Optical and magneto-optical absorption of negatively charged excitons in three- and two-dimensional semiconductors

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The line shape of the optical and magneto-optical absorption of negatively charged excitons in three- and two-dimensional (2D) semiconductors has been studied. The absorption coefficients have been determined using envelope wave functions obtained by variational means. At zero field, the charged exciton lines are disposed at the low-energy side of the threshold frequency with a rapidly decreasing long tail. In the two-dimensional case, the maximum corresponds to the threshold frequency, while in the 3D case, this maximum is shifted to lower transition energies. The magnetic field gives rise to a Landau quantization of the spectra, which reduces to a series of sharp lines in the two dimensional case. [S0163-1829(98)02639-3]

I. INTRODUCTION

Charged excitons (or excitonic trions) are excitonic complexes that may result in semiconductors from the binding of an electron (e) or a hole (h) with an exciton (X). The existence of two kinds of charged excitons has been suggested first by Lampert[1] in analogy with existing atomic and molecular systems. The negatively charged exciton, or excitonic ion $X^-(eeh)$ is the analogous of the H^- hydrogen ion, while the positively charged exciton, or excitonic molecule ion $X_2^+(hhe)$ is the analogous of the H_2^+ hydrogen molecule ion. Original optical properties are expected due to their mobility and their charge, in particular, when submitted to an external electric or magnetic field. Excitonic trions have been first observed in three-dimensional (3D) semiconductors: Ge,[2,3] Si,[4] and CuCl.[5] However, because the 3D charged exciton binding energies are very weak, these observations have been possible only at very low temperatures. However, more recently, the possibility of growing artificial structures like quantum wells, where the quantum confinement effects become predominant and enhance the Coulombic correlations, has given new possibilities of observation of these complexes even at room temperature, giving rise to the possibility of technologic applications for optoelectronic devices. In particular, negatively charged excitons have been observed in different types of semiconductor quantum wells (QW).[6–9]

From the theoretical point of view, the binding energies of charged excitons have been estimated using variational calculations, in the case of 3D semiconductors,[10–14] 2D semiconductors,[15–17] semiconductor QW,[18] and semiconductor quantum dots.[19] The influence of an external magnetic field on the binding energy of the negatively charged exciton has been studied in the case of 3D (Ref. 20) and 2D (Ref. 21) semiconductors. However, to our knowledge, there does not exist any study concerning the optical properties of charged excitons. In order to identify the charged exciton lines, it may be interesting to know whether these lines are different from exciton or bound exciton lines, to know the influence of the geometric and quantum confinement, and also their behavior in an external magnetic field.

It is the aim of the present paper to give an insight on the shape of the absorption lines of negatively charged excitons in 3D and 2D semiconductors with or without an external magnetic field. In the following section, we outline the theory of the one-photon dipolar absorption corresponding to transitions from a free-electron initial state to a negatively charged exciton final state. We make precise our approximations and obtain an expression of the absorption coefficient with and without an external magnetic field. In Sec. III, we study the zero-field absorption, and show how the 3D and 2D cases are different. Crudely speaking, the absorption coefficient is proportional to the density of states of the final state. So, because a charged exciton may be considered as a charged mobile particle localized at the center of mass of the complex, we expect a quasi-free-particle behavior. But due to the Coulomb correlation, this free-particle behavior is modified by an envelope oscillator strength that decreases strongly on the low-energy side of the threshold transition energy. This behavior is quite analogous for 2D and 3D materials. However, because the free-particle 2D and 3D densities of states are different, the final behavior is quite different for 2D and 3D excitonic trions. In Sec. IV, we take into account an external magnetic field. In this case, an additional confinement effect arises. In 3D semiconductors, there appears a quantization of the motion of the center of mass in the plane perpendicular to the magnetic field that gives rise

to Landau levels. In 2D semiconductors, with the field perpendicular to the plane, the quantization effects are total, and the spectra is expected to reduce to Dirac peaks. Finally, in the last section we outline our conclusions.

II. ABSORPTION COEFFICIENT

In this section we present the main results of the theory of the electric dipolar absorption corresponding to a transition from a free-electron state (e) to the ground state of a negatively charged exciton X^- consisting of two electrons (1,2) and one hole (h). We take into account the influence of an external uniform magnetic field. Because the formalism of the 3D and 2D cases are quite analogous, we treat explicitly only the 3D case, from which we deduce the 2D case. In the present study we consider only direct-gap semiconductors with spherical bands at $\mathbf{k}=0$. For the sake of simplicity, we do not take into account all the details and possible degeneracies of the band structure, which we describe by an isotropic two-band model, and restrict ourselves to the linear low-density regime. Because this theory is a natural extension of the well-known theory of the optical absorption of excitons,[22,23] we present only its main results. We do not take into account the influence of the temperature restricting ourselves to one-photon transitions at 0 K.

