

## The impurity photoionization cross-section in the bulk and low dimensional electronic systems

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The effects of a strong magnetic field, a weak electric field, the central-cell correction, the electron mass anisotropy and the electron-phonon interaction on the dependence of the photoionization cross-section on photon energy of a shallow donor impurity are investigated with the use of a variational method in the bulk case. In the low dimensional systems such as quantum well and quantum-well wires, we have studied the effect of electron-phonon interaction on the binding energy and the impurity photoionization cross-section. We have also shown that the photoionization cross-sections are affected by the sizes of the wire and the height of the barrier in finite quantum-well wires.

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### I. INTRODUCTION

Impurities in semiconductors are characterized by their optical properties such as concentration, thermal emission rate, energy, capture cross-section and optical cross-section. We concentrate on the last property, i.e. on the photoionization cross-section which is one of the most important optical properties. The photoionization cross-section as a function of photon energy is generally determined both by the wavefunction that describes the impurity in its ground state and the potential which links the charge carrier (electron or hole) to the (donor or acceptor) impurity and the (conduction or valence, respectively) band of the host crystal. The main obstacle one encounters in this problem in calculating the transition cross-section is the lack of knowledge of the impurity wavefunction.

Over the past decades, a number of experimental and theoretical studies<sup>1-2</sup> has been devoted to the calculation of the photoionization cross-section for excitation of shallow or deep bound charge carrier from the impurities to the bands in the bulk semiconductors. As a matter of fact, the early 1950 s<sup>3</sup> witnessed the beginning of these studies.

In recent years, studies in the low dimensional systems such as quantum well (QW) in which the electron is confined in one dimension and is free to move in the two other dimensions of the well and such as quantum-well wire (QWW) in which the electron motion along the length of the wire is that of a quasi-free electron and it is quantized in the two dimensions perpendicular to the wire, are very interesting problems. The presence of ionized impurities in these structures and their small sizes play a fundamental role in some physical properties such as optical and transport mechanism properties at low temperature. This role becomes increasingly important as the dimensions of these structures become small and it is thus quite different from that in the bulk case. Some theoretical and few experimental studies<sup>4-10</sup> have been advanced for optical properties such as the photoionization cross-section in these microstructures.

Various effects such as external perturbations, central-cell correction, electron mass anisotropy and electron-phonon coupling have a drastic influence on the behaviour of the photoionization cross-section. The strength of these effects depends on the nature of the studied crystal.

For semiconducting materials of high dielectric constant and low effective mass such as germanium, the effect of the strong magnetic field is well observed in these materials. In this paper, we will first show what we expect to happen to the photoionization cross-section as the magnetic field is introduced.

In silicon where the central-cell correction is important even for a shallow impurity, we will investigate the effect of a weak electric field on the binding energy and the photoionization cross-section taking into account the chemical nature of the impurity by means of a semi-empirical short-range potential.

In anisotropic polar semiconductor crystals II-VI such as CdS, which present many valley at the bottom of the conduction band ( $k_c \neq 0$ ) and which are characterized by an intermediate electron-phonon coupling constant, the effects of electron mass-anisotropy and the electron-phonon interaction will be incorporated in calculating the transition cross-section.

As in the bulk case, the study of the behaviour of the photoionization cross-section as a function of the excitation energy in QW and QWWs will gives useful information on impurity states. We therefore study the effect of the electron-interaction with the bulk longitudinal- optical (LO) phonons on the binding energy and the photoionization cross-section of an isolated donor impurity in QW and QWW structures with infinite confining potential. The photoionization cross-section of a shallow hydrogenic impurity in finite-barrier QWW as a function of the sizes of the wire and the potential-barrier heights of the confining potential has been calculated.

### II. PHOTOIONIZATION CROSS-SECTION THEORY

Under the action of an electromagnetic wave, the transition of an electron residing in the ground state of a donor impurity into a conduction band with absorption of a photon occurs only if the energy of the incoming photon  $\hbar\omega$  is larger than the optical photoionization threshold  $E_g$ . The photoionization cross-section associated with an impurity atom is calculated by using the formula of the perturbation theory in the well-known dipole approximation<sup>3</sup>:



$$\sigma(\hbar\omega) = \left[ \left( \frac{E_{\text{eff}}}{E_0} \right)^2 \frac{n_r}{\varepsilon} \right] \frac{4\pi^2}{3} \alpha_{\text{FS}} \hbar\omega \times \sum_f |\langle \psi_i | r | \psi_f \rangle|^2 \delta(E_f + E_i - \hbar\omega) \quad (1)$$

