CHAPTER 3

PHOTOIONIZATION OF A DONOR IMPURITY IN A QUANTUM WELL: EFFECT OF AN ELECTRIC FIELD

Abstract

Recently several authors have investigated the photoionization of impurities in quantum well systems. The cross section profile depends upon the type of polarization of the incident radiation. There has not been sufficient work either on magnetic superlattices or on the effects of electric field on photoionization cross section. In the present work, cross sections are calculated for the $GaAs/Al_xGa_{1-x}As$ quantum well system in external electric fields with finite and infinite barriers. Results are compared with available data in the literature.
I. Introduction

Among the several properties of low dimensional semiconductor systems, photoionization of donors in a quantum well has not drawn sufficient attention experimentally. In the work of Takihawa et al. the photoionization manifests as a shoulder near the exciton resonance peak [1]. Apart from this, there doesn’t seem to be any other experimental data available in low dimensional semiconductor systems.

From a theoretical point of view, several authors have investigated the photo-ionization cross sections of shallow donors in the GaAs quantum well of a GaAs/Al\(_x\)Ga\(_{1-x}\)As quantum well system and in a quantum well wire [2,3,4]. The behaviour of the cross section as a function of incident energy is totally different in the two cases of radiation, being x-polarized or z-polarized (along the growth direction in the quantum well case). It has also been shown that in a magnetic field the cross section values are lowered. This is attributed to additional confinement of the carrier [3].

In the present work the interest is two fold: (i) the cross section is calculated in a quantum well system as there are some errors in the works of El-Said and Tomak [2] and Sali et al. [4] and (ii) reporting the results for cross section under the influence of an external electric field. The calculations have been performed with infinite and finite barriers which are described in the next section. The results and discussion are provided in section III.
II. Theory

1. Donor ionization energy

When the electric field is applied to the donor situated at the middle of the finite well, the Hamiltonian is given by,

\[ H = \frac{p^2}{2m^*} + e\xi z + V(z) - \frac{e^2}{\varepsilon r} \]  

(1)

where \( \xi \) is the electric field.

Without the donor, the sub-band energies are obtained using

\[ H_1 = -\hbar^2 \frac{\partial^2}{2m^* \partial z^2} + e\xi z + V(z) \]  

(2)

where \( V(z) = \begin{cases} 0 & |z| \leq \frac{L}{2} \\ V & |z| > \frac{L}{2} \end{cases} \)

Employing a trial wave function,

\[ \Psi_1 = \begin{cases} A_1(1-b\xi z)\cos(\alpha_1z) & |z| \leq \frac{L}{2} \\ A_1C_1(1-b\xi z)\exp(-\beta_1z) & |z| > \frac{L}{2} \end{cases} \]  

(3)

In Eq.(3), ‘\( b \)’ is the variation parameter, \( V(z) \) is the barrier height and \( C_1=\cos(\alpha_1L/2) \exp(\beta_1 L/2) \)

The eigen value of the Hamiltonian in Eq.(3) gives the first sub band energy( \( E_1 \)) given by

\[ (E_1/V)^{1/2}=\cos(m*E_1 L^2/2 \hbar^2)^{1/2} \]  

(4)

The second sub band energy (\( E_2 \)) is obtained using the trial function
\[ \Psi_2 = \begin{cases} 
    A_2 (1 - b \xi z) \sin(\alpha_2 z) & |z| \leq \frac{L}{2} \\
    A_2 C_2 (1 - b \xi z) \exp(-\beta_2 z) & |z| > \frac{L}{2} 
\end{cases} \]

where \( A_1 \) and \( A_2 \) are the normalization constants,

\[ C_2 = \sin(\alpha_2 L/2) \exp(\beta_2 L/2) \]

and

\[ \frac{[(V-E_2)/E_2]^{1/2}}{\csc(m^* E_2 L^2/2 \hbar^2)^{1/2}} \quad (5) \]

The donor states are obtained using the Hamiltonian \( H \) in the presence of an electric field with

\[ \Psi_1 = \begin{cases} 
    A_1 (1 - b \xi z) \exp(-\rho \alpha/a) \cos(\alpha_1 z) & |z| \leq \frac{L}{2} \\
    A_1 C_1 (1 - b \xi z) \exp(-\beta_1 z) \exp\left(-\frac{\rho}{a}\right) & |z| > \frac{L}{2} 
\end{cases} \]  

where \( \alpha_1, \alpha_2, \beta_1 \) and \( \beta_2 \) have the same expressions as in Ref.[3] and \( H_{\text{min}} \) is the eigen value of Eq.(1) with the variation parameter 'a'.

