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Effect of the parabolic confinement potential on the binding energy of a donor in a double-step barrier quantum dot

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Abstract The effect of the parabolic confinement potential due to electrons on the binding energy of a donor impurity centered in a double-step potential barrier quantum dot has been investigated within the effective mass approximation, as a function of the dot radius(R). Calculations are performed for several states using a numerical method both with and without the parabolic confinement potential. The results show that as the dot radius increases, the effect of the parabolic potential depends very much on the state and is quite complex.

Keywords Quantum dot, donor impurity, confined systems

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1. Introduction

In recent years, there has been a great deal of interest in studying the properties of hydrogenic impurities in quantum dots. An understanding of the physics of impurity states in semiconductor quantum-dot structures is important for several device applications. A number of investigations on the binding energy of hydrogenic impurities in spherical quantum dots have been reported during the last few years [1-14]. Usually, the barrier potential is taken to be infinite beyond the radius of the quantum dot.

Recently, Betancur, Mikhailov and Oliveira [15] have calculated energies of the ground and some excited states of on-centre donors (D^0) in spherical quantum dots, within the effective mass approximation, as functions of the dot radius and for different potential shapes. They used a trigonometric sweep method for a numerical solution of the radial Schrödinger equation in a quantum dot with any arbitrary spherical potential. One of the potential barriers considered by these authors is relevant for a structure consisting of a GaAs quantum dot surrounded by two concentric spherical layers of $Ga_{0.7}Al_{0.3}As$ and $Ga_{0.55}Al_{0.45}As$. Such structures have been discussed to obtain a high optical nonlinearity for inter-band and inter-sub-band transitions [16]. For such a structure, Betancur *et al* [15] have represented the barrier potential by a double-step barrier model which consists of a small rectangular potential inside a large rectangular potential. These authors have calculated the properties of the D^0 shallow donors in a quantum dot with such a double-step potential barrier and two peaks in the binding energy were found, which is quite interesting.

The question of the confining potential of electrons in a quantum dot was considered by Kumar, Laux and Stern [17] who self-consistently calculated the electron states in GaAs / AlGaAs heterostructures with confinement in all three dimensions and they found that the evolution of levels with increasing magnetic field is similar to that found for a parabolic potential. Thus, the confinement potential due to electrons could be described by a simple one-parameter adjustable parabolic potential. Peeters [18] pointed out that this is a consequence of the generalized Kohn theorem which is valid for a harmonic confinement potential.

It was of interest to examine the effect of the parabolic confinement potential due to electrons on binding energies in a structure like that of a GaAs quantum dot surrounded by two concentric spherical layers of $Ga_{0.7}Al_{0.3}As$ and $Ga_{0.55}Al_{0.45}As$, which has been considered by Betancur *et al* [15] and for which the double-step potential barrier model is valid.

In the present paper, we first present results on the binding energies of several states of an on-centre hydrogenic donor in such a quantum dot structure as a function of the radius of the dot, taking into account the Coulomb potential and the double-step potential barrier. Next, we obtain results on the binding energies taking into account the parabolic confining potential due to electrons also. The difference between the two binding energies gives the contribution due to the parabolic potential. The behaviour of this contribution is studied as a function of the radius of the dot.

2. Theory and calculations

We shall use atomic units such that the unit of length is the reduced Bohr radius $a_0 = \hbar^2\varepsilon_0/m^*e^2$, and the unit of energy is reduced Rydberg $Ry = m^*e^4/2\hbar^2\varepsilon_0^2 = e^2/2\varepsilon_0 a_0$. Here, m^* is the effective mass and ε_0 is the dielectric constant of the material of the quantum dot. In these units, the Hamiltonian can be written as

$$H = -\nabla^2 - \frac{2}{r} + \gamma_p^2 r^2 + V_0 \qquad (1)$$

where $\gamma_p = \hbar\omega_p/2\ Ry$, ω_p being the harmonic oscillator frequency. V_0 is the double-step spherical rectangular barrier potential used by Betancur *et al* [15], which is as follows :

$$V_0 = 0 \text{ for } r \le 0.3R$$
$$= 40\ Ry \text{ for } 0.3R < r < R$$
$$= 80\ Ry \text{ for } r > R. \qquad (2)$$

We have calculated the eigenenergies by numerical integration of the Schrödinger equation using Numerov's method and the logarithmic mesh for the $1s$, $2s$, $2p$, $3s$ and $3p$ states of the donor. To see the effect of the confining potential due to electrons, two sets of calculations were carried out: without the $\gamma_p^2 r^2$ term and with it. The value of γ_p is usually considered to be less than 1. Here we have taken two values of γ_p, namely 0.4 and 0.8. The $\gamma_p^2 r^2$ term was assumed to be zero for $r > R$. Calculations were carried out for a large number of values of R.