where  $n_r$  is the optical index of refraction,  $\varepsilon$  is the dielectric constant,  $\alpha_{\text{FS}} = e^2/\hbar c$  is the fine structure constant. The factor  $E_{\text{eff}}/E_0$  is the so-called effective field ratio, which takes into account the fact that the dielectric field  $E_{\text{eff}}$  which is effective in inducing a transition is different from the average field  $E_0$  in the medium<sup>11</sup>.  $\langle \psi_i | r | \psi_f \rangle$  is the usually position matrix element between the envelope functions  $|\psi_i\rangle$  and  $|\psi_f\rangle$ , respectively, of the impurity ground state and the continuum final state.  $E_i$  and  $E_f$  are, respectively, the ionization energy of the impurity level and the energy of the final state.

### A. Photoionization cross-section in the bulk case

#### 1. Effect of a strong magnetic field on the photoionization cross-section

The strength of the magnetic field  $B$  is characterized by the value of the effective magnetic field parameter  $\gamma$  which depends on the host crystal parameters (effective mass  $m$  and dielectric constant  $\varepsilon$ )

$$\gamma = \varepsilon_0^2 \hbar^3 B / (m^2 c e^3) \quad (2)$$

where  $c$  is the velocity of light.

In the effective mass approximation, the energy level of an electron bound to a coulombic donor impurity subjected to a uniform magnetic field  $B=(0,0,B)$  in a material having a prolate-spheroid conduction band, such as germanium, is given by the solution of the Schrödinger equation with the Hamiltonian<sup>12</sup>

$$H = -\nabla^2 - \frac{2}{r} + \gamma L_z + \frac{\gamma^2}{4} (x^2 + y^2) \quad (3)$$

in which we have introduced  $a^* = \varepsilon_0 \hbar^2 / m e^2$ ,  $R^* = m e^4 / 2 \varepsilon_0^2 \hbar^2$  and  $\gamma$  described above, respectively, as the units of length, energy, and magnetic field.  $r$  denotes the position of the electron and  $L_z$  is the  $z$ -component of the orbital angular momentum.

The calculation of the impurity photoionization cross-section requires the knowledge of the ground state and the final state wavefunctions.

For the initial ground state, we use a normalized trial wavefunction proposed for the first time by Yafet, Keyes, and Adams<sup>13</sup> in the following form:

$$\psi_i(r) = \frac{1}{((2\pi)^{3/2} a_t^2 a_l)^{1/2}} \times \exp\left[-\frac{(x^2 + y^2)}{4a_t^2} + \frac{z^2}{4a_l^2}\right] \quad (4)$$

where  $a_t$  and  $a_l$  are variational parameters, which may be thought of as the effective bohr radii of the donor ground state.

For the final state, we use a plane wave

$$\psi_f(r) = 1/\sqrt{V} \exp(ik \cdot r) \quad (5)$$

where  $k$  is the wave vector of the electron and  $V$  is the volume of the crystal.

At zero magnetic field, the transverse and longitudinal effective Bohr radii  $a_t$  and  $a_l$ , respectively, are comparable, we therefore choose as a trial wavefunction corresponding to the coulombic potential the Gaussian function given by

$$\psi_0(r) = 1/\sqrt{\pi^{3/2} a^3} \exp[-r^2/(2a^2)] \quad (6)$$

where  $a$  is a variational parameter.

At zero magnetic field, we obtained for the photoionization cross-section:

$$\sigma(\hbar\omega) = \left[ \left( \frac{E_{\text{eff}}}{E_0} \right)^2 \frac{n}{\varepsilon_0} \right] \frac{8\pi^{3/2} \alpha_{\text{SF}}}{3} a^7 b^{5/2} \times x(x-1)^{3/2} \exp[-a^2 b(x-1)] \quad (7)$$

where  $x = \hbar\omega/E_i$  and  $b = 2mE_i/\hbar^2$ .

For a strong magnetic field, the effective Bohr radii  $a_t$  and  $a_l$  are not comparable, the diamagnetic forces are centripetal in the  $xy$  plane, they tend to compress the impurity atom in the transverse dimensions. The photon energy dependence of the photoionization cross-section associated with the donor impurity in the presence of the magnetic field is calculated.<sup>1</sup>

#### 2 Effect of a weak electric field on the photoionization cross-section

The strength of the electric field  $\zeta$  is characterized by the value of the effective electric field parameter  $\eta = e |a^* \zeta| R^*$ .

