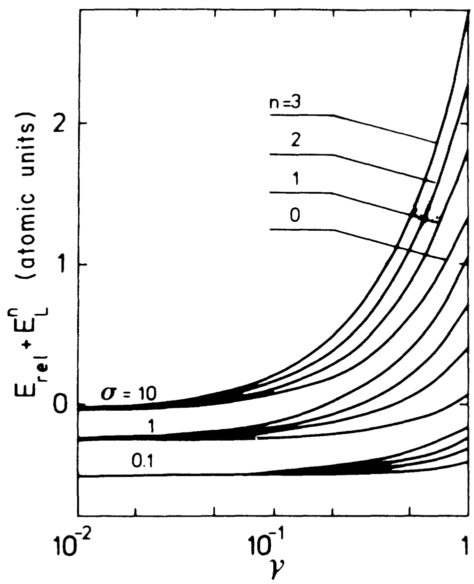

FIG. 4. Discrete part $E_{\rm rel}+E_L^n$ of the total energy vs the effective magnetic field γ corresponding to the four lowest Landau levels.

the magnetic field. This is due to the shrinking of the orbitals when the magnetic field takes higher values. In Fig. 3 we have reported the relative energies with respect to the sum of the fundamental Landau energies $E_L^0(e,e,h)$ of the three noninteracting particles. It appears, as expected, that the Coulomb interaction is enhanced by the magnetic field. Figure 4 shows how the quantified motion of the center of mass in the plane perpendicular to the magnetic field lifts the degeneracy of the energy levels. Because the present study does not take into account the linear Zeeman contribution, the levels reported in Fig. 4 undergo an additional splitting, not reported here. To our knowledge, there exists no experimental study of the influence of a magnetic field on the energy of an excitonic trion. The expected transition energies between a free electron (hole) and an X^- $(X_2{}^+)$ trion are given by

$$h\nu_{X^-}=h\nu_X+W_{X^-}-\frac{\hbar^2K_z^2}{2m_e^*}\frac{\sigma+1}{2\sigma+1}+E_L^n(X^-)-E_L^{n'}(e)\ ,$$

$$h\nu_{X_2{}^+}=h\nu_X+W_{X_2{}^+}-\frac{\hbar^2K_z^2}{2m_e^*}\frac{\sigma+1}{\sigma+2}+E_L^n(X_2{}^+)-E_L^{n'}(e)\ ,$$

(4.14)

where $h\nu_X$ is the fundamental exciton discrete transition energy in a magnetic field. $-W_{X^-}(-W_{X_2{}^+})$ stands for the binding energy of the excitonic trion X^- $(X_2{}^+)$, defined by

$$E_{\rm rel}(X^-)=E_X+W_{X^-}\ . \tag{4.15}$$

This latter can be obtained using our values of the relative energies (Fig. 1) and the exciton binding energies as reported for instance by Cabib *et al.*[18] The Landau energies $E_L^n(X^-)$ and $E_L^{n'}(e)$ appearing in (4.14) are given by

$$E_L^n(X^-)=(n+\tfrac{1}{2})\hbar\omega_e\frac{\sigma}{1+2\sigma}\ ,$$

$$E_L^{n'}(e)=(n'+\tfrac{1}{2})\hbar\omega_e\ , \tag{4.16}$$

$$\omega_e=e\mathcal{H}/m_e^*c,\quad n,n'=0,1,2\ldots\ .$$

In the present study we have restricted ourselves to isotropic, spherical, and nondegenerate electron and hole bands. This approximation becomes questionable for materials with $(j=\frac{3}{2})$-type hole band structure. In this case the best results would probably arise from the use of an experimental "mean" hole mass deduced, for instance, from the observed exciton spectra.

The above splitting into Landau levels is the main result of the present study. We hope that it may be used to distinguish experimentally the excitonic trions from excitons and other excitonic complexes. The most important splitting is expected in materials with small electron and hole effective masses.

[1]M. A. Lampert, Phys. Rev. Lett. 1, 450 (1958).
[2]V. B. Timofeev, in *Excitons,* edited by E. I. Rashba and M. D. Sturge (North-Holland, Amsterdam, 1982), p. 349.
[3]G. A. Thomas and V. B. Timofeev, in *Handbook on Semiconductors,* edited by T. S. Moss and M. Balkanski (North-Holland, Amsterdam, 1980), Vol. 2, p. 45.
[4]G. Munschy and B. Stébé, Phys. Status Solidi B **64**, 213 (1974).
[5]G. Munschy and B. Stébé, Phys. Status Solidi B **72**, 135 (1975).

[6]B. Stébé and G. Munschy, Solid State Commun. **17**, 1051 (1975).
[7]Z. A. Insepov and G. E. Norman, Zh. Eksp. Teor. Fiz. **69**, 1321 (1975) [Sov. Phys.—JETP, **42**, 674 (1975)].
[8]B. Stébé and C. Comte, Solid State Commun. **19**, 1237 (1976).
[9]B. Stébé and C. Comte, Phys. Rev. B **15**, 3967 (1978).
[10]Z. A. Insepov, G. E. Norman, and L. Yu Shurova, Zh. Eksp. Teor. Fiz. **71**, 1960 (1976) [Sov. Phys.—JETP **44**, 1028 (1976)].
[11]T. Kawabata, K. Muro, and S. Narita, Solid State Commun. **23**, 267 (1977).
[12]G. A. Thomas and T. M. Rice, Solid State Commun. **23**, 359 (1977).
[13]B. Stébé, T. Sauder, M. Certier, and C. Comte, Solid State Commun. **26**, 637 (1978).
[14]A. E. Zhidkov and Ya E. Pokrovskii, Pis'ma Zh. Eksp. Teor. Fiz. **30**, 499 (1979) [JETP Lett. **30**, 468 (1979)].
[15]M. H. Johnson and B. A. Lippmann, Phys. Rev. **76**, 828 (1949).
[16]R. S. Knox, *Theory of Excitons* (Academic, New York, 1963).
[17]V. M. Edel'shtein, Zh. Eksp. Teor. Fiz. **77**, 760 (1979) [Sov. Phys.—JETP **50**, 384 (1979)].
[18]D. Cabib, E. Fabri, and G. Fiorio, Solid State Commun. **9**, 1517 (1971).