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Numerical Calculation of the Ionization Energy of Donors in a Cubic Ouantum well and Wire

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***Abstract*—**The ionization energy in semiconductor systems in nano scale was investigated by using effective mass approximation. By introducing the Hamiltonian of the system, the variational technique was employed to calculate the ground state and the ionization energy of a donor at the center and in the case that the impurities are randomly distributed inside a cubic quantum well. The numerical results for GaAs/GaAlAs show that the ionization energy strongly depends on the well width for both cases and it decreases as the well width increases. The ionization energy of a quantum wire was also calculated and compared with the results for the well.

***Keywords*—**quantum well, quantum wire, quantum dot, impurity state

I. Introduction

Experimental growth techniques such as molecular beam epitaxy, chemical vapor deposition and electron lithography in recent years has motivated interests in semiconductor-confined nanostructures for their utility in electronic and optoelectronic devices.

In the past few decades, a large amount of work, both theoretical and experimental, has been devoted to the study of the nature of impurity state in quantum well structures. The ideal system for studying two dimensional carriers in semiconductors is $GaAs/Ga_{1-x}Al_xAs$ quantum well systems (QW). The measurements are leading to the electronic and optical properties of such nanostructures. Recently, different authors have investigated semiconductor-metal transition in guasi-2D GaAs/GaAlAs system are demonstrated the transition for very narrow wells [1,2]. A similar model was used by the present authors to investigate the semiconductor-metal transition in many valley semiconductors [3]. In this paper, the ionization energy of a donor in a center of a cubic quantum well and quantum wire, in the case where the donor is located at the center and where the impurities are distributed are compared. In this regard a proper trial wave function is used to calculate numerically the ground state and ionization energy of the donor in a quantum well and wire by variational technique.

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II. Model and Calculations

The Hamiltonian of the system is given by [4]:

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 - \frac{e^2}{\varepsilon(r)r} + V(r) \tag{1}$$

Where m^* and $\varepsilon(r)$ are the effective mass and the dielectric function of GaAs, respectively. The second term is the screened coulomb potential and $V(r)$ is the confining potential.

For a quantum box the confining potential is given as:

$$V(r) = \begin{cases} 0 & |x, y, z| \le L \\ \infty & otherwise \end{cases} \tag{2}$$

Using the Thomas-Fermi screening function, $\varepsilon(r)$ is given as:

$$\varepsilon^{-1}(r) = \exp(-\lambda r)/\varepsilon_0 \tag{3}$$

Where ε_0 is the static dielectric constant of GaAs and λ is the screening parameter given by $\lambda^2 = 4\pi e^2 n(\xi)$ where $n(\xi)$ is the density of states at the Fermi level. Since an exact solution of the Schrodinger equation for the given Hamiltonian is not possible, here the variational method with a trial wave function

$$\psi(r) = N\exp(-\alpha r^2) r^2 \sqrt{(L^2 - x^2)}\sqrt{(L^2 - y^2)}\sqrt{(L^2 - z^2)} \tag{4}$$

Satisfying the boundary condition, with α as a variational parameter is used to calculate the ground state energy of the donor impurity in the well. The expectation value of H is given by:

$$\langle H \rangle = \langle T \rangle + \langle V \rangle \tag{5}$$

Where:

$$\langle T \rangle = \frac{\langle \psi | T | \psi \rangle}{P} = \frac{\int_{-L}^{L} \psi \left(-\frac{\hbar^2}{2m^*}\right) \nabla^2 \psi}{P} \quad (6)$$

where P is given as:

$$P = \langle \psi | \psi \rangle = \int_{-L}^{L}\int_{-L}^{L}\int_{-L}^{l} \left(N^2 \exp(-2\alpha r^2) r^4 (L^2 - x^2)(L^2 - y^2)(L^2 - z^2)\right) dx dy dz \quad (7)$$

$$\langle V \rangle = \frac{\langle \psi | V | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\int_{-L}^{L}\int_{-L}^{L}\int_{-L}^{l} \psi \frac{-e^2}{\varepsilon(r) r} \psi dx dy dz}{P} =$$

$$\frac{\int_{-L}^{L}\int_{-L}^{L}\int_{-L}^{l} \frac{-e^2}{\varepsilon(r) r} \left(N^2 \exp(-2\alpha r^2) r^4 (L^2 - x^2)(L^2 - y^2)(L^2 - z^2)\right) dx dy dz}{P} \quad (8)$$

When the impurities are distributed randomly the Anderson localization comes into play [5,6]. Considering $P(r_i) = A\exp(-\beta r_i)$ as the probability of finding an impurity at r_i when another impurity is at the origin, the potential energy can be written as [4]:

$$V_d(r) = \left(\frac{-e^2}{\varepsilon_0 r}\right) e^{-\lambda r} + \left(\frac{-e^2}{\varepsilon_0 r}\right) e^{-\delta r} + \left(\frac{e^2\beta}{\varepsilon_0} - \frac{e^2\beta^3}{2\varepsilon_0\delta^2} + \frac{e^2\beta^2 r}{2\varepsilon_0} - \frac{e^2\beta^2 r}{2\varepsilon_0\delta}\right) e^{-\delta r} \quad (9)$$

Where $\delta = \beta + \lambda$. Therefore $V_0(r) = \frac{-e^2}{\varepsilon(r) r}$ in Eq.(5) can be replaced by $V_d(r)$ if Anderson localization is considered. In Eq. (9), β as given in ref.[6] is 0.95.