The Hamiltonian describing the state of a shallow donor impurity in the presence of an electric field  $\zeta$  which is taken to be parallel to the  $z$  direction and taking into account the chemical nature of the impurity is given by<sup>14</sup>

$$H = -\nabla^2 - \frac{2}{r} - \eta \cos(\theta) - \frac{2}{r} (\varepsilon_0 - 1) (e^{-Kr} + \frac{\delta}{2} r e^{-\delta r}) \quad (8)$$

where  $\theta$  is the angle between the  $z$  axis and the position vector  $r$  and the last term describes the central-cell correction.

The parameter  $K$  (characteristic for each material) in the first part of this potential model arising from the relaxation of the electron gas due to the excess charge of the impurity<sup>15</sup> for silicon is determined by the fit of the numerical results

carried out by Vinsome and Richardson<sup>16</sup> by the analytic expression of the  $q$ -dependent optical dielectric constant<sup>17</sup>

$$\epsilon_0(q) = \frac{\epsilon_0(q^2 + K^2)}{\epsilon_0 q^2 + K^2} \quad (9)$$

The second part of Eq.(4) accounts for the electron screening at larger distance from the nucleus.<sup>18</sup> The value of  $\delta$  is determined for each impurity by requiring the calculated binding energy to agree with the observed one for that impurity.

To obtain the ground state energy, we follow a variational treatment and we use a normalized trial wavefunction proposed by Cahay and Kartheuser<sup>19</sup> in the following form

$$\psi_i = N\psi_0 \left\{ 1 + \left[ \frac{b}{a} + \frac{c}{a^2} r \right] \eta \cdot r \right\} \quad (10)$$

where  $N$  is a normalization constant given by

$$N^2 = \left\{ 1 + [b^2 + \frac{15}{2}c^2 + 5bc] \eta^2 \right\}^{-1} \quad (11)$$

with  $a$ ,  $b$  and  $c$  as variational parameters.

The initial ground state wavefunction without the electric field effect is as a normalized trial wavefunction given by

$$\psi_0 = \frac{1}{\sqrt{\pi a^3}} e^{-r/a} \quad (12)$$

The final state is described by a plane wave.

Taking into account the above considerations, we have obtained an analytic expression for the photoionization cross-section.<sup>20</sup>

### 3. Effect of the electron mass-anisotropy and the electron-phonon coupling on the photoionization cross-section

For anisotropic polar semiconductors such as CdS, the minimum of the conduction band is at  $k_c \neq 0$ . The effective mass tensor is anisotropic, and symmetry allows a longitudinal effective mass  $m_l$  in the direction of  $k_c$  and a transversal effective mass  $m_t$  perpendicular to it. The effective mass Hamiltonian of a donor impurity center taking into account the electron mass-anisotropy and the electron-phonon interaction can be written as

$$H = -\frac{\hbar^2}{2m_t} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \lambda \frac{\partial^2}{\partial z^2} \right) - \frac{e^2}{\epsilon_0 r} + \sum_q \hbar\Omega a_q^\dagger a_q + \sum_q [V_q a_q e^{iq \cdot r} + V_q^* e^{iq \cdot r}] \quad (13)$$

where  $\lambda = m_t/m_l$  is the ratio between the transverse and the longitudinal effective electron mass,  $a_q^\dagger$  and  $a_q$  are creation and annihilation phonon operators for the LO phonon of energy  $\hbar\Omega$  and wave vector  $q$ , respectively. According to Fröhlich et al,<sup>21</sup> we have

$$V_q = -\frac{ie}{q} \left[ \frac{2\pi \hbar\Omega}{V} (1/\epsilon_\infty - 1/\epsilon_0) \right] \quad (14)$$

where  $\epsilon_\infty$  is the high-frequency dielectric constant.

The donor impurity wavefunction  $|\psi_i\rangle$  in the ground state that satisfies the Schrödinger equation with the effective mass Hamiltonian (13) is described in the adiabatic approximation<sup>22</sup> by

$$|\psi_i(r)\rangle = |1S\rangle U |0\rangle \quad (15)$$

with

$$U = \exp \left[ \sum_q (g_q a_q^\dagger - g_q^* a_q) \right]$$

and  $|0\rangle$  is the phonon vacuum state, i.e.  $a_q |0\rangle = 0$ , and

$$g_q = -V_q^* \rho_q / \hbar\Omega.$$

$\rho_q$  is the electronic charge distribution described by the Fourier transform

$$\rho_q = \langle 1S | e^{iq \cdot r} | 1S \rangle \quad (16)$$

$|1S\rangle$  is the electron ground state wave function of the coulomb Hamiltonian<sup>23</sup> given by

$$\langle r | 1S \rangle = (\pi a_t^2 a_l)^{-1/2} \times \exp \left[ -\left( \frac{x^2 + y^2}{a_t^2} + \frac{z^2}{a_l^2} \right)^{1/2} \right] \quad (17)$$

in which  $a_t$  and  $a_l$  are the variational parameters.

