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PHOTOIONIZATION CROSS-SECTION OF SHALLOW DONORS IMPURITIES AT ALL MAGNETIC FIELDS

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Abstract

The dependence of the photoionization cross-section for shallow donors on photon energy is calculated. The effects of strong and weak magnetic fields are considered by means of a variational wave function which is a linear combination of the cylindrical wave function and the oscillator one. Simple analytical expressions, valid for all magnetic fields, are obtained. It has been found that the photoionization cross-section is strongly affected by the magnetic field. We give some results for Germanium.

I- Introduction

Photoionization cross-section measurements in semiconductors give useful information on impurity states: energy, nature of defect. Several works have proposed how to explain the behaviour of the photoionization cross-section spectrum in doped semiconductors as a function of the photon energy at zero-magnetic field [1-9]. These models are principally different by the impurity potential nature and by the wave function describing its ground state. In a previous paper [1], we have presented a theoretical model, in order to calculate the photoionization cross-section of semi-deep level impurity as a function of photon energy in polar semiconductors, which takes into account the interaction between the charge carriers and the longitudinal optical phonon and the influence of central-cell correction by means of a semi-empirical short range potential.

The study of a magneto-donor is an interesting problem which has not completely solved in semiconductor physics. To represent the ground state wave function of a shallow donor in the presence of a magnetic field, we use the Hasse variational technique. For a weak magnetic field, it is adequate to choose a cylindrical wave function [10] which is close to the hydrogen-like one. While for a strong magnetic field it is preferable to adopt a harmonic oscillator wave function proposed by Yafet-Keys and Adam [11]. Several other functions and other analytical methods [12-14] have been proposed in order to solve the problem of the impurity plunged into a magnetic field. Dexter [15] has proposed a wave function containing three variational parameters, but this wave function presents a Bohr radius higher than unity at low fields, which has no physical sense. In order to have a wave function valid for all magnetic fields, we propose a wave function which is a linear combination of the cylindrical wave function and the oscillator one. This wave function has been used successfully to calculate the Lande g-factor [16], the ground state energy of a bound polaron [17] and the absorption coefficient corresponding to the electric-dipole-induced spin resonance [10,18].

Very few papers discuss the effects of a magnetic field on the photoionization process of a shallow donor. The effect of a strong magnetic field on photoionization cross-section has been investigated by using the (YKA) function [19,20]. Our aim in the present work, is to calculate the photoionization cross-section of a shallow donor in a magnetic field by using the combinational wave function. The effects of the electron-phonon interactions are neglected.

The paper is organised as follows: In section II, we calculate the photoionization cross-section as a function of the photon energy for a shallow donor and for all magnetic fields. Numerical results and discussions are presented in section-III. We give some results for Germanium and a comparison has been made with Refs [19,20].

II- General Formalism

In the well-known dipolar approximation, the photoionization cross-section of a donor impurity in semiconductors is given by [1]:

$$\sigma(\hbar\omega)=\left[\left(\frac{\mathrm{Eeff}}{\mathrm{E}}\right)^2 \frac{n}{\varepsilon}\right]\frac{4\pi^2}{3}\,\alpha\;\hbar\omega\sum_f\left|\left\langle\Psi_i\right|\vec{r}\left|\Psi_f\right\rangle\right|^2\delta\left(E_i+E_f-\hbar\omega\right) \tag{1}$$

where n, ε_0 and α are the optical refraction index, the optical dielectric constant and the fine structure constant, respectively. E_{eff} / E is the effective field ratio. $|\psi_i\rangle$ ($|\psi_f\rangle$) and E_i (E_f) are the state wave function of the impurity (final state) and the corresponding energy, respectively.

The effective Hamiltonian of a donor impurity in the presence of an external magnetic field is given by:

$$\mathrm{H}=-\nabla_{\mathrm{r}}^2-\frac{2}{\mathrm{r}}+\frac{\gamma^2}{4}(x^2+y^2)+\gamma.\mathrm{L_Z} \tag{2}$$

where the unit of the energy is the effective Rydberg and the unit of length is the effective Bohr radius given by:

$$R^{*} = \frac{m^{*} e^{4}}{\hbar^{2} \varepsilon_{o}^{2}} \quad \text{and} \quad a^{*} = \frac{\hbar^{2} \varepsilon_{o}}{m^{*} e^{2}}$$

