EFFECTS OF THE CONFINEMENT AND THE ELECTRIC FIELD ON THE EXCITED STATES OF A IMPURITY IN QUANTUM DOTS WITH PARABOLIC CONFINEMENT

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ABSTRACT

In this article we present the study of some excited states of a donor shallow hydrogenic impurity in the center of a spherical GaAs-(Ga,Al)As quantum dot with potential parabolic confinement and under the influence of an electric field. Using the approach of the effective mass, inside an outline variational, we calculate the binding energy of the ground state and of the p-like states. We define the isotropic parabolic confinement $V(r) = \beta^2 r^2$ with a β parameter chosen in such a way that the resultant energy of the ground state was the same one than that of a spherical quantum dot of radius R with rectangular potential in the absence of the impurity.

INTRODUCTION

Quantum dots (QD) have revolutionized semiconductor physics and have been constituted in one of the more studied semiconductor nanoestructures [1,2]. Novel physics and important applications have emerged. Certain classes of semiconductor quantum dots being actually fabricated exhibit a nearly parabolic confinement for both the electron and the hole [3,4]. These structures show interesting physical properties which do not depend only on the degree of confinement but also on external electric fields and of impurities [5,6,7].

In this work we calculate the energy of the ground state of a spherical GaAs-(Ga,Al)As quantum dot with parabolic confinement (PQD) as well as the binding energy for few exited states of an on-center donor impurity as a function of the radius of the PQD and as a function on an applied electric field. Our calculations are made using the effective mass approximation within a variational procedure.

THEORY

The Hamiltonian associated with a hydrogenic impurity in a spherical GaAs-(Ga,Al)As PQD in the presence of an electric field may be written in spherical coordinates as:

$$H = \frac{-\hbar^2}{2m^*}\nabla^2 + \frac{1}{2}m^*\omega^2 r^2 + |e|\xi\, r\cos\theta - \frac{e^2}{4\pi\varepsilon_0\varepsilon\, r} \qquad [1]$$

where m^* is the electronic effective mass in the PQD, ω is the parabola frequency, ε_0 is the vacuum permittivity, ε is the relative permittivity of the PQD material and ξ is the external electric field applied in the z-direction.

Inclusion of the impurity into the system gives us a differential equation that cannot be solved by the separable variable method. Thus, it is necessary to use a variational

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approach to approximate the wave functions and eigenvalues implied by the Hamiltonian. We are interested in the calculation of the first few excited states thus we assume as the trial wave functions for this states

$$\psi_\lambda = \psi(r,\theta,\varphi)\,\zeta_{n\ell m}(r,\lambda_{n\ell m},\alpha_{n\ell m}) \qquad [2]$$

where:

$$\zeta_{n\ell m}(r,\lambda_{n\ell m},\alpha_{n\ell m}) = \begin{cases} e^{-\lambda_{1s} r} & \textbf{like 1s} \quad \mathbf{n=1, \ell=0, m=0} \\ (1-\alpha\, r)e^{-\lambda_{2s} r} & \textbf{like 2s} \quad \mathbf{n=2, \ell=0, m=0} \\ \mp r\, e^{-\lambda_{2\mathbf{p}\pm1} r} \sin\theta & \textbf{like 2p} \quad \mathbf{n=2, \ell=1, m=\pm 1} \\ r\, e^{-\lambda_{2\mathbf{p0}} r} \cos\theta & \textbf{like 2p} \quad \mathbf{n=2, \ell=1, m=0} \end{cases} \qquad [3]$$

The numbers n, l and m are the quantum numbers. In this work we consider n = 1,2 with l = 0,1 and m = -1,0,1. Here the λ_{nlm} , α_{nlm} are variational parameters and the respective values are calculated by requiring that the $\zeta_{n\ell m}(r,\lambda_{n\ell m},\alpha_{n\ell m})$ form a set of orthogonal functions in all space. The binding energy of a hydrogenic impurity, E_b, is defined as the energy of the ground state without the impurity, E_0, less the energy of the state considering the presence of the impurity:

$$E_b = E_0 - min_\lambda \frac{\langle \psi_\lambda | H | \psi_\lambda \rangle}{\langle \psi_\lambda | \psi_\lambda \rangle} \qquad [4]$$

where min_λ means the minimun value of the energy of the impurity with respect to the respective variational parameter.

To calculate the second term of this expression we write the Hamiltonian and the wave function in reduced atomic units, which corresponds to an effective Rydberg (unit of energy) and an effective Bohr radius (unit of length):

$$\tilde{H} = -\tilde{\nabla}^2 + \tilde{\beta}^2\, \tilde{r}^2 + F\, \tilde{z} - \frac{2}{\tilde{r}} \qquad [5]$$

$$\psi_\lambda = Exp\left[-\frac{F^2}{8\tilde{\beta}^3} - \frac{F\,\tilde{r}\cos\theta}{2\tilde{\beta}} - \frac{\tilde{\beta}\,\tilde{r}^2}{2} \right] \zeta_{n\ell m}(\tilde{r},\tilde{\lambda}_{n\ell m},\tilde{\alpha}_{n\ell m}) \qquad [6]$$

where $\tilde{r}^2 = \frac{r^2}{a^{*2}}$, $F = \frac{\xi}{R_y^* / e\, a^*}$, $\tilde{\lambda} = a^*\lambda$ and $\tilde{\beta} = a^{*2}\beta$.