The ionization energy is given by :

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

$$E_{sub} = \left(\frac{\hbar^2}{2m^*}\right)\left(K_m^2 + K_n^2 + K_l^2\right)$$

$$K_m = \frac{m\pi}{L}, K_n = \frac{n\pi}{L}, K_l = \frac{l\pi}{L}, (m,n,l = 1,2,3,....) \quad (10)$$

III. RESULT AND DISSCUSION

The numerical results obtained by Matlab are presented in Figs.1 to 5. Fig.1 and 2 show the ionization energy as a function of the size for a cubic well and a wire with square cross section. As it is seen from the figures, the ionization energy for both, the quantum well and the wire, decreases as the size increases, and approaches to zero for the size larger than 400A°, where the well and wire indicate metallic behavior. Our results are quite similar in shape, but smaller in value, than those reported by J. Peter *et al* [4, 7] where a cosine form for the trial function has been employed.

The effects of randomness in impurity distribution, for the quantum well and wire, are given in Fig. 3 and 4,respectively. As it is seen from the figures the randomness enhances the ionization energy for both cases.

To see the effect of impurities in the ionization energy clearly, the results for the case where the donor is located at the center and where the impurities are distributed in the wire are compared and shown in Fig. (5). as it is seen from the figure the ionization energy is higher when the impurities are spread in the wire.

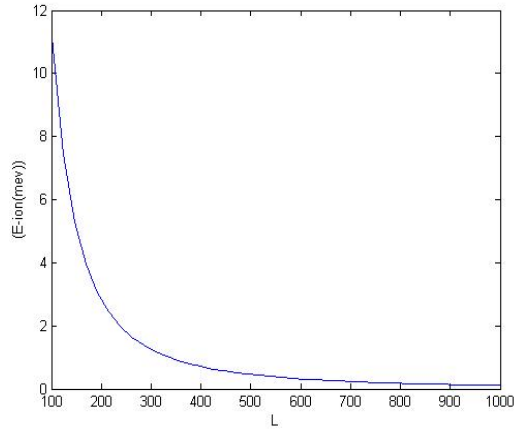

Fig.1 Variation of the ionization energy as a function of size in angstrom for a cubic well

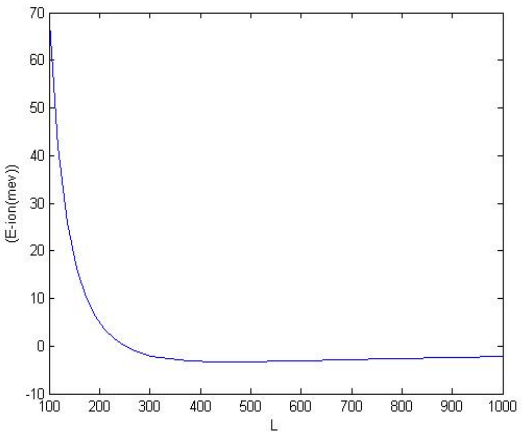

Fig.2. Variation of the ionization energy as a function of size in angstrom for a square wire

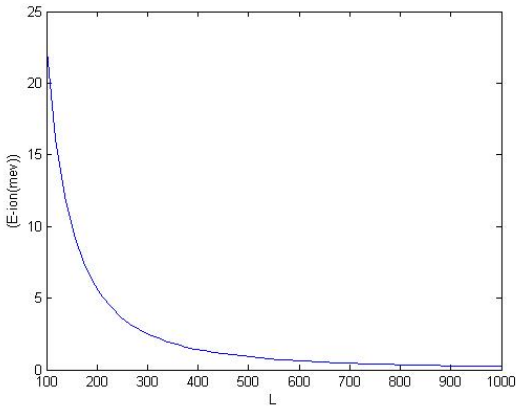

Fig.3 Variation of ionization energy as function of size in angstrom for cubic well in presence of impurities.

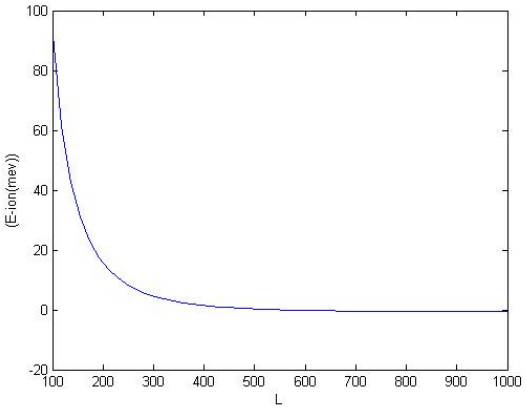

Fig. 4 Variation of ionization energy as function of size in angstrom for square wire in presence of impurities.

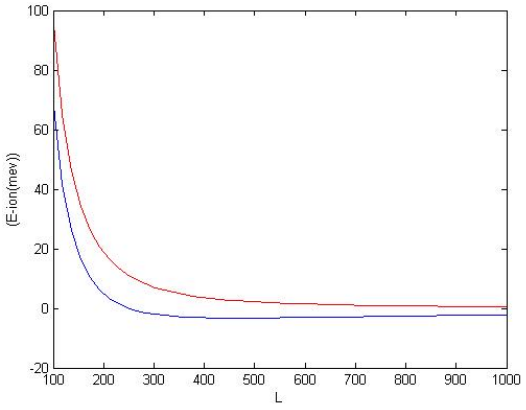

Fig. 5 The effect of confinement of the carrier in quantum wire. for random impurity distribution $(V_d(r))$ and screened potential without considering the random distribution of impurities $(V_0(r))$.

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