Different transition processes may be suggested. Here we consider a transition between a free-electron state from the top of the valence band and a negatively charged exciton ground state. Thus the electron-photon initial and final states correspond, respectively, to a free-electron state $|\Phi_i\rangle$ with $N_{\mathbf{q}\nu}$ photons and a negatively charged exciton ground state $|\Phi_f\rangle$ with $N_{\mathbf{q}\nu}-1$ photons:

$$|i\rangle = |\Phi_i ; N_{\mathbf{q}\nu}\rangle \quad \text{and} \quad |f\rangle = |\Phi_f ; N_{\mathbf{q}\nu}-1\rangle \quad (1)$$

with

$$|\Phi_i\rangle = a_\lambda^\dagger |\Phi_0\rangle,$$

$$|\Phi_f\rangle = \frac{1}{\sqrt{2}} \sum_{\lambda_1 \lambda_2 \lambda_h} C_{\lambda_1 \lambda_2 \lambda_h} a_{\lambda_1}^\dagger a_{\lambda_2}^\dagger d_{\lambda_h}^\dagger |\Phi_0\rangle. \quad (2)$$

$|\Phi_0\rangle$ denotes the ground state of the crystal electronic ground state at $T=0$ K, which in our model corresponds to a full valence band and an empty conduction band. $a_\lambda^\dagger$ and d_λ are, respectively, the creation and annihilation operators of electrons and holes in the states $|\lambda\rangle$. In the first-order envelope function approximation, the electron and hole wave functions may be written as a product of the periodic part of the conduction- and valence-band wave functions c and v at $\mathbf{k}=0$ with an envelope function f associated with the motion of the electrons or the holes:

$$\varphi_{e\lambda}(\mathbf{r}) = c(\mathbf{r}) f_{e\lambda}(\mathbf{r})$$

and

$$\varphi_{h\lambda}(\mathbf{r}) = v^*(\mathbf{r}) f_{h\lambda}(\mathbf{r}). \quad (3)$$

We assume that the functions f_λ, c and v satisfy the orthogonality relations:

$$\frac{1}{\Omega} \int_\Omega d^3 r f_{h\lambda}^*(\mathbf{r}) f_{e\lambda'}^*(\mathbf{r}) = \delta_{\lambda\lambda'},$$

$$\frac{1}{\Omega_0} \int_{\Omega_0} d^3 r c^*(\mathbf{r}) v(\mathbf{r}) = 0, \quad (4)$$

where Ω_0 is the volume of the unit cell, and $\Omega = L_x L_y L_z$ denotes the crystal volume.

The coefficients $C_{\lambda_1 \lambda_2 \lambda_h}$ are the envelope wave functions of the charged exciton in the $\mathbf{k}$ space related to the envelope wave function ϕ in the r space by a Fourier transformation. The envelope wave function accounts for the Coulomb interaction and is obtained as a solution of the Schrödinger equation:

$$\left[\frac{\hbar^2}{2m_e^*} \left(\mathbf{p}_1 + \frac{e}{c} \mathbf{A}_1 \right)^2 + \frac{\hbar^2}{2m_e^*} \left(\mathbf{p}_2 + \frac{e}{c} \mathbf{A}_2 \right)^2 \right.$$
$$\left. + \frac{\hbar^2}{2m_h^*} \left(\mathbf{p}_h - \frac{e}{c} \mathbf{A}_h \right)^2 + V_c \right] \phi = E\phi, \quad (5)$$

where the potential vectors A_i of the electrons and the hole are expressed as a function of the uniform magnetic field $\mathbf{H}$:

$$\mathbf{A}(r_i) = \tfrac{1}{2} \mathbf{H} \times r_i. \quad (6)$$

The interactions between the three particles are modeled by a Coulomb potential that is screened by a quite phenomenological dielectric constant κ:

$$V_c = \frac{e^2}{\kappa} \left(\frac{1}{r_{12}} - \frac{1}{r_{1h}} - \frac{1}{r_{2h}} \right). \quad (7)$$

We have previously obtained variational solutions of Eq. (5) for 3D semiconductors, without[10] and with[20] an external magnetic field, and in for 2D semiconductors, without[17] and with[21] an external magnetic field perpendicular to the plane.

The absorption coefficient α may be defined as usual as the energy dissipation per unit volume divided by the energy density and by the energy velocity:

$$\alpha = \frac{n}{c N_{\mathbf{q}\nu} \Omega} W_{abs}^{if}, \quad (8)$$

where n is the real part of the refractive index of the crystal of volume, and c is the velocity of the light in the vacuum. The transition probability per unit time W_{abs}^{if} is given by

$$W_{abs}^{if} = \frac{2\pi}{\hbar} \sum_{i,f} |\langle f|H_{abs}|i\rangle|^2 \delta(\mathcal{E}_f - \mathcal{E}_i - \hbar\omega), \quad (9)$$

where $\mathcal{E}_i$ and $\mathcal{E}_f$ are the initial- and final-state energies of the crystal electronic system interacting with a photon of energy $\hbar\omega$. The interaction Hamiltonian describing the absorption of the light reads

