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The Effect of Spatially Dependent Screening On the Donor Ionization Energy in a Quantum Wire

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Abstract

The effect of the spatially dependent screening on the ionization energy of a shallow donor in a 1D quantum well wire made of $Ga_{1-x}Al_x/GaAs$ superlattice is presented. A variational approach is used to obtain ionization energy of the on-centre impurity at the origin of the well and the results obtained are compared with the existing values.

1. Introduction

With the development of Molecular Beam Epitaxy (MBE), considerable attention is being paid to the fabrication and understanding of the physical properties of pure and doped 1D and 2D quantum systems whose dimensions are of the order of de Broglie wavelength of electrons [1-3]. Sakaki [6-8] suggested fabrication of ultrathin semiconducting wires whereby the electrons behave essentially as a quasi-one-dimensional electron gas. For such 1D structures, Sakaki [6-8] took into account the scattering of the carriers by ionized impurities located at a fixed distance outside the structure. He suggested that the carrier mobility should benefit from the bi-dimensional confinement in thin Quantum Well Wires (QWW). He also calculated the mobility limited by coulombic scattering and acoustic phonon scattering and found mobility figures in excess of $10^{-6}\mathrm{cm}^2\mathrm{V}^{-1}\mathrm{s}^{-1}$ at low temperatures. It was then concluded that such a high mobility system could serve as a promising material for use in a variety of electronic devices. Later, Lee and Spector [9] used a more realistic model to determine the mobility limited by scattering from either remote or background impurities. Petroff et.al. [10] fabricated quantum well wires and observed an enhanced cathoduluminescence in these structures.

Nevertheless, the problem of hydrogenic impurities has attracted some attention in quasi bi-dimensional (2D) systems (e.g. semiconducting quantum wells) [11-3]. The

relevance of carrier confinement in quasi 2D problems indicates that more dramatic effects should occur when an impurity is placed in a quasi-unidimensional 1D environment. Thus, variational calculations of the ground state binding energy of hydrogenic impurity has been carried out for such wires. Lee and Spector [14] found that the binding energy diverged with decreasing well width for an axial impurity by modelling the wire as an infinite cylindrical well with a step function electronic probability density. Brum [15] considered axial, edge and corner impurities in an infinite rectangular well and obtained similar results. Bryant [16] found that the binding energy has a peak value at some finite well thickness when he used the finite cylindrical well model with an axial impurity. Also, Bryant [17] studied the effect on the impurity's binding energy by changing the cross-sectional form of the wire. He studied a rectangular well of varying dimensions on the basis of an infinite well model and compared the results to those for a cylindrical well. It was found that for wires of equal cross-sectional area the binding energies are nearly equal between cylindrical and rectangular wells, provided the rectangular form does not deviate too far from a square shape. Brown and Spector [18] calculated the binding energy of a hydrogenic impurity in or near a quantum well wire. Investigations have been carried out in the impurity states in Q1D and Q2D systems, in external perturbation [19, 20]. Costa and Albuquerque [21] applied the effective-mas approximation to the calculation of impurity binding energy. Porras-Montenegro et.al. [21] calculated the binding energies of hydrogenic impurities in both infinite and finite GaAs-(GaAl)As cylindrical quantum-well wires as functions of the wire radius and of the impurity location in the well for different radii of the wires using a variational procedure within the effective-mass-approximation. Recently, Porras-Montenegro [22] reported that using a variational procedure within the effective-mass approximation, the spatially dependent screening increases the binding energies of shallow hydrogenic impurity states in GaAs-(GaAl)As quantum-well-wires.

In this paper, the ionization of a hydrogenic impurity in the centre of the quantum well wire $Ga_{1-x}Al_xAs/GaAs$ superlattice will be determined using a variational approach. To this end, an investigation of the effect of spatially dependent screening on the ionization energy of a shallow donor in such a system will be explored. In Section 2 the brief theory of the infinite rectangular quantum well wire is outlined, numerical results and conclusion are presented in Section 3.

2. Theory

The Hamiltonian for a donor electron confined by a two dimensional square well potential in the $x-y$ plane and free to move in the z-direction is

$$H = \frac{\hbar^2\nabla^2}{2m^*} + V_W(x,y) - \frac{e^2}{4\pi\epsilon(r)r}, \tag{1}$$

where

$$r = \sqrt{x^2+y^2+z^2} \tag{2}$$

and m^* is the effective mass of the electron in the GaAs well and $\epsilon(r)$ is the spatially

varying dielectric function which is described below. $V_W(x,y)$ is given by

$$V_W(x,y) = \begin{cases} 0 & |x| \text{ and/or } |y| \leq L_x/2 \text{ or } L_y/2. \\ \infty & \text{otherwise.} \end{cases} \tag{3}$$