The isotropic parabolic confinement $V(r) = \beta^2 r^2$ is defined with a β parameter chosen in such a way that the resultant energy of the ground state is the same than that of a spherical quantum dot of radius R with rectangular potential, V_b (eV) = 1.247x for

R>r, x = 0.3. The binding energy of ground and exited states are obtained numerically by means of the equations above and the possible infrared transitions are conditioned by $\Delta l = \pm 1$ and the respective energies are obtained from $(E_b(n,l)- E_b(n^{'},l'))$.

RESULTS

Our results are presented in reduced atomics units, which corresponds to an effective Bohr radius as the unit of length and to an effective Rydberg as the unit of energy. The effective mass for shallow donor impurities is $m^* = 0.0665m_e$, where m_e is the free-electron mass. For donor impurities these atomic units are $1\ a^* \sim 100$ Å and $1\ Ry^* \sim 5.72$ meV, respectively.

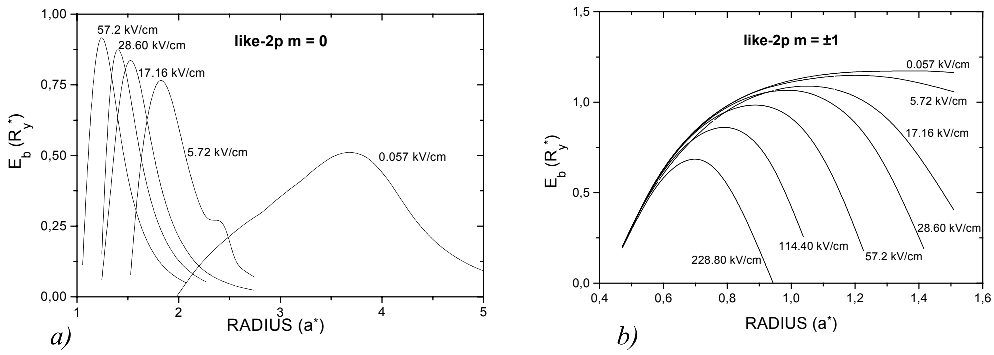
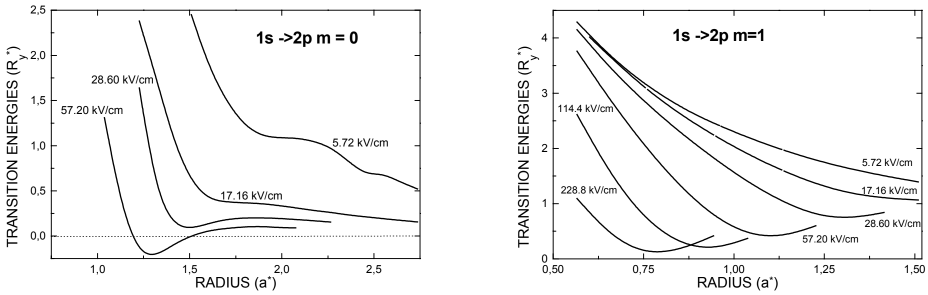


Figure 1. a) Binding energy -2p m = 0 like state and b) 2p m = ± 1 like state as a function of the radius for different values of the applied electric field.

In the figure 1.a, we show the binding energy 2p m = 0 like state as a function of the radius for different values of the applied electric field. As the electric field increases, the 2p m = 0 state is more bounded for PQD with radius small and their maximum increases.

In the figure 1.b, we show the binding energy 2p m = ±1 like state as a function of radius for different values of the applied electric field. These states are degenerates. As the electric field increases, these 2p m = ±1 like states are bounded but for PQD with radius smalls.

In the figure 2.a, we display the infrared transition energies 2p m = 0 like state as a function of radius for different values of the applied electric field. It is observed that these energies increase with the PQD confinement. Also, these energies decrease with the applied electric field. Note that for PQD with radius in the interval ($1.2\ a^*$, $1.5\ a^*$) and electric field equal a 57.20 kV/cm, the transition energies are negative. This means that transition is reversed and occurs from a 2p m = 0 to a 1s like state. The behaviors of these graphics show that this phenomenon is also observed for electric field bigger than that 57.20 kV/cm.



a. b.

Figure 2. a) Infrared transition energies 2p m = 0 like state and b) Infrared transition energies 2p m = ±1 like state as a function of radius for different values of the applied electric field.

In the figure 2 b, we show the infrared transition energies 2p m = ±1 like state as a function of radius for different values of the applied electric field. It is observed that these energies increase with the PQD confinement. Also, these energies decrease with the applied electric field and not are observed transition energies negatives for electric fields until 228.8 kV/cm

CONCLUSIONS

We have calculated the binding energy and the transition energies of some excited states of a donor impurity in a spherical GaAs-(Ga,Al)As quantum dot with parabolic confinement as a function of the radius of the quantum dot and as a function of the intensity of an applied electric field. Our results show that the electric field produces variations in the donor binding energy of the 1s and 2p like states. We found that the binding energy for the 1s state increase with quantum confinement and diminish with the applied electric field. The electric field is determinant for the existence of bound donor impurity excited states and resolve the degenerancy for 2p like states. Also, we found some reverse transition between 1s and 2p m = 0 like states.

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