The dimensionless parameter γ is a measure of the magnetic field strength defined by:

$$\gamma = \frac{\hbar \omega_{c}}{2 R^{*}} = \mu_{B} \frac{m_{o} B}{m^{*} R^{*}}$$

where m* is the band effective mass, μ_B is the Bohr magneton and B is the intensity of the magnetic field. Our aim is to find a simple solution for the wave function covering all magnetic field domains. For a low field, the magnetic energy is smaller than the Coulomb energy (i.e. γ « 1), and in order to take into account the lengthening of the electronic wave function along the magnetic field, we will choose the following cylindrical envelope function (CYL) [10] :

$$\left| \psi_{CYL} \right\rangle = \sqrt{\frac{1}{\pi a_{t}^{2} a_{l}}} \exp - \left(\frac{x^{2} + y^{2}}{a_{t}^{2}} + \frac{z^{2}}{a_{l}^{2}} \right)^{\frac{1}{2}} \tag{3}$$

For a high field, the magnetic energy is greater than the Coulomb interaction, (i.e. γ »1), so it is useful to consider a trial function which is close to the harmonic-oscillator one, proposed by Yafet, Keys and Adams (YKA) [11]:

$$\left| \psi_{YKA} \right\rangle = \sqrt{\frac{1}{2^{3/2} \pi^{3/2} a_{t}^{2} a_{l}}} \exp - \left(\frac{x^{2} + y^{2}}{4 a_{t}^{2}} + \frac{z^{2}}{4 a_{l}^{2}} \right) \tag{4}$$

a_t and a_l are variational parameters corresponding, respectively, to the transverse and the longitudinal effective Bohr radius. These parameters are obtained by minimising the energy corresponding to these wave functions. When γ goes to zero, the (CYL) wave function tends to the spherical wave function (i.e. $a=a_t=a_l$). Barticevic et al. [14] have proposed a trial function available in the adiabatic approximation, and have solved the problem numerically. Other wave functions which tend to the hydrogenic wave function have been proposed by Brandi et al. [12]. A numerical solution for the problem has been proposed by Cabib et al. [13]. However, this method does not propose a simple wave function where the variational parameters have precise physical meaning. Dexter has proposed the following wave function for studying the polarizability of a hydrogenic impurity [15]:

$$\left|\psi_{DEX}\right\rangle = \sqrt{\frac{2^{3\lambda-2}}{\lambda(3\lambda-1)!\,\pi a_t^2 a_l}}\ \exp\left[-\left(\frac{x^2+y^2}{4a_t^2}+\frac{z^2}{4a_l^2}\right)^{1/2\lambda}\right] \qquad (5)$$

where a_t ,a_l and λ are variational parameters. We note that, for $\lambda=1$ we find the (CYL) wave function (Eq.(3)), and for $\lambda=1/2$ the (YKA) wave function (Eq.(4)). The results obtained for different wave functions and magnetic field are presented in Ref [16]. But any of these functions can give good results for all magnetic field domains. To solve this problem, we propose the following linear combination:

$$\left|\psi_{COM}\right\rangle = A\left|\psi_{CYL}\right\rangle + B\left|\psi_{YKA}\right\rangle \qquad (6)$$

where A and B are real constants depending on the magnetic field strength. Taking into account the following normalisation condition:

$$A^2 + 2\,AB\,I + B^2 = 1 \qquad (7)$$

where I is given by:

$$I = \frac{2^5}{\sqrt{2^{\frac{3}{2}}\pi^{\frac{1}{2}}}} J \qquad (8)$$

with :

$$J = \int_0^{+\infty} t^2 e^{-2t-t^2}\,dt = -\frac{1}{2} + \frac{3\sqrt{\pi}}{4} e\left[1-\Phi(1)\right] \qquad (9)$$

and

$$\Phi(x) = erf(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}\,dt \qquad (10)$$

The ground state energy E_{COM} corresponding to ψ_{COM} is then given by:

$$E_{COM} = A^2 E_{CYL} + 2AB\,E_{INT} + B^2 E_{YKA} \qquad (11)$$

where E_{CYL}, E_{YKA} are respectively, the energy corresponding to the (CYL) and the (YKA) wave functions, the expressions of these energies are given in Ref [17]. E_{INT} is the interaction term given by:

$$E_{INT} = \langle \psi_{CYL} | H | \psi_{YKA} \rangle \tag{12}$$

The (COM) wave function has the advantage of possessing three variational parameters. The ground state energy, the transverse, the longitudinal Bohr radius and the value of the parameter A corresponding, respectively, to the Dexter and (COM) wave functions for different values of γ are listed in table-1. We remark that the energy obtained by the (COM) wave function gives good results in the strong and the weak magnetic field limits, while the Dexter wave function presents a Bohr radius (a_t and a_l) higher than unity for the weak magnetic field case which has no a physical sense. In spite of this, the Dexter function is more used in the literature.