$$\mathcal{H}_{abs} = \frac{1}{mn} \sqrt{\frac{2\pi\hbar}{\omega\Omega}} \sum_{\mathbf{q}\nu} \sum_\lambda a_\lambda^\dagger d_\lambda^\dagger b_{\mathbf{q}\nu} \varepsilon_{\mathbf{q}\nu} \cdot \mathbf{D}. \quad (10)$$

where m denotes the non relativistic free-electron mass. $b_{\mathbf{q}\nu}$ is the annihilation operator of a photon with wave vector $\mathbf{q}$, polarization ν, and circular frequency ω. $\varepsilon_{\mathbf{q}\nu}$ represents the

polarization vector of the radiation. $\mathbf{D}$ represents the $\mathbf{k}=0$ band to band dipolar momentum:

$$\mathbf{D}=e\int_\Omega d^3 r c^*(\mathbf{r})\mathbf{p}v(\mathbf{r}), \qquad (11)$$

which depends only on the particular band structure. It may be supposed to be nonzero if we assume that direct band to band transitions are allowed at $\mathbf{k}=0$. We have neglected the terms corresponding to the creation followed by the annihilation of the same particle in a given band, so that intraband transitions are not taken into account. This approximation is justified because we consider only optical excitation energies comparable to the band gap at $T=0$ K. Finally we get, in the case of a given polarization ε,

$$\alpha=\frac{8\pi^2}{nm^2 c\Omega\omega}\sum_{if}|\varepsilon\cdot\mathbf{D}|^2 I\delta(\mathcal{E}_i-\mathcal{E}_f-\hbar\omega), \qquad (12)$$

where

$$I=\left|\sum_{\lambda'} C_{\lambda'\lambda\lambda'}\right|^2 \qquad (13)$$

denotes the ''envelope oscillator strength,'' which depends only on the envelope wave function of the charged exciton.

At this point it is important to remark that we suppose that the initial free-electron state $|\Phi_i\rangle$ in Eq. (2) corresponds to extra electrons not generated by band to band transitions, so that the number of electrons in the valence band remains unchanged. In this scheme, at zero temperature, the Fermi thermal distribution for the ''free'' electrons reduces to unity provided that their energies are lower than their Fermi energy, as we assume in the present study. As a consequence, the electron density of states as well as the absorption coefficient α do not depend on the temperature. The physical situation described by the assumption of both zero temperature and electrons in the conduction band may, for instance, correspond to extra carriers generated by injection or by nonthermal previous ionization of impurities.

III. ZERO-FIELD OPTICAL ABSORPTION

In this section we will establish the expression of the absorption coefficient of the charged exciton [Eq. (12)] without taking into account the external magnetic field for 3D and 2D semiconductors. In this case the envelope parts of the free electron and hole basis functions defined in Eq. (3) reduces to simple plane wave functions $\exp(i\mathbf{k}\cdot\mathbf{r})$.

We study first the case of bulk semiconductors. The charged exciton envelope oscillator strength [Eq. (13)] depends on the ground-state envelope wave functions ϕ in the $\mathbf{r}$ space that is related to its Fourier transform $C_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_h}$ in the $\mathbf{k}$ space by

$$C_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_h}=\frac{1}{\Omega^{3/2}}\int_\Omega d^3 r_1 d^3 r_2 d^3 r_h$$

$$\times\phi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_h)\exp[-i(\mathbf{k}_1\cdot\mathbf{r}_1+\mathbf{k}_2\cdot\mathbf{r}_2-\mathbf{k}_h\cdot\mathbf{r}_h)]$$

$$(14)$$

where $\mathbf{r}_1,\mathbf{r}_1,$ and $\mathbf{r}_h$ are the position vectors of the three particles. The envelope function ϕ may be written as the product of the center of mass contribution and the relative envelope function ϕ_{rel}:

$$\phi(\mathbf{r},\mathbf{R},\mathbf{R}_0)=\frac{1}{\Omega^{1/2}}e^{i\mathbf{K}_0\cdot\mathbf{R}_0}\phi_{rel}(\mathbf{r},\mathbf{R}), \qquad (15)$$

where $\mathbf{K}_0$ is the wave vector of the center of mass; $\mathbf{r}$, $\mathbf{R}$, and $\mathbf{R}_0$ are, respectively, the relative and center-of-mass coordinates defined by

$$\mathbf{r}=\mathbf{r}_2-\mathbf{r}_1, \qquad \mathbf{R}=\frac{\mathbf{r}_1+\mathbf{r}_2}{2}-\mathbf{r}_h,$$

$$\mathbf{R}_0=\frac{m_e^*}{M_0}(\mathbf{r}_1+\mathbf{r}_2)+\frac{m_h^*}{M_0}\mathbf{r}_h. \qquad (16)$$