The electric field affects both the sub-band energy and the ionization energy. The ionization energy of the donor is,

\[ E_{\text{ion}} = E_1 - \langle H_{\text{min}} \rangle \quad (7) \]

2. Photoionization cross section

a. Polarization along the z-direction

For shallow impurities with low binding energies, the standard dipole approximation in the bulk case holds good and the photoionization cross section is given by [2],

\[ \sigma(\hbar \omega) = \left( \frac{E_{\text{eff}}}{E} \right)^2 \frac{n}{\epsilon} 4 \pi^2 \frac{\alpha}{3} \hbar \omega \sum_f \langle \Psi_f | \overrightarrow{F} | \Psi_i \rangle^2 \delta[E_f - (E_i + \hbar \omega)] \quad (8) \]
where \( \frac{E_{\text{eff}}}{E} \) is the effective field ratio, \( n \) the refractive index, \( \varepsilon \) the dielectric constant of GaAs and \( \alpha \) the fine structure constant. Since the transition to the first sub-band is forbidden by symmetry, the final eigen state in the presence of the electric field, omitting the influence of the Coulomb potential is,

\[
\Psi_f = \begin{cases} 
A_1(1-b\xi z)\exp(ik_1\rho)\sin(\alpha_2 z) & |z| < \frac{L}{2} \\
A_2 \frac{C_1}{\sqrt{S}}(1-b\xi z)\exp(ik_1\rho)\exp(-\beta_2 z) & |z| > \frac{L}{2}
\end{cases}
\]  

where \( S \) is the surface area. Thus

\[
\langle \Psi_f | \Psi_f \rangle = \frac{\hbar^2}{m(E_r - E_f)} \left\{ \langle \Psi_f \frac{\partial}{\partial z} \Psi_f \rangle_{|z| < \frac{L}{2}} + \langle \Psi_f \frac{\partial}{\partial z} \Psi_f \rangle_{|z| > \frac{L}{2}} \right\} 
\]

\[
= \frac{\hbar^2}{m(E_r - E_f)} (A + B)
\]

where

\[
A = \left( \frac{-2\pi A_1 A_2}{\sqrt{S}} \right) \int_0^{\frac{L}{2}} \int_{-\frac{L}{2}}^{\frac{L}{2}} b\xi (1-b\xi z)\sin(\alpha_2 z)\cos(\alpha_1 z)\exp(ik_1\rho)\exp\left(-\frac{\rho}{a}\right)\rho d\rho dz
\]

\[
+ \left( \frac{-2\pi A_1 A_2}{\sqrt{S}} \right) \int_0^{\frac{L}{2}} \int_{-\frac{L}{2}}^{\frac{L}{2}} \alpha_1 (1-b\xi z)^2 \sin^2(\alpha_2 z)\exp(ik_1\rho)\exp\left(-\frac{\rho}{a}\right)\rho d\rho dz
\]

and

\[
B = \left( \frac{-4\pi A_1 A_2 C_1 C_2}{\sqrt{S}} \right) \int_0^{\frac{L}{2}} \int_{-\frac{L}{2}}^{\frac{L}{2}} \beta_1 (1-b\xi z)\exp(-\beta_1 z)\exp(-\beta_2 z)\exp(ik_1\rho)\exp\left(-\frac{\rho}{a}\right)\rho d\rho dz
\]

\[
+ \left( \frac{-4\pi A_1 A_2 C_1 C_2}{\sqrt{S}} \right) \int_0^{\frac{L}{2}} \int_{-\frac{L}{2}}^{\frac{L}{2}} \beta_1 (1-b\xi z)^2 \exp(-(\beta_1 + \beta_2) z)\exp(ik_1\rho)\exp\left(-\frac{\rho}{a}\right)\rho d\rho dz
\]

and \( E_r - E_f = \hbar \omega \)

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with \( E_i = \frac{\hbar^2 k^2}{2m^*} + E_2 \).

Also,
\[
E_i = \langle H_{\text{min}} \rangle + \hbar \omega,
\]
where \( E_i \) refers to the initial energy of the system.

**b. Polarization along the x-direction**

In this case the dipole transition to the first sub band is allowed, hence

\[
\Psi_f = \begin{cases} 
A_1 (1 - b \xi z) \exp(i k_{\parallel} \rho) \cos(\alpha, z) & |z| \leq \frac{L}{2} \\
\left( \frac{A_1 C_1}{\sqrt{S}} \right) (1 - b \xi z) \exp(i k_{\parallel} \rho) \exp(-\beta, z) & |z| > \frac{L}{2}
\end{cases}
\]

A standard result is
\[
\exp(i k_{\parallel} \rho) = J_0(k_{\parallel} \rho) + 2 \sum_{m=1}^{\infty} J_m(k_{\parallel} \rho) \cos(m[\theta - \theta_k])
\]
where \( J_0, J_m \) are the Bessel functions, \( \theta_k \) is the direction of vector \( k_{\parallel} \).