According to (13), the expectation value  $\langle \psi_i | H | \psi_i \rangle$  leads to an analytic expression.<sup>2</sup>

In the photoexcitation of an electron from the ground state of a hydrogenic donor to the conduction band, the final state in (1) is described in the Lee-Low-Pines<sup>24</sup> approximation

$$|\psi_f(r)\rangle = |f\rangle e^{S_1} e^{S_2} |\{n_q\}\rangle \quad (18)$$

where

$$S_1 = -i \sum_q q \cdot r a_q^\dagger a_q \quad (19)$$

$$S_2 = \sum_q (f_q a_q^\dagger - f_q^* a_q) \quad (20)$$

and  $|\{n_q\}\rangle$  is the state of  $n$  emitted phonons.

For the electronic part, the final state of the electron is taken to be a plane wave.

The term  $f_q$  that describes the polarization in the final state is taken to be

$$f_q = -V_q^* / [\hbar\Omega + \frac{\hbar^2}{2m_t} (q_x^2 + q_y^2 + \lambda q_z^2)] \quad (21)$$

After application of the first and the second Lee-Low-Pines transformations, we obtained for the free polaron final state energy



$$E_f = \frac{\hbar^2}{2m_t} (k_x^2 + k_y^2 + \lambda k_z^2) + \hbar\Omega - \alpha_t \hbar\Omega \sin^{-1}(\sqrt{1-\lambda}) / \sqrt{1-\lambda} \quad (22)$$

in which

$$\alpha_t = \frac{e^2}{\hbar} \left( \frac{m_t}{2\hbar\Omega} \right)^{1/2} (1/\epsilon_\infty - 1/\epsilon_0) \quad (23)$$

The photoionization cross-section as a function of photon energy  $\hbar\omega$  obtained for the bound polaron associated with  $n$  phonons emission taking into account the electron mass anisotropy and the electron-LO phonon interaction has been calculate,<sup>2</sup> since its expression is long and we don't write it here.

## B. Photoionization cross-section in the low dimensional electronic systems

### 1. Effect of the electron-LO phonon interaction on the photoionization cross-section in a quantum well

The motion of the electron coupled to a coulombic impurity and interacting with the bulk longitudinal optical phonons is described by the Fröhlich Hamiltonian in the framework of the effective mass approximation

$$H = H_{3D} + V(z) \quad (24)$$

where

$$H_{3D} = \frac{p^2}{2m} - \frac{e^2}{\epsilon_0 r} + \sum_q \hbar\Omega a_q^+ a_q + \sum_q [V_q a_q e^{iq \cdot r} + V_q^* a_q^+ e^{-iq \cdot r}] \quad (25)$$

and  $V(z)$  is the potential-energy barrier which confines the carrier in the well

$$V(z) = \begin{cases} \infty & \text{if } |z| \geq L/2 \\ 0 & \text{otherwise} \end{cases} \quad (26)$$

Here  $L$  denotes the layer thickness.

The envelope function of the electron-phonon system in the ground state is as (15).

For the electronic part, we choose a separable trial wavefunction in  $z$  and  $(x, y)$  as

$$\langle r | 1S \rangle = \sqrt{\frac{2}{\lambda^2 \pi}} \phi(z) e^{-\rho/\lambda} \quad (27)$$

where

$$\phi(z) = \sqrt{2/L} \cos(\pi z/L) \quad (28)$$

is the ground state wavefunction which describes the electron confinement in the  $z$ -direction while the exponential factor accounts for the motion of the electron in the  $(x, y)$  plane. The parameter  $\lambda$  is to be determined by minimizing

the expectation value of the Hamiltonian that is,  $\langle \psi_i | H | \psi_i \rangle$ .