$M_0=2m_e^*+m_h^*$ is the mass of the center of mass. m_e^* and m_h^* are, respectively, the effective masses of the electron and the hole at $\mathbf{k}=0$. The envelope oscillator strength [Eq. (13)] may then be written as

$$I(\mathbf{k})=\delta_{\mathbf{K}_0\mathbf{k}}\left|\int_\Omega d^3 r e^{-i\mu\mathbf{K}_0\cdot\mathbf{r}}\phi_{rel}(\mathbf{r},\mathbf{r}/2)\right|^2, \qquad (17)$$

where the mass parameter $\mu=1+\sigma/1+2\sigma$ depends only on the effective mass ratio $\sigma=m_e^*/m_h^*$. It appears, as expected, that the transitions are only allowed if the wave vectors $\mathbf{k}$ and $\mathbf{K}_0$ of the free electron and the center of mass are identical. The absorption coefficient [Eq. (12)] reduces thus to a single summation that we replace by an integral in $\mathbf{k}$ space:

$$\alpha=\frac{2}{m^2\pi nc\omega}|\varepsilon\cdot\mathbf{D}|^2\int d^3 k I(\mathbf{k})\delta(\mathcal{E}_f-\mathcal{E}_i-\hbar\omega), \qquad (18)$$

where we have introduced a factor of 2 in order to take into account the spin degeneracy. The initial and final excitation energies $\mathcal{E}_i$ and $\mathcal{E}_f$ of the crystal electronic system are given by

$$\mathcal{E}_i=\mathcal{E}_0+\epsilon_{c0}+E_e(\mathbf{k}),$$

$$\mathcal{E}_f=\mathcal{E}_0+2\epsilon_{c0}-\epsilon_{v0}+E(\mathbf{K}_0), \qquad (19)$$

where $\mathcal{E}_0$ is the fundamental crystal electronic energy corresponding to full valence bands and empty conduction bands at $T=0$ K. ϵ_{c0} and ϵ_{v0} are, respectively, the one-electron band energies of the bottom and the top of the conduction and valence bands. $E_e=\hbar^2 k^2/2m_e^*$ is the free-electron energy while the total charged exciton energy E is related to its relative energy E_{rel} by

$$E=E_{rel}+\frac{\hbar^2 K_0^2}{2M_0}. \qquad (20)$$

We can still remark from Eq. (18) that the charged exciton lines, are not sharp lines contrary to what happens for excitons or impurity bound excitons. Indeed, due to the mobility of the center of mass, the charged exciton lines behave like free electrons if the envelope oscillator strength $I(\mathbf{k})$ is constant. However, as it results from Eq. (17), this latter case

depends strongly on the envelope wave function, and we show below that it will strongly modify the free-electron-like behavior of the center of mass. Using the properties of the Dirac function, we can express the absorption coefficient as the product of a crystalline part α_{cryst} that does not depend on the transition energy by an envelope part α_{env}:

$$\alpha(\hbar\omega) = \alpha_{cryst}\alpha_{env}(\hbar\omega),$$

$$\alpha_{cryst} = \frac{8\sqrt{2}m_e^{*3/2}}{ncm^2\hbar^2}|\varepsilon\cdot\mathbf{D}|^2,$$

$$\alpha_{env}(\hbar\omega) = \frac{1}{\mu^{3/2}}\frac{\sqrt{\hbar\omega_0 - \hbar\omega}}{\hbar\omega}I(Q). \quad (21)$$

We have introduced the threshold transition energy $\hbar\omega_0$ corresponding to zero center of mass momentum:

$$\hbar\omega_0 = \epsilon_g + E_{rel}, \quad (22)$$

where $\epsilon_g = \epsilon_{c_0} - \epsilon_{v_0}$ denotes the band gap at $\mathbf{k}=0$. Now we obtain the result that the envelope oscillator strength [Eq. (17)] depends only on the transition energy difference $\Delta\hbar\omega = \hbar\omega_0 - \hbar\omega$ through the quantity Q defined by

$$Q^2 = \frac{2m_e^*}{\mu\hbar^2}(\hbar\omega_0 - \hbar\omega). \quad (23)$$

So it appears that because only positive values of $\Delta\hbar\omega$ are allowed, the absorption bands of negatively charged excitons are disposed on the low-frequency side of the threshold transition energy $\hbar\omega_0$. This particular behavior distinguishes charged exciton spectra from exciton or impurity bound-exciton spectra. In order to get qualitative insight into the dependence of α on $\Delta\hbar\omega$ near the threshold transition energy $\hbar\omega_0$, we can assume that the photon energy $\hbar\omega$ is nearly constant. In the limit of three noninteracting particles, the envelope oscillator strength is constant, and the behavior of the absorption coefficient is dominated by the square-root function $\sqrt{\Delta\hbar\omega}$, leading to an increase of α at increasing $\Delta\hbar\omega$. This behavior is analogous to that of free electrons. However, the Coulomb interaction may not at all be neglected so that the influence of the envelope oscillator strength will be predominant.