Here
\[
< \Psi_f | \frac{\partial}{\partial x} | \Psi_i > = \frac{-2\pi A_1 A_3}{a \sqrt{S}} (C + 2D)
\]

where
\[
C = \int_{\frac{-L}{2}}^{\frac{L}{2}} (1 - b \xi z)^2 \cos^2(\alpha, z) J_1(k_{\parallel} \rho) \exp\left( -\frac{\rho}{a} \right) \rho d\rho dz
\]

and
\[
D = \int_{\frac{-L}{2}}^{\frac{L}{2}} (1 - b \xi z)^2 \exp(-2\beta, z) J_1(k_{\parallel} \rho) \exp\left( -\frac{\rho}{a} \right) \rho d\rho dz
\]

using
\[
k_{\parallel}^2 = \frac{2m^*}{\hbar^2} [H_{\text{min}} + \hbar \omega - E_1],
\]

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we obtain

\[
\sigma(h\omega) = \left( \frac{E_{\text{eff}}}{E} \right)^2 \frac{n 4\pi^2 \alpha \hbar \omega}{3 \pi \hbar^2} m^* S \frac{\hbar^2}{m^* (E_m - E_f)^2} \left| < \Psi_f \left| \frac{\partial}{\partial x} \right| \Psi_i > \right|^2
\]

c. Infinite well model

In the infinite well case, the following expressions are valid:

\[
\Psi_i = \begin{cases} 
A_i (1 - b_\xi z) \exp \left( -\frac{\rho}{a} \right) \cos \left( \frac{\pi z}{L} \right) & |z| \leq \frac{L}{2} \\
0 & |z| > \frac{L}{2}
\end{cases}
\]

(14)

with

\[ V(z) = \begin{cases} 
0 & |z| \leq \frac{L}{2} \\
\infty & |z| > \frac{L}{2}
\end{cases} \text{ in Eq.(1)}

The first sub-band energy is determined using

\[ \Psi_1 = N_1 (1 - b_\xi z) \cos \left( \frac{\pi z}{L} \right) \text{ in Eq.(2)} \] and

the second sub-band energy is obtained using

\[ \Psi_2 = N_2 (1 - b_\xi z) \sin \left( \frac{2\pi z}{L} \right) \text{ in Eq.(2)} \]

For x- polarization, \[ \Psi_f = \frac{N_1}{\sqrt{S}} (1 - b_\xi z) \exp(ik_{\perp,\rho}) \cos \left( \frac{\pi z}{L} \right) \]

with \[ E_f = \hbar^2 k_{\perp,\rho}^2 + E_1 \].

For z- polarization, \[ \Psi_f = \frac{N_4}{\sqrt{S}} (1 - b_\xi z) \exp(ik_{\perp,\rho}) \sin \left( \frac{2\pi z}{L} \right) \]

with \[ E_f = \hbar^2 k_{\perp,\rho}^2 + E_2 \] and \[ E_f = H_{\text{min}} + \hbar \omega \].

Here, \( N_1, N_2, N_3, N_4 \) are the normalization constants.
III. Results and Discussion

The results are presented in Figs. 1 to 4 and in Table 1. Fig. 1 shows the decrease of ionization energy with well width for finite and infinite wells. In the presence of an electric field, the decrease is faster. Also the ionization energy is higher in the case of infinite well. As \( L \to 0 \) in the infinite well model without the electric field, \( E_{ion} \) should reach \( 4R^* \). The chosen wave function has this correct behaviour and so the present results are reliable for an infinite well case. However, for the case of finite well, \( E_{ion} \to R^* \) which is the 3D limit. The choice of the wave function seems to be poor in this limit.

The variation of ionization energy with electric field is displayed for an infinite well in Fig. 2. Even a strong field of \( 10^7 \) V/m does not produce appreciable change in the ionization energy for a narrow well of 100 Å. However, for a fairly wider well the ionization energy decreases for fields of higher intensity. This behaviour is attributed to the boundary condition imposed on the wave function at the walls. The electric field tries to accelerate the particle towards the wall whereas the boundary condition works against it. The decrease in ionization energy in an electric field for a wider well is a cumulative effect of

(i) the well becoming asymmetric in an electric field thereby reducing the sub-band energy and

(ii) the electric field working against the Coulomb attraction due to the donor ion, which has been assumed to be at the center of the well, in the present work.

Fig. 3 gives the variation of photo-ionization with photon energy. In an electric field, the threshold energy for cross section is reduced. This is due to
Fig. 1 Ionization energy as a function of well width
Fig. 2 Variation of ionization energy with electric field in the infinite well model.
Fig. 3 The photoionization cross section as a function of photon energy for finite and infinite wells when the radiation is x-polarized for $L=200\text{ Å}$.
the fact that the well becomes asymmetrical in an electric field inducing electron tunneling. When compared to an infinite well model, in a finite well the peak value is reduced. This is due to

(i) the finite well behaving as a 3D system and
(ii) the choice of our trial function.