For the final state of an electron on the conduction band, we simply take a plane wave function [1]. We obtain the following analytical expression of the photoionization cross-section:

$$\sigma_{COM} = A^2\sigma_{CYL} + B^2\sigma_{YKA} + 2AB\sigma_{INT} \tag{13}$$

where

$$\sigma_{CYL} = 32\sigma_0 \frac{1}{\left(1+a_t^2 b^2\right)^6} \frac{1}{1280d^5(d-1)} \left\{ -128 + 16d + 18d^2 + 23d^3 + 35d^4 + 35d^5 \frac{Arctg\sqrt{d-1}}{\sqrt{d-1}} \right\} \tag{14}$$

$$\sigma_{YKA} = \sigma_0 \sqrt{2\pi} \frac{e^{-2b^2a_t^2}}{\alpha} \left\{ 0.5\sqrt{\frac{\pi}{\alpha}} erf\left(\sqrt{\alpha}\right) - e^{-\alpha} \right\} \tag{15}$$

are respectively, the CYL (Eq.(3)) and the YKA (Eq.(4)) contributions to the photoionization cross-section.

$$\sigma_{INT} = \sigma_0 \frac{16}{2^{3/4}} \sqrt{\pi} e^{-b^2 a_l^2} \int_0^1 \frac{x^2 e^{-\alpha/2\, x^2}}{\left(1 + b^2 a_t^2 + \frac{\alpha}{2} x^2\right)^3} dx$$

(16)

is the contribution of the interaction term,

with

$$\sigma_0 = 32\pi \left[\left(\frac{E_{eff}}{E_0} \right)^2 \frac{n}{\varepsilon} \right] \alpha_{sf} a_t^2 a_l^5 a^{*2} \xi_i^{5/2} x (x-1)^{3/2}$$

(17)

$\xi_i = \frac{E_i}{R^*}$, $x = \frac{\hbar\omega}{E_i}$, $b = \sqrt{\xi_i (x-1)}$, $d = \frac{1 + b^2 a_l^2}{1 + b^2 a_t^2}$

$\alpha = 2b^2 \left(a_l^2 - a_t^2\right)$ and $E_i = \gamma - E$.

III- Results and discussion

The value of γ depends on the effective mass m* of the donor and the dielectric constant ε_0. From the experimental point of view, there is an upper limit γ_{max} of γ for each crystal. Table-2 displays the maximum values of γ for some semiconductors in the hydrogen-like approximation (for B=5T). Since for the majority of crystals, γ_{max} is less than unity, we use the (CYL) wave function to describe the orbital part of the ground state of the donor (for example for Ge: γ=0.222 for B= 5T). For narrow gap semiconductors γ_{max} is larger than unity, the oscillator wave function (YKA) is adequately useful (for example for InSb: γ=40 for B= 5T). Whereas for GaAs, it is suitable to use the (COM) wave function (γ = 0.77 for B= 5T).

For comparison with Ref [20], we have applied this model for a shallow donor impurity in Germanium. The following material parameters are used in the calculations: m*=0.15m_0 and ε_0=15.36 [21]. The calculation of the cross-section requires knowledge of the quantity E_{eff}, which is the effective field at the impurity site. It is quite difficult to calculate E_{eff}. The ratio E_{eff} /E has therefore generally been treated as an adjustable parameter to fix the absolute values of σ. It is clear that this factor does not affect the shape of σ. In this work, this ratio is taken to be approximately equal to one [1].