The ground state binding energy of the electron-phonon system can be written as

$$E_i = \frac{\pi^2}{L^2} - \min \langle \psi_i | H | \psi_i \rangle \quad (29)$$

We consider the photoionization as an optical transition of an electron from the ground state of a hydrogenic impurity to one of the conduction subbands where the electron is free to move in the  $(x, y)$  plane. The polaron final state is described in the Lee-low-Pines approximation equation (18) taking into account the character bidimensional by

$$S_1 = -i \sum_q q_\perp \cdot \rho a_q^+ a_q \quad (30)$$

and

$$S_2 = \sum_q (f_q a_q^+ - f_q^* a_q) \quad (31)$$

The term  $f_q$  describing the polarization in the final state is taken to be

$$f_q = -V_q^* \exp(-iq_z \cdot z) / (\hbar\Omega + \frac{\hbar^2 q_\perp^2}{2m}) \quad (32)$$

where  $\rho = (x, y)$  and  $q_\perp = (q_x, q_y)$ .

Without the impurity coulombic potential and the electron-phonon coupling, the eigenstates corresponding to the Hamiltonian  $H$  are<sup>25</sup>

$$\langle r | f \rangle = \begin{cases} \left( \frac{2}{LS} \right)^{1/2} \exp(ik_\perp \cdot \rho) \cos(k_p z), & p \text{ odd} \\ \left( \frac{2}{LS} \right)^{1/2} \exp(ik_\perp \cdot \rho) \sin(k_p z), & p \text{ even} \end{cases} \quad (33)$$

with  $k_p = p\pi/L$ ,  $p \geq 1$ .  $S$  is the layer surface and  $k_\perp = (k_x, k_y)$  is the two dimensional wave vector of the electron in the plane of the surface.

For light polarized in the  $x$ -direction, the first allowed dipole transition is to the first conduction subband, as a consequence, the electron final state wavefunction used may be taken as

$$\langle r | f \rangle = \left( \frac{2}{LS} \right)^{1/2} \exp(ik_\perp \cdot \rho) \cos(k_1 z) \quad (34)$$

By using Eq.(1), we obtained an expression of the photoionization cross-section for the impurity ground state-first conduction subband transition expressed in.<sup>8</sup>

## 2. Photoionization of impurities in quantum-well wires

### 2.1 Photoionization of shallow donor impurities in finite-barrier quantum-well Wires

The problem we are interested in is a system consisting of an electron bound to a donor ion inside a quantum-well wire of GaAs surrounded by  $\text{Ga}_{1-x}\text{Al}_x\text{As}$ , which is assumed to have rectangular cross-section and finite height of the electron confining potential. The motion of the electron coupled to a coulombic impurity (located at  $\mathbf{r}_i = 0$ ) is described by the effective mass Hamiltonian

$$H = \frac{p^2}{2m} - \frac{e^2}{\epsilon r} + V(x, y) \quad (35)$$

The value of the static dielectric constant  $\epsilon$  is assumed to be the same in GaAs and  $\text{Ga}_{1-x}\text{Al}_x\text{As}$  ( $\epsilon = 13.1$ ). The quantity  $m$  is the effective mass, which is different in the two semiconductors and is defined as<sup>26</sup>

$$m = \begin{cases} m_1 = 0.067m_0 & \text{in the GaAs} \\ m_2 = (0.067 + 0.083x)m_0 & \text{in the } \text{Ga}_{1-x}\text{Al}_x\text{As} \end{cases} \quad (36)$$

where  $m_0$  is the free electron mass and  $x$  is the Al concentration.

The electron confining potential  $V(x, y)$  is taken as<sup>26</sup>

$$V(x, y) = \begin{cases} 0, & |x| < L_x/2, |y| < L_y/2 \\ V_{0x}, & |x| > L_x/2, |y| < L_y/2 \\ V_{0y}, & |y| > L_y/2 \end{cases} \quad (37)$$

$V_{0x}$  and  $V_{0y}$  are the conduction band discontinuities at the interfaces between the two semiconductors and  $L_x$  and  $L_y$  are the dimensions of the wire. The values of the potential-well heights  $V_{0x}$  and  $V_{0y}$  are determined from the Al concentration  $x$  in GaAs- $\text{Ga}_{1-x}\text{Al}_x\text{As}$  using the following expression<sup>27</sup> gap discontinuity  $\Delta E_G$ ,  $\Delta E_G = 1.04x + 0.47x^2 \text{ eV}$ . The values of  $V_{0x}$  and  $V_{0y}$  are taken to be 60% of  $\Delta E_G$ .