In order to evaluate the envelope oscillator strength [Eq. (17)] we use the Hylleraas-type variational wave function determined previously[10] for the charged exciton ground state:

$$\phi_{rel}(s,t,u) = \mathcal{N}\psi(ks,kt,ku), \quad (24)$$

$$\psi(s,t,u) = e^{-s/2}\sum_{mnp}c_{mnp}s^m t^n u^p, \quad (25)$$

where $\mathcal{N}$ is a normalization constant; the scaling factor k and the coefficients c_{mnp} are variational parameters that have been determined by minimizing the mean value of the relative energy E_{rel}; m, n, and p are positive integers or zero, with n even due to the symmetry of the envelope wave function by interchanging the two electrons; s, t, and u are elliptic coordinates related to the three mutual distances
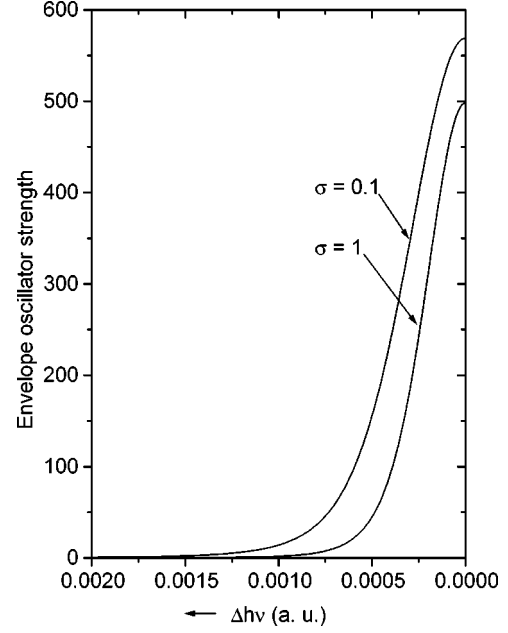

FIG. 1. Plot of the 3D zero-field envelope oscillator strength I against the transition energy difference $\Delta h\nu = \Delta\hbar\omega = \hbar\omega_0 - \hbar\omega$ for two values of $\sigma = m_e^*/m_h^*$. The transition energies are expressed in "atomic units" $2(1+m_e^*/m_h^*)|E_X|$, where E_X is the 3D exciton binding energy.

$$s = r_{1h} + r_{2h}, \quad t = r_{1h} - r_{2h}, \quad u = r_{12}; \quad (26)$$

$$0 \leq s, \quad -u \leq t \leq u, \quad 0 \leq u \leq s. \quad (27)$$

Thus we get the following expression for $\phi_{rel}(\mathbf{r},\mathbf{r}/2)$ in Eq. (17):

$$\phi_{rel}(\mathbf{r},\mathbf{r}/2) = \mathcal{N}e^{-(kr/2)}\sum_{mnp}c_{mnp}(kr)^{m+n+p}, \quad (28)$$

so that the envelope oscillator strength reads

$$I^{1/2}(\Delta\hbar\omega)$$

$$= \mathcal{N}\frac{4\pi}{k^3}\sum_{mnp}c_{mnp}2^{m+n+p+2}(m+n+p+1)!$$

$$\times\frac{1}{\beta}\left(\frac{1}{1+4\beta^2}\right)^{m+n+p+2}$$

$$\times\sum_{2l=0}^{m+n+p+1}(-1)^l C_{2l+1}^{m+n+p+2}(2\beta)^{2l+1} \quad (29)$$

with $\beta = \mu\{[Q(\Delta\hbar\omega)]/k\}$, and where C_i^j denotes the binomial coefficients.

In Fig. 1 we have plotted the variations of the envelope oscillator strength I against $\Delta\hbar\omega$ for significant values of the mass ratio σ, using a 34-term wave function defined by the condition $m+n+p\leq5$. It appears, as expected, that I remains not at all constant, and decreases strongly with $\Delta\hbar\omega$. This behavior is quite analogous for different values of σ. In Fig. 2 we have plotted the variations of the envelope part α_{env} of the absorption coefficient [Eq. (22)] for $\sigma=0.1$ and $\sigma=1$. We remark that the behavior of α_{env} is dominated by the envelope oscillator strength I and not by that of the
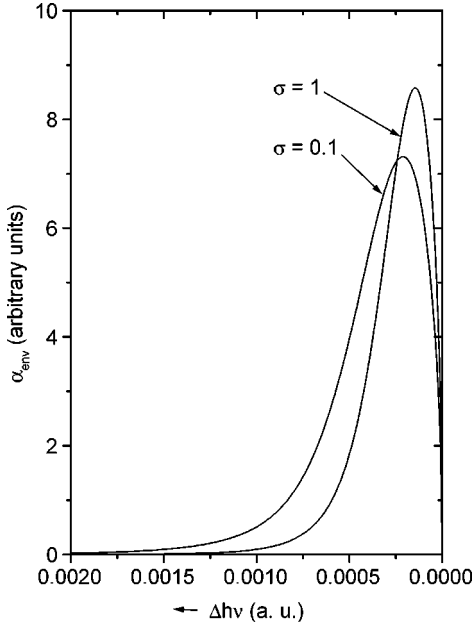
FIG. 2. Plot of the 3D zero-field envelope absorption coefficient α_{env} against the transition energy difference $\Delta h\nu = \Delta\hbar\omega = \hbar\omega_0 - \hbar\omega$ for two values of $\sigma = m_e^*/m_h^*$. The transition energies are expressed in atomic units $2(1+m_e^*/m_h^*)|E_X|$, where E_X is the 3D exciton binding energy.