3. Results and discussion

The binding energy E_b of the impurity is defined as the energy of the system without the impurity present E_0, minus the energy with the impurity (E) :

$$E_b(n, \ell) = E_0(n, \ell) - E(n, \ell). \qquad (3)$$

First we consider the case when there is no confinement due to electrons. In Figure 1, we show the binding energies for the $1s$, $2s$ and $3s$ states, and in Figure 2 for the $2p$ and $3p$ states as a function of R. Betancur *et al* [15] have obtained results for $1s$, $2s$ and $2p$ states (their Figure 8). Our results for these states fully confirm theirs except on one important point. The curve labelled $2p$ in their Figure 8 is actually for the $2s$ state, and similarly the one labelled $2s$ is actually for the $2p$ state. Our Figure 1 shows two peaks for the $1s$ and $2s$ states, but the behaviour of the $3s$ state is more complicated. There are two close peaks, followed by a minimum and a peak and then the binding energy continues to decrease. It will be noticed in Figure 2 that $2p$ and $3p$ states show a similar behaviour, both having two peaks.

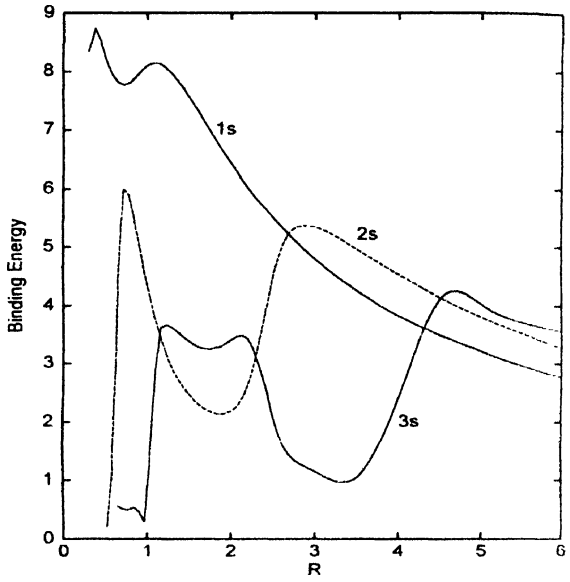

Figure 1. Binding energies for the $1s$, $2s$ and $3s$ states as a function of the radius R. The curve for the $2s$ state has been drawn with broken lines for the sake of clarity.

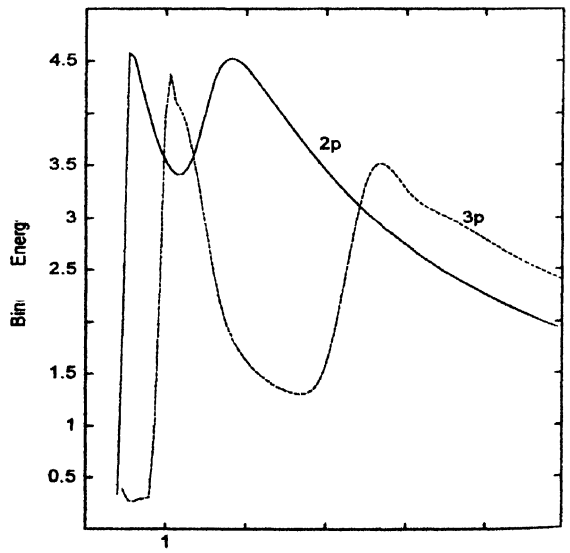

Figure 2. Binding energies for the $2p$ and $3p$ states as a function of the radius R. The curve for the $3p$ state has been drawn with broken lines for the sake of clarity.

Next, we consider the effect of the parabolic confinement potential due to electrons on the binding energy. We define the binding energy difference, ΔE, as follows