Ionization Energy of a shallow Donor in GaAs Quantum Dot using Effective – Mass approximation

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Abstract— **The purpose of the present work is we work out the Ionization energy values of a donor in a QOD system of $GaAs - Ga_{1-x}Al_xAs$ with square and rectangular cross sections, assuming the donor at the centre of the box. This problem has been studied by means of the effective-mass approximation. The present calculations are performed for different well widths and for different electric field strengths in square and rectangular cross sections.**

Keywords— Quantum dot, ionization energy, shallow donor, Quasi –Zero dimension

INTRODUCTION

In the last decade semiconductor heterostructures have received a great deal of attention because of their intrinsic physical interest and their technological applications in electronic devices. In recent years much attention has been focused on quasi-zero dimensional (QOD) semiconductor structures called quantum dots or boxes. The most often employed semiconductors are of the III-V compound type, as in the $GaAs - Ga_{1-x}Al_xAs$ system, which is the most thoroughly studied and one of the greatest technological promises. In a $GaAs - Ga_{1-x}Al_xAs$ quantum dot the difference in the band gap of the two semiconductors acts as an additional square-well potential which confines the carries (both electrons and holes) in all three directions.

Also there has been increasing interest in the study of electronic properties of QOD system. There are many papers that treat the energy-level structure of related system. Of particular current interest are, electron states in a quantum dot in a magnetic field(Aravind Kumar et al 1990),excitons in parabolic (Weiming Que 1992) and square confinement (Bryant 1988), biexciton states (Hu et al 1990), magneto-optics (Peeters 1990) and intraband absorption of infrared radiation (Milanovic and Ikonic 1989), to cite some examples.

THEORETICAL FRAMEWORK

Calculation of Ionization energy in the presence of an electric field

Let us consider a QOD system with impenetrable walls formed by restricting GaAs layer in all three dimensions. The quantum well exists in the GaAs region of the $GaAs / Ga_{1-x}Al_xAs$ super lattice system. So the donor electron is thus confined to move in all the three directions in the quantum dot of infinite strength.

The Hamiltonian of the donor electron within the frame work of the effective - mass approximation, in a GaAs quantum dot in the presence of an electric field is given by

$$H = \frac{P^2}{2m^*} + V_w(x,y,z) + e\,\vec{F}.\vec{r} - \frac{e^2}{4\pi \epsilon_0 \epsilon_r} \quad \ldots\ldots. (1)$$

Where m^* is the effective mass of the electron in the conduction band minimum (Γ) of GaAs, 'e' is the electronic charge, ϵ_0 is the permittivity of free space, ϵ_r is the static dielectric constant of GaAs and $\vec{F}$ is the electric field. V_w is the confining well potential given by

$$V_w(x, y, z) = \infty, x \geq \frac{L}{2} \text{ and/or } y \geq L/2$$

$$\text{and/or } z \geq L/2$$

$$0, \text{ Otherwise} \ldots\ldots\ldots(2)$$

$\vec{F}$ is the electric field vector making an angle θ with the position vector $\vec{r}$. The donor electron is situated at the centre of the box. Here we consider that applied electric field direction is [100]. In the case of a box of square and rectangular cross-sections the electric field strength along [100] direction is just $F_x = F$. Other two components F_y & F_z are zero. F denotes the magnitude of the applied electric field and F_x, F_y & F_z refer to strength of it along x, y and z axes.

Following the work of Sukumar and Navaneethakrishnan (1990), the variational anastz we use is written as

$$\psi(x, y, z) = N \cos\frac{\pi x}{A} \cos\frac{\pi y}{B} \cos\frac{\pi z}{C} e^{(-\alpha r)(1+\lambda F X)} \ldots\ldots\ldots\ldots\ldots(3)$$

With α and λ as variational parameters. A, B and C refer to well thickness (L) along x, y and z axes.

We obtain

$$< \psi|H|\psi >= \langle H \rangle = \langle KE \rangle + \langle PE \rangle + \langle EE \rangle$$

$$\langle H \rangle = T_1 + T_2 + T_3 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4)$$