FIG. 3. Plot of the 2D zero-field envelope absorption coefficient α_{env} against the transition energy difference $\Delta h\nu = \Delta\hbar\omega = \hbar\omega_0 - \hbar\omega$ for different values of $\sigma = m_e^*/m_h^*$. The transition energies are expressed in atomic units $2(1+m_e^*/m_h^*)|E_X|$, where E_X is the 3D exciton binding energy.

square-root function, contrary to what happens for free electrons where the absorption coefficient depends mainly on the electronic joint density of states. As a result, in bulk semiconductors, the negatively charged excitons bands are displayed at the low-energy side of the main absorption threshold $\hbar\omega_0$ with a maximum followed by a rapidly decreasing tail. This behavior may be used to distinguish the charged excitons from free or impurity bound excitons the spectra of which reduce to sharp lines.

It is interesting to compare the above 3D results with those we may obtain in the case of strictly 2D semiconductors. Our 3D theory may be easily extended to the 2D case. The only differences arises from the fact that the integrals over to the crystal volume Ω have to be replaced by integrals over the crystal surface S. The 3D absorption coefficient [Eq. (21)] becomes, in the 2D case,

$$\alpha(\hbar\omega) = \alpha_{cryst}\alpha_{env}(\hbar\omega),$$

$$\alpha_{cryst} = \frac{8\pi m_e^*}{ncm^2\hbar}|\varepsilon\cdot\mathbf{D}|^2,$$

$$\alpha_{env}(\hbar\omega) = \frac{1}{\mu}\frac{1}{\hbar\omega}I(Q), \qquad (30)$$

where Q is still given by Eq. (23). But we remark that α_{env} no longer depends on the square root of the transition energy difference $\Delta\hbar\omega$. This is due to the fact that the free electron density of states reduces to a constant in a 2D medium. Thus, the absorption coefficient depends now only on the envelope oscillator strength I.

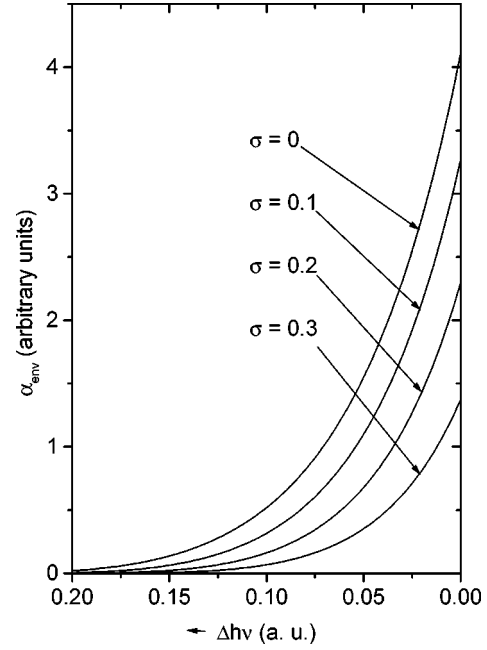In order to compute this latter, we use the 2D analogous function[17] of the 3D case [Eq. (25)]. We obtain

$$I^{1/2}(\Delta\hbar\omega) = \mathcal{N}\frac{8\pi}{k^2}\sum_{mnp}c_{mnp}2^{m+n+p}$$

$$\times\int_0^\infty J_0[2r\beta(\Delta\hbar\omega)]e^{-r}r^{m+n+p+1}dr, \qquad (31)$$

where J_0 is a Bessel function depending on the transition energy $\Delta\hbar\omega$ through the quantity β, which has the same meaning as in Eq. (29). In Fig. 3 we have reported the variations of the 2D envelope absorption coefficient $\alpha_{env}(\hbar\omega)$, [Eq. (30)], for significant values of the mass ratio σ, using a 22-term wave function defined by the condition $m+n+p \leq 4$. It appears that the charged exciton bands are decreasing functions disposed on the low-energy side of the threshold transition energy $\hbar\omega$. But, contrary to what happens in the 3D case, the absorption coefficient does not exhibit a maximum below the threshold transition energy. This result is due to the fact that the 2D free-electron density of states is constant.

IV. MAGNETOABSORPTION

In the present section we study the optical absorption of negatively charged excitons under the influence of an external uniform magnetic field directed along the z axis.