Lee and Spector [14] and Brum [15] have obtained the eigenvalues and eigenfunctions of equation (1) using the spatially constant dielectric function in place of $\epsilon(r)$. We follow Brum [15] and write the approximate eigenfunctions of H in the form

$$\Psi(x,y,z) = \frac{2N}{\sqrt{L_x L_y}} \cos\frac{n\pi x}{L_x} \cos\frac{n\pi y}{L_y} e^{-r/\lambda}, \tag{4}$$

where N is a normalization constant and λ is a trial parameter. The on-centre impurity is considered at the origin (mid-point) of the well and taken a box such that $L_x = L_y = 1$. Only the eigenstate associated with the lowest subband $n = m = 1$ is investigated. This yields

$$\begin{aligned} \langle H \rangle = \frac{\hbar^2}{2m^*\lambda^2} - \frac{1}{C}\frac{\hbar^2\pi^2}{2m^*L^2}\frac{4N^2}{L^2}\int_{-L/2}^{L/2}\int_{-L/2}^{L/2} dxdy \left[\cos\frac{\pi x}{L} - \cos\frac{\pi y}{L}\right]^2 \\ \times\sqrt{x^2+y^2}K_1\left(\frac{2}{\lambda}\sqrt{x^2+y^2}\right) - \frac{e^2A}{C}, \end{aligned} \tag{5}$$

where

$$A = \frac{4N^2}{L^2}\int_{-L/2}^{L/2} \epsilon^{-1}(r) dxdy \cos^2\frac{\pi x}{L}\cos^2\frac{\pi y}{K}_0\left[\frac{2}{\lambda}\sqrt{x^2+y^2}\right] \tag{6}$$

and

$$C = \frac{4N^2}{L^2}\int_{-L/2}^{L/2} dxdy \cos^2\frac{\pi x}{L^2}\cos^2\frac{\pi y}{L}\sqrt{x^2+y^2}K_1\left[\frac{2}{\lambda}\sqrt{x^2+y^2}\right], \tag{7}$$

where $K_0(x)$ and $K_1(x)$ are the zeroth and first order modified Bessel function, respectively.

In the work of Brum, the second term in the kinetic energy was omitted. It can be seen that this term does not vanish. The ionization energy is given by

$$E_{ion} = E_{sub} - \langle H \rangle_{\min}, \tag{8}$$

where

$$E_{sub} = \frac{\hbar^2\pi^2}{2m^*}\left(\frac{n^2}{L_x^2} + \frac{m^2}{L_y^2}\right) = \frac{\hbar^2\pi^2}{m^*L^2} \tag{9}$$

and $\langle H \rangle_{\min}$ is found variationally by evaluating the integrals numerically. The integral is evaluated by replacing the integrals in xy by integrals over r and θ, such that $L^2 = \pi R^2$.

The spatially varying dielectric function used is defined in the form

$$\epsilon^{-1}(r) = \begin{cases} A + Br & r \leq R_0 \\ K^{-1} & r \geq R_0, \end{cases} \tag{10}$$

where $A = 1$ and $B = \frac{1}{R_0}(\frac{1}{K} - 1)$. Also, A and B values are obtained by demanding $\epsilon(r) = 1$ and $r = 0$ and $\epsilon(r) = K(0)$ at $r = R_0$. This spatially varying dielectric function is an approximate form which is valid in the study of donors in the bulk of 3D semiconductor systems [24, 25]. K is the dielectric constant of GaAs. R_0 is the screening radius which is assumed to be half the nearest neighbour distance in accordance with the earlier workers [19, 20]. For very thin wells, one has to use a spatially varying dielectric function which is pertinent to quasi 1D systems [26].

3. Numerical Results and Conclusion

The donor ionization energy is computed with equation (8) and calculations show that the inclusion of the second term in the kinetic energy modifies the binding energy by about 25%. The ionization energies E_i, are computed for well-widths varying from 0 to 50 nm with spatial variation of the dielectric function. The result is displayed in Figure 1 and it is observed that as $L \to \infty$, the ionization energies approach 1 effective Rydberg viz: $m^* e^4/2n^2\hbar^2 K$ $(n = 1)$, the 3D result. Lee and Spector [14] found $E_i = 17.8$ meV for on-centre impurity QWW of infinite barrier height at radius $L = 10$ nm; Brum [15] found $E_i = 24.4$ meV for on-centre at $L = 10$ nm; whereas, in the present approach, $E_i \approx 63$ meV for on-centre at $L = 10$ nm.

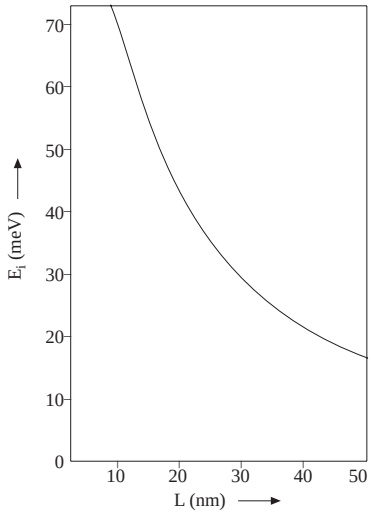

Figure 1. Donor ionization energy E_i for a square quantum well wire of GaAs ($L_x = L_y = 1$) versus L with spatial variation in dielectric function. The impurity is at on-centre.

The present work differs from the work of Brum in the sense that the second term in the kinetic energy which is shown in equation (5) is omitted in the work of Brum. Moreover, the present work has used spatially varying dielectric function as reported in refs. 24 & 25, rather than the spatially constant dielectric function used by Brum. Both differences explain why the present value of E_i is about two and half times larger than

the results obtained by Brum [15].

This paper is concluded with a remark on the use of the effective mass theory (EMT) for confined systems. The potential energy does not change very much over a distance of approximately the effective Bohr radius viz. $\hbar K/m^* e^2$. For extremely thin wells, the use of spatially varying dielectric function pertinent to a 3D system should be alright.

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