With,

$$T_1 = \langle \frac{P^2}{2m^*} \rangle = \frac{\hbar^2\alpha^2}{2m^*} - \frac{\hbar^2\pi^2}{2m^*}\left(\frac{1}{A^2} + \frac{1}{B^2} + \frac{1}{C^2}\right) + \frac{\hbar^2\pi^2N^2}{2m^*}\left(\frac{1}{A^2} + \frac{1}{B^2} + \frac{1}{C^2}\right) I_3 + \frac{N^2\hbar^2\pi^2\lambda^2F^2}{2m^*A^2} I_4$$

$$+ \frac{N^2\hbar^2\pi^2\lambda^2F^2}{2m^*}\left(\frac{1}{A^2} + \frac{1}{B^2}\right) I_5 + \frac{N^2\hbar^2\pi\alpha}{2m^*}\left(\frac{1}{A} + \frac{1}{B} + \frac{1}{C}\right) I_6 + \frac{N^2\hbar^2\pi\alpha\lambda^2F^2}{2m^*A} I_7 + \frac{N^2\hbar^2\pi\alpha\lambda^2F^2}{2m^*}\left(\frac{1}{B} + \frac{1}{C}\right) I_8 + \frac{N^2\hbar^2\lambda^2F^2}{2m^*} I_1 - \frac{N^2\hbar^2\pi\lambda^2F^2}{2m^*A} I_9 - \frac{N^2\hbar^2\alpha\lambda^2F^2}{m^*} I_{10}$$

$$T_2 = \langle \frac{-e^2}{4\pi\epsilon_0\epsilon r} \rangle = \frac{-e^2N^2}{4\pi\epsilon_0\epsilon}[I_{11} + \lambda^2F^2I_{10}]$$

$$T_3 = \langle e\,\vec{F}.\vec{r} \rangle = 2N^2\lambda eF^2I_2$$

The normalization constant N is given by the expression

$$N = [I_1 + \lambda^2F^2I_2]^{-1/2}$$

Where $I_1, I_2, I_3, I_4, I_5, I_6, I_7, I_8, I_9, I_{10}$ and I_{11} are volume integrals.

The integrals appearing in I_1 to I_{11} can be evaluated numerically. In all these integrals the lower limit is zero and the upper limit is L/2 i.e. (A/2, B/2, C/2). By varying α and λ, $\langle H \rangle_{min}$ is obtained. To calculate $\langle H \rangle_{min}$, first we switch off the electric field strength and minimize the expression (1) by varying the variational parameter 'α'. In this process we calculate different α values for different well widths in the absence of the electric field. Using these calculated α values for different well widths $\langle H \rangle_{min}$ is obtained for different well widths and when $F \neq 0$, by varying the electric field dependent parameter λ. The calculations were performed for various electric field strengths as well as for different geometries of the dot, viz [L, L, L], [L, L, L/2]. L ranges from 10 nm to 50 nm in our calculations.

The donor ionization energy is defined as

$$E_{ion} = E_{SUB} - \langle H \rangle_{min} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(6)$$

CONCLUSIONS:

Considering the square [L, L, L] and rectangular [L, L, L/2] cross sections we arrive at the following conclusions. It is noticed that for a given electric field strength (both in the range of 10^7 and 10^6 V/m, the ionization as well as the sub band energies decrease with the increase of well width both in square and rectangular cross section.

For a given box dimension whether it is square or rectangular cross section, both the donor and sub band energies decrease with increasing electric field intensity, the decrease being more significant for larger well widths.

The insignificant change in the donor ionization energies for smaller well widths as the field intensity is increased from zero, is a common feature in low dimensional system. It is understood that the boundary condition prevents the electron localizing near the edge, the shift arising due to the electric field. The electric field also has to do work on the electron against the attractive donor potential. As the well width increases, the confinement becomes progressively poor resulting in larger changes. Our results show that the ionization energy increases as the dimension is reduced irrespective of cross section.

An interesting result of the present work is that when the strength of the electric field is increased to 10^7 V/m, for well widths larger than 20 nm, we have found that the ionization energy is negative both in square and rectangular boxes. It is well known that for a well of finite strength and for larger electric fields one has only quasi bound or unbound states in a quantum well (Bastard et al 1983). Such a situation does not arise in the present work since we have restricted our calculations to wells of infinite strength. A zero ionization energy would mean that the donor state is in the continuum of the n=1 sub band. A negative value for the ionization energy means that the ground state sub band moves downwards faster than the donor ground state for such a large electric field. However, a transition from the ground state of the donor to the n=2 (first excited) sub band in the QOD is still possible which will make the ionization energy positive, provided this sub band does not descend rapidly with electric field. This indeed is the case as can be easily demonstrated using the results of Ahn and Chuang (1987) in a quantum well, where it is shown that the n = 2 sub band shows a slight increase upwards for small fields and show a decrease for larger fields. This conclusion ,i.e., the donor states are no longer associated with the ground state sub band for electric fields >= 10^7V/m appears difficult to be verified experimentally, as the barrier heights in reality are finite.An infinite well model is generally employed as it reduces the amount of numerical work.

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