Let us first discuss the case of bulk semiconductors. In the effective mass approximation the envelope parts of the electron and hole basis wave functions defined in Eq. (3) read

$$f_\lambda(\mathbf{r}) = e^{i(k_x x + k_z z)}e^{-(eHxy/2c\hbar)}g_l(y), \qquad (32)$$

where $g_l(y)$ are the linear harmonic oscillator wave functions. Now, $\lambda \equiv (k_x, k_y, l)$ where l is the Landau quantization index. In our previous study we have shown that at sufficiently low magnetic fields the in-plane center-of-mass motion can be separated from the relative function. Thus the envelope wave function reads

$$\phi(\mathbf{r}, \mathbf{R}, \mathbf{R}_0) = \exp[i(K_{0x}X_0 + K_{0z}Z_0)]\phi_{rel}(\mathbf{r}, \mathbf{R})\Phi^L(Y_0),$$
(33)

where K_{0x} and K_{0z} are the x and z components of the center-of-mass wave vector. X_0, Y_0, and Z_0 are the components of the position vector R_0 of the center of mass. $\Phi^L(Y_0)$ stands for the eigenstates of the Schrödinger equation of the linear harmonic oscillator. L is the Landau-level quantization integer corresponding to the center-of-mass in-plane motion. ϕ_{rel} is the relative wave function that we have determined using the variational method.

In order to get an expression of the envelope oscillator strength I defined in Eq. (13), we use the same method as above in the zero-field case, but restricting ourselves to low magnetic fields. In this case, we may assume that the spatial extension of the relative motion is very smaller than that of the center-of-mass motion. With these assumptions we obtain

$$I(k_x, k_z, l)$$
$$= \delta_{\mathbf{K}_{0x}, k_x} \delta_{\mathbf{K}_{0z}, k_z} \delta_{L,l}$$
$$\times \left| \int_\Omega d^3r \, \exp[-i\mu(K_{0x}x + K_{0z}z)]\phi_{rel}(\mathbf{r}, \mathbf{r}/2) \right|^2.$$
(34)

As expected, the transitions are allowed only if the selection rules $L = l$, $K_{0x} = k_x$, $K_{0z} = k_z$ are satisfied. On the other hand, because we may assume that the oscillatory in-plane motion of the center of mass is confined within a surface $S = L_x L_y$, the possible values of K_{0x} are restricted by the condition $0 \leq K_{0x} \leq eHL_y/c\hbar$. The absorption coefficient defined in Eq. (12) may thus be written as

$$\alpha = \frac{4}{nm^2 c \omega L_y}|\varepsilon \cdot \mathbf{D}|^2 \sum_l \int_0^{eHL_y/c\hbar} dk_x$$
$$\times \int_0^\infty dk_z I(k_x, k_z, l)\delta(\mathcal{E}_f - \mathcal{E}_i - \hbar\omega).$$
(35)

The initial- and final-state energies are now given by

$$\mathcal{E}_i \equiv \mathcal{E}_0 + \epsilon_{c0} + \frac{\hbar^2 k_z^2}{2m_e^*} + (l + 1/2)\hbar\omega_e,$$

$$\mathcal{E}_f \equiv \mathcal{E}_0 + 2\epsilon_{c0} - \epsilon_{v0} + \frac{\hbar^2 K_{0z}^2}{2M_0}$$
$$+ (L + 1/2)\hbar\omega_{cm} + E_{rel}.$$
(36)

$\hbar^2 k_z^2/2m_e^*$ denotes the electron kinetic energy along the z axis. $(l + 1/2)\hbar\omega_e$ is the energy of an electron Landau level, $\omega_e = eH/m_e^*c$ being the electron cyclotron frequency. E_{rel} is the charged exciton relative energy in a magnetic field.

$\hbar^2 K_{0z}^2/2M_0$ is the kinetic energy of the center of mass along the field direction and $\omega_{cm} = eH/M_0 c = (\sigma/1 + 2\sigma)\omega_e$ is the cyclotron frequency of the center of mass. Using the properties of the δ function, we obtain finally the following expression of the absorption coefficient:

$$\alpha(\hbar\omega) = \alpha_{cryst}\alpha_{env}(\hbar\omega),$$

$$\alpha_{cryst} = \frac{2\sqrt{2}m_e^{*1/2}}{ncm^2 L_y}|\varepsilon \cdot \mathbf{D}|^2,$$

$$\alpha_{env}(\hbar\omega) = \frac{1}{\mu^{1/2}}\frac{1}{\hbar\omega}\sum_l \frac{1}{\sqrt{\Delta\hbar\omega}}$$
$$\times \int_0^{eHL_y/c\hbar} dk_x I[k_x, Q(\Delta\hbar\omega), l], \quad (37)$$

where the transition energy difference $\Delta\hbar\omega$ is now given by

$$\Delta\hbar\omega = \epsilon_g + E_{rel} - \mu(l + 1/2)\hbar\omega_e - \hbar\omega.$$
(38)

The quantity $Q(\Delta\hbar\omega)$ is given by Eq. (23).