The wavefunction that describes the impurity in the ground state is taken to be<sup>26</sup>

$$\psi_i(\mathbf{r}) = \sqrt{\frac{\lambda}{2}} \varphi(x) \varphi(y) \exp\left(-\frac{\lambda|z|}{2}\right) \quad (38)$$

where  $\lambda$  is a variational parameter and

$$\varphi(x) = \begin{cases} A_x \cos(K_{1x} L_x/2) e^{K_{2x} L_x/2} e^{-K_{2x}|x|} & , |x| > L_x/2 \\ A_x \cos(K_{1x} x), & -L_x/2 < x < L_x/2 \end{cases} \quad (39)$$

$A_x$  is a normalization constant of  $\varphi(x)$ ,  $K_{1x} = (2m_1 E_x / \hbar^2)^{1/2}$  and  $K_{2x} = [2m_2 (V_{0x} - E_x) / \hbar^2]^{1/2}$ .

The parameters  $K_{1x}$  and  $K_{2x}$  are determined by the matching conditions at the interfaces. It is assumed that  $\varphi(x)$  and  $\frac{1}{m} \frac{\partial \varphi}{\partial x}$  are continuous across the interface, then

$K_{1x}$  and  $K_{2x}$  must satisfy the following relation

$$m_1 K_{2x} = m_2 K_{1x} \tan(K_{1x} L_x/2) \quad (40)$$

Similar function is used for  $\varphi(y)$ .

For light polarized in the  $z$ -direction, the final state wavefunction of the first conduction subbands is

$$\psi_f(\mathbf{r}) = 1/\sqrt{L} \varphi(x) \varphi(y) \exp(ik_z z) \quad (41)$$

where  $L$  is the length of the wire and  $\varphi(x)$  and  $\varphi(y)$  are taken to be the same as in the initial ground state. Thus, we obtained for the transition from the impurity ground state to the first subbands wavefunction relative to the  $x$  and  $y$  transverse directions of the wire an analytical expression of the photoionization cross-section.<sup>9</sup>

### 2-2 Effect of the electron-LO phonon interaction on the photoionization in infinite quantum-well wire.

The motion of an electron bound to a donor ion, inside a rectangular wire of sizes  $L_x$  and  $L_y$  and interacting with the bulk longitudinal optical phonons is described by the Fröhlich Hamiltonian :

$$H = H_{3D} + V(x, y) \quad (42)$$

where  $V(x, y)$  is the infinite confining potential

$$V(x, y) = \begin{cases} 0 & \text{for } |x| \leq L_x/2, |y| \leq L_y/2 \\ \infty & \text{otherwise} \end{cases} \quad (43)$$

For the electron-phonon system, we choose a pekar-type trial envelope function<sup>22</sup> which is separable into the particle  $|1S\rangle$  and the phonon part equation (15).

Without electron-phonon coupling, we take a separable electronic wavefunction  $|1S\rangle$  as

$$\langle 1|1S\rangle = \left(\frac{4}{L_x L_y}\right)^{1/2} \cos(\pi x/L_x) \cos(\pi y/L_y) \times \phi(z) \quad (44)$$

where  $\phi(z)$  is the electron wavefunction for the motion along the wire axis

$$\phi(z) = \left(\frac{2}{\lambda^2 \pi}\right)^{1/2} \exp(-z^2 / \lambda^2) \quad (45)$$

and  $\lambda$  is a variational parameter.



We consider the photoionization as an optical transition from the impurity ground state to the final subband state where the electron is free to move along the length of the wire. We describe the polaron final state of this transition in the Lee-Low-Pines approximation<sup>24</sup> taking into account the character unidimensional by

$$S_1 = -i \sum_q q_z z a_q^+ a_q \quad (46)$$

and

$$S_2 = \sum (f_q a_q^+ - f_q^* a_q) \quad (47)$$

Without the impurity potential and the electron-phonon coupling, the eigenstates of the Hamiltonian  $H$  are

$$\psi_f(n_x, n_y, k_z, r) = \frac{1}{\sqrt{L}} \exp(ik_z z) X_{n_x}(x) \quad (48)$$

$X_{n_x}(x)$  and  $Y_{n_y}(y)$  are chosen to be the solutions for the one-dimensional infinite wells defined by the rectangular well.

For example,

$$X_{n_x}(x) = \begin{cases} \sqrt{2/L_x} \cos(k_{n_x} x), & n_x \text{ odd} \\ \sqrt{2/L_x} \sin(k_{n_x} x), & n_x \text{ even} \end{cases} \quad (49)$$

where  $K_{n_x} = n_x \pi / L_x$ ,  $n_x \geq 1$ . Similar functions are used for  $Y_{n_y}$ .