In figure-1, the dependence of the photoionization cross-section as a function of the photon energy $\hbar\omega$ is plotted for different values of γ of the magnetic field. For a weak magnetic field, the photoionization cross-section rises from zero, reaches a maximum and decreases for higher energies of the photon. This performance is similar to the true hydrogenic model [1]. When the magnetic field increases, the value of $\hbar\omega$, at which the cross-section reaches a maximum, moves towards greater energies with a decreasing of its intensity. The overall shape of the photoionization cross-section curve for strong magnetic field ($\gamma = 10$) is alike to the Lucovsky model [9] where the effects of long range Coulomb potential are neglected. Due to the increased localization of the impurity ground state wave function, the increasing of the magnetic field strength leads to less overlapping between the wave functions of the initial and the final states. We have also compared in this figure our results with those calculated by Sali et al [20] using (YKA) wave function. We found that the values of σ_{max} obtained by (COM) wave function are always higher than the values of σ_{max} obtained by (YKA) wave function [20], the difference $\Delta\sigma = \sigma_{max}(COM) - \sigma_{max}(YKA)$ increases with decreasing the magnetic field. Numerical values of this difference are given in table-3. Considering the (COM) wave function the values of $\hbar\omega$ at which the cross-section reaches a maximum moves towards lower energies.

We notice, from table-2, that for the majority of crystals γ_{max} is less than unity, so the (Y.K.A) function used in Ref [20] is not appropriate to calculate the photoionization cross-section in the presence of a magnetic field (especially for Germanium). Our results seems to be more reliable and adequate for all magnetic fields. Comparison with experimental results was not possible because experimental data are not available. However, in order to obtain theoretical results with a good agreement with experimental data, it would be important to take into account the electron-longitudinal-phonon interaction effects [1]. Calculations including the polaron and magnetic field effects are in progress.

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Table Captions

Table-1: The ground state energy (in units of R*), the tranverse and longitudinal Bohr radius (in units of a*) the value of the parameters A and λ correspond respectively, to the Dexter and (COM) wave function for different values of γ.

Table-2: Values of γ_{max} for a magnetic field B equal 5 T.

Table-3: Comparisons of the intensity of the maximum values of the photoionization σ_{max} cross-section calculated in the present work and those calculated by Ref [20].

Table.1

γ	wave function of the Dexter				Combination wave function			
	a_t	a_l	λ	E	a_t	a_l	A	E
0.2	1.004	1.013	0.979	-0.981	0.978	0.988	0.982	-0.980
0.4	1.006	1.039	0.937	-0.928	0.929	0.960	0.964	-0.926
0.6	1.002	1.061	0.895	-0.852	0.875	0.929	0.945	-0.845
0.8	0.990	1.076	0.858	-0.759	0.824	0.900	0.929	-0.746
1	0.974	1.086	0.828	-0.654	0.744	0.828	0.811	-0.656
2	0.882	1.086	0.736	-0.244	0.591	0.726	0.683	-0.247
3	0.804	1.063	0.689	0.701	0.505	0.667	0.448	0.698
4	0.741	1.037	0.660	1.478	0.448	0.627	0.372	1.147
5	0.691	1.012	0.641	2.287	0.407	0.597	0.322	2.283
10	0.538	0.921	0.593	6.585	0.299	0.511	0.218	6.580
30	0.338	0.760	0.547	25.080	0.178	0.400	0.130	25.076
50	0.268	0.690	0.530	53.837	0.127	0.344	0.091	53.833
80	0.215	0.629	0.525	73.245	0.110	0.323	0.070	73.241
100	0.193	0.602	0.521	92.753	0.099	0.308	0.059	92.750

Table-2

	Ge	InSb	GaAs	CdSe	ZnSe	GaP
ε_0	15.36	17.9	12.75	10.02	8.33	10.28
m*	0.15	0.013	0.067	0.12	0.17	0.34
γ_{max}	0.222	40	0.77	0.148	0.051	0.019

Table-3

γ=0.2			γ=2			γ=5			γ=10		
σ_{max}com $cm^2 10^{-15}$	σ_{max}YKA $cm^2 10^{-15}$	$\Delta\sigma$ $cm^2 10^{-15}$	σ_{max}com $cm^2 10^{-15}$	σ_{max}YKA $cm^2 10^{-15}$	$\Delta\sigma$ $cm^2 10^{-15}$	σ_{max}com $cm^2 10^{-15}$	σ_{max}YKA $cm^2 10^{-15}$	$\Delta\sigma$ $cm^2 10^{-15}$	σ_{max}com $cm^2 10^{-15}$	σ_{max}YKA $cm^2 10^{-15}$	$\Delta\sigma$ $cm^2 10^{-15}$
16.24	12.13	4.11	11.86	9.80	2.06	6.42	5.64	0.78	4.00	3.81	0.19