This result is in contradiction with the results of Ilawai and El-Said [3] who used hydrogenic trial function which is not suitable as $L \rightarrow 0$ in an infinite well model. However, in the finite well model, a hydrogenic function is more suitable in this limit. The overall behaviour is in agreement with the results of El-Said and Tomak [5]. However, in the present model, the numerical values are of the same order as in ref [3]. There doesn’t seem to be accurate experimental data available at present to compare the results.

The photo-ionization cross sections in the case of z-polarization are given in Fig.4. Again the thresholds are found shifted to lower energies in an electric field. However, the order of magnitude of the values are the same. The behaviour of the cross section versus photon energy is in overall agreement with other available works in the literature [3].

In Table 1 a comparison of the cross sections in the infinite and finite well models is made. Here also the threshold gets shifted to lower energies. But the numerical values for finite well are one order less than those of infinite well.

As remarked earlier, the expression for cross section [in Eq.(11) of Ref.[2]] contains an error. The expression for cross section of Ref.[2] is,

$$\sigma(\hbar \omega) = \left( \frac{E_{\text{eff}}}{E} \right)^2 \frac{(n/k)(4\pi^2 \alpha/3)}{\hbar \omega \pi/a^4} [(I_2-I_3)]^2$$
Fig. 4 The photoionization cross section as a function of photon energy for z-polarization for an infinite well (L=200Å)
TABLE 1 Photoionization cross sections in finite and infinite well models for a well of width 150Å (Radiation z-polarized)

(a) Infinite well

<table>
<thead>
<tr>
<th>Photon energy (meV)</th>
<th>$\sigma/L^2$ $\xi=0$ V/cm</th>
<th>Photon energy (meV)</th>
<th>$\sigma/L^2$ $\xi=100$ KV/cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>86.029</td>
<td>0.0356</td>
<td>76.4538</td>
<td>0.03499</td>
</tr>
<tr>
<td>87.306</td>
<td>0.0204</td>
<td>79.2437</td>
<td>0.01147</td>
</tr>
<tr>
<td>88.425</td>
<td>0.0134</td>
<td>81.4147</td>
<td>0.00592</td>
</tr>
<tr>
<td>89.545</td>
<td>0.00926</td>
<td>84.6713</td>
<td>0.00268</td>
</tr>
<tr>
<td>91.784</td>
<td>0.00491</td>
<td>86.8424</td>
<td>0.001727</td>
</tr>
</tbody>
</table>

(b) Finite well

<table>
<thead>
<tr>
<th>Photon energy (meV)</th>
<th>$\sigma/L^2$ $\xi=0$ V/cm</th>
<th>Photon energy (meV)</th>
<th>$\sigma/L^2$ $\xi=100$ KV/cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>60.043</td>
<td>0.005806</td>
<td>36.579</td>
<td>0.00551</td>
</tr>
<tr>
<td>61.569</td>
<td>0.00277</td>
<td>37.85</td>
<td>0.002897</td>
</tr>
<tr>
<td>62.595</td>
<td>0.001824</td>
<td>38.821</td>
<td>0.001905</td>
</tr>
<tr>
<td>64.648</td>
<td>0.000903</td>
<td>40.762</td>
<td>0.000938</td>
</tr>
<tr>
<td>66.7</td>
<td>0.000506</td>
<td>42.703</td>
<td>0.000521</td>
</tr>
</tbody>
</table>
where the dimensions of $I_2$ and $I_3$ do not match in the expressions given by them. Hence the numerical results are not reliable, though the overall behaviour is in agreement with our present work. Expression (9) of Ref. [3] is also in error. The correct expression should be

$$[(V-E_2)/E_2]^{1/2} = -\cot(m^*E_2L^2/2h^2)^{1/2}$$

Hence, in addition to the numerical data for cross section, their observation of reduction in cross section in a magnetic field also requires close scrutiny. The effect of a magnetic field leads to interesting results as one has to compare the inter sub-band separation with the Landau level separation. The former is unaffected in a magnetic field when it is applied along $z$-direction (growth direction). However, the field that is used in Ref. [3] is 6.74 Tesla for a well width of $2.5a^*$ which is about 250 Å. For this case, the Landau level separation is 11.663 meV while the inter sub-band separation is 21.543 meV. Hence, transition to higher Landau levels should be considered. Also for such strong fields, it has been shown [6] that a hydrogenic function yields poor results. Hence a product Gaussian or a linear combination of hydrogenic functions has to be used. The effect of magnetic field has been investigated in Ref. [3] where it is shown that the cross section reduces in a magnetic field, due to the additional confinement of the carrier. These points are further discussed in the next chapter on semimagnetic quantum well systems.
References