By minimizing the final state energy  $E_f = \langle \psi_f(r) / H + e^2 / \epsilon_0 r / \psi_f(r) \rangle$  with respect to the variational function  $f_q$ , we take  $f_q$  as

$$f_q = - \frac{V_q^* \langle f / \exp(-iq_\perp \rho) / f \rangle}{(\hbar\Omega + \frac{\hbar^2 q_z^2}{2m})} \quad (50)$$

where  $q_\perp = (q_x, q_y)$  and  $\rho = (x, y)$ .

For light polarized in the  $z$ -direction, the first allowed dipole transition is to the first subbands  $n_x = 1$  and  $n_y = 1$  for which the final state electronic wavefunctions  $|f\rangle$  may be taken as

$$\langle r | f \rangle = \frac{1}{\sqrt{L}} \left( \frac{2}{\sqrt{L_x L_y}} \right) \exp(ik_z z) \times \cos(\pi x / L_x) \cos(\pi y / L_y) \quad (51)$$

Taking into account the above considerations, we have<sup>10</sup> obtained an expression of the excitation energy dependence of the photoionization cross-section  $\sigma(\hbar\omega)$  associated with a transition from a shallow donor impurity to the first subbands  $n_x = 1$  and  $n_y = 1$  and for  $n$  phonons emission.

### III. RESULTS AND DISCUSSIONS

The effective field ratio  $E_{\text{eff}}/E_0$  used to calculate the theoretical cross-section is generally evaluated by the adjusting the theoretical curve such that the maximum value of the cross-section is the same as that of the experiment. This is due to the complexity of calculating the effective field parameter  $E_{\text{eff}}$  at the impurity site. The factor  $E_{\text{eff}}/E_0$  may be generally smaller than unity for shallow impurity levels and greater than unity for deep impurities. As it is well known, this factor does not affect the shape of the cross-section and according to our knowledge, unfortunately, no experimental results on the photoionization cross-section of the shallow impurity level is available, and a comparison with experiment is not yet possible. We therefore calculated the photoionization cross-section for an effective field ratio equal to unity.

The numerical results of the photoionization cross-section as a function of photon energy at zero magnetic field and for different values of  $\gamma$  are applied to germanium.<sup>1</sup> With increasing magnetic field, the value of  $\hbar\omega$  at which the cross-section reaches a maximum moves to greater energies, the magnitude of the cross-section becomes slightly smaller and the photoionization cross-section falls off very slowly like the  $\delta$ -function potential model<sup>28</sup> for higher photon energies. This is due to the fact that as the magnetic field increases, the effective bohr radius becomes larger than the transverse one, and this makes the impurity ground state wavefunction to be deeper, more precisely, cigar-shaped.

For the electric field effect, we have calculated<sup>20</sup> the binding energy and the photoionization cross-section in the presence of an applied weak electric field with and without the account of central-cell correction. We have found that the short-range potential has a large effect on the binding energy for very weak applied fields and a small effect for increasing electric field. As expected, the magnitude of the cross-section becomes smaller with central-cell correction effect because of increasing binding energy and smaller effective Bohr radius, this leads the ground state level to be more deeper. The peak values of the cross-section with and without central-cell corrections effect occur at photon energies at about  $1.3 E_i$  and  $1.4 E_i$ , respectively.

We also find that as the value of the parameter  $\eta$  increases, the value of  $\hbar\omega$  at which  $\sigma(\hbar\omega)$  reaches a maximum becomes smaller and moves near the threshold.. With increasing electric field, the extension of the ground state wavefunction is shrinked, this increases the magnitude of the cross-section.

For a same given value of  $\eta$ , the cross-section and its associated peak with the combined effect of central-cell correction and electric field are found to be, respectively, larger and smaller than those with only the electric field effect, this is well achieved for the very weak fields where the central-cell correction effect is important.

The numerical results of the photoionization cross-section as a function of photon energy  $\hbar\omega$  for both the isotropic and anisotropic hydrogenic models with zero phonon and one LO phonon for a shallow donor impurity are applied to CdS.<sup>2</sup> These results show that the action of the electron-phonon interaction is to lower the cross-section, to push the value of  $\hbar\omega$  associated with the peak value of the cross-



section towards higher photon energies, and to increase the optical photoionization threshold energy because of increasing binding energy with the electron-LO phonon coupling for both the isotropic and anisotropic hydrogenic models. The combined effect of the electron mass-anisotropy and the electron-phonon coupling has a drastic effect on the photoionization cross-section.

The results we have obtained<sup>8</sup> through a numerical minimization of the energy with and without the electron-interaction with the lattice through LO phonon coupling in the GaAs/Ga<sub>1-x</sub>Al<sub>x</sub>As quantum-well structures show that the general characteristic features and implications of the present calculations agree well with those obtained by Erçelebi and Tomak<sup>29</sup> using a non separable wavefunction for the smaller well thickness. These results clearly show the validity of the electronic separable wavefunction for thin well sizes.

For a CdTe quantum-well in which the electron-LO phonon coupling constant is intermediate, we have calculated the binding energy of the ground state and the impurity photoionization cross-section with and without taking into account the electron-LO phonon coupling.<sup>8</sup> We have found as expected that the polaronic effect is more pronounced in the thin layer size and the binding energy increases as the layer thickness decreases.

The zero photoionization threshold of the cross-section we have obtained in the quasi-two-dimensional systems<sup>8</sup> does not occur at the ionization energy  $\hbar\omega = E_i$ , as predicted in the bulk three dimensional systems when using plane wave for the final state,<sup>1,2,20</sup> but is splitted in two terms corresponding to the ionization energy  $E_i$  of the impurity level and the lowest subband energy of the square well potential  $\hbar^2\pi^2/(2mL^2)$ . This enhancement of the optical photoionization threshold is due to the additional electron confinement in the direction perpendicular to the well. When  $L$  goes to infinity, the electron is free to move in all the space and the zero phonon threshold reduces as expected to the ionization energy. The photoionization cross-section in QW rises sharply at zero absorption, peaks at lower photon energies, and then increases as photon energy increases. The effect of electron-phonon coupling on the photoionization in quantum well exhibits the same behaviour as in the bulk case, but in a more pronounced manner, especially when the layer thickness of the well is small.

For an infinite square ZnSe wire of dimensions  $L_x = L_y = 1(a^*)$  and a rectangular one of dimensions  $L_x = 1(a^*)$  and  $L_y = 1.5(a^*)$  where  $a^*$  is the effective Bohr radius of ZnSe, we have<sup>10</sup> found that the zero optical photoionization threshold energy  $E_s^0$  obtained is a sum of the ionization energy  $E_i$  and the electron confinement energy of the final state of the transition, i.e.,  $E_s^0 = E_i + \hbar^2\pi^2/(2mL_x^2) + \hbar^2\pi^2/(2mL_y^2)$ . Clearly, it is seen that the photoionization energy in the quasi-one-dimensional quantum wire is greater than that in comparable two-dimensional quantum well.<sup>8,4</sup> The enhancement of the

optical photoionization threshold is due to the additional electron confinement in QWWs. We have also found that the magnitude of the cross-section decreases and the optical photoionization threshold energy increases with decreasing confinement length of the QWW. These effects are more pronounced for the one-phonon results than for the zero phonon case. Moreover, we have shown<sup>10</sup> that the effects of electron-phonon coupling on the cross-section are more significant for small confinement lengths of QWW ( $L_y = 1(a^*)$ ) than for slightly larger confinement of QWW ( $L_y = 1.5(a^*)$ ).

For a single shallow hydrogenic impurity placed at the center of the wire material GaAs sandwiched between two finite layers of Ga<sub>1-x</sub>Al<sub>x</sub>As, we have<sup>9</sup> studied the photoionization cross-section as a function of photon energy  $\hbar\omega/E_s$  for two choices of the alloy composition of Ga<sub>1-x</sub>Al<sub>x</sub>As,  $x=0.15$  and  $x=0.30$  and for different values of the dimensions of the wire. As we have noted by fixing two directions of the wire and as the Al content  $x$  increases, the confining well depth increases, making the wire more one-dimensional. So the binding energy increases and, as a consequence, the maximum value of the photoionization cross-section decreases.

For a same value of the Al concentration  $x$ , as one direction of the wire ( $L_x$ ) increases, the peak value of the cross-section increases because of decreasing binding energy. The numerical values of the cross-section in the infinite confining potential are smaller than those in the finite potential case. These results are more pronounced as the photon energy increases. We also note that the optical photoionization threshold energy in infinite confining potential is greater than in finite potential of the confinement. This is logical because the bound states in the infinite-well wires have higher binding energies than in the finite-well wires. In conclusion, we have shown that the impurity photoionization cross-section are very sensitive to the magnetic field, the electric field, the central-cell correction, the mass anisotropy, the electron-phonon coupling and their combined effect in a bulk semiconductors and to the electron-phonon coupling in a quasi-bidimensional and a quasi-unidimensional systems. We have also shown that the Al concentration or the height of the barrier affect drastically the photoionization cross-section in a finite quantum-well wire.

## ACKNOWLEDGMENTS

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