In order to compute the envelope oscillator strength we have chosen the same 34-term trial wave function[20] [Eq. (25)] as in the case of the zero-field case. Though this function is only well adapted in the zero-field limit, we expect that it will lead to an acceptable estimation of the absorption coefficient in the case of low magnetic fields if we vary the scaling factor as well as the linear parameters in order to minimize the mean value of the relative energy. In Fig. 4 we have reported our results in the case of an effective mass ratio $\sigma = 0.1$ and for two values of the effective magnetic field $\gamma = \hbar\omega_e/(2|E_D|)$, where E_D is the 3D donor impurity ground-state binding energy. It appears, as expected, that the absorption coefficient decreases strongly with $\Delta\hbar\omega$. This is due to the fact that, on the one hand, the center-of-mass behavior is dominated by the $1/\sqrt{\Delta\hbar\omega}$ function, which is related to a 1D free-electron density of states. Indeed, due to the magnetic field, the center-of-mass motion remains free only along the field direction. On the other hand, as in the zero-field case, the envelope oscillator strength decreases with $\Delta\hbar\omega$. Finally, the observed quantization is due to the quantization of the center-of-mass motion in the plane perpendicular to the field direction, and is quite analogous to the Landau quantization for free electrons.

In the case of 2D semiconductors, using the same method, we obtain in the case of a magnetic field perpendicular to the semiconductor surface:

$$\alpha = \frac{8\pi}{nm^2 c\omega L_y}|\varepsilon \cdot \mathbf{D}|^2 \sum_l \delta(\Delta\hbar\omega)\int_0^{eHL_y/c\hbar} dk_x I(k_x, l),$$
(39)

where the envelope oscillator strength reads now

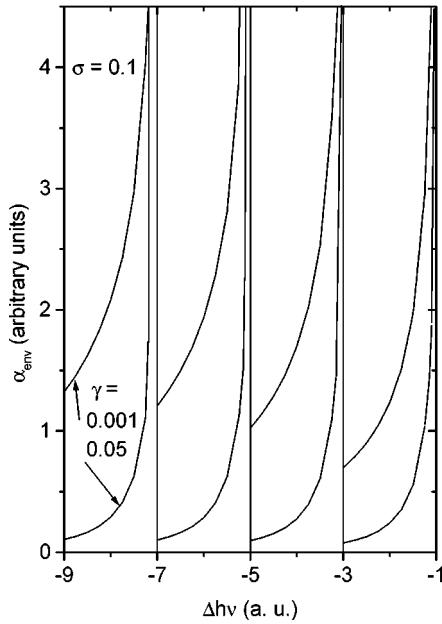FIG. 4. Plot of the 3D absorption coefficient α_{env} against the transition energy difference $\Delta h \nu = \Delta \hbar \omega = \hbar \omega_0 - \hbar \omega$ for two values of the effective magnetic field γ and $\sigma = m_e^*/m_h^* = 0.1$. The transition energies are expressed in atomic units $2(1+m_e^*/m_h^*)|E_X|$, where E_X is the 3D exciton binding energy.

$$I(k_x,l) = \delta_{K_{0x},k_x} \delta_{L,l}$$
$$\times \left| \int_S d^2r \, e^{-i\mu(K_{0x}x)} \phi_{rel}(\mathbf{r},\mathbf{r}/2) \right|^2. \quad (40)$$

It appears that, in this case, the absorption spectrum reduces to a series of sharp lines located below the threshold transition line and separated by the energy $\frac{1}{2}\mu \hbar \omega_e$ corresponding to integer positive or zero values of l. This behavior is due to the fact that the perpendicular magnetic field gives rise to a total quantization of the electron and center-of-mass motions.[21]

V. SUMMARY

In this study we have shown how the shape of the absorption coefficient of charged excitons with and without an external magnetic field may be used to distinguish them from excitons or localized bound excitons. In the zero-field case, the charged excitons lines are never sharp lines, because of the mobility of the center of mass. The behavior of the absorption coefficient is dominated, on the one hand, by that of the envelope oscillator strength, resulting from the relative Coulomb correlation, which decreases strongly with the transition energy difference $\Delta \hbar \omega$. On the other hand, it depends, crudely speaking, on the density of states associated with the ''free'' charged center of mass. This latter behavior is different in the 3D and the 2D cases, like what happens in the case of free electrons, where the densities of states are, respectively, proportional to the square root of the energy or equal to a constant. In a magnetic field, the absorption coefficient depends mainly on the behavior of the ''free'' center of mass in a magnetic field, giving rise to a Landau quantization in the 3D as well as the 2D cases. Only the shape of the absorption coefficient is different in the two cases due to the differences of the densities of states. In a semiconductor QW, we expect an intermediate situation. In particular, if the field is perpendicular to the plane, we expect sharp lines, because the combined effects of the magnetic and quantum confinement in the field direction give rise to a total confinement. We hope that the present study will be useful in order to characterize charged exciton lines in semiconductors.

ACKNOWLEDGMENT

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