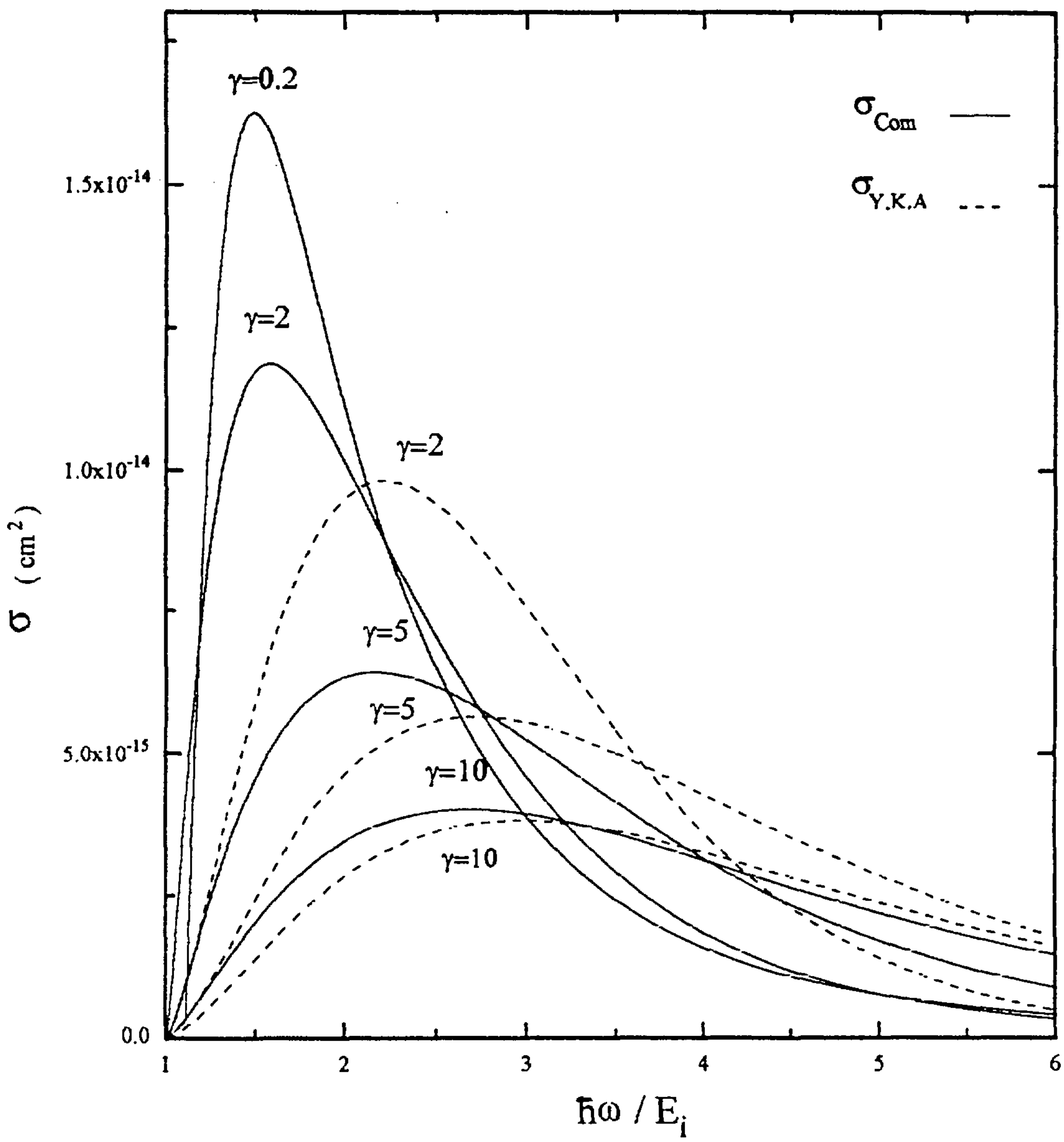

Figure-1: Photoionisation cross-section as a function of photon energy for a shallow donor in Germanium and for different values of magnetic field ($\gamma = 0.2$, 2, 5 and 10) using the (COM) wave function (solid line) and the (YKA) wave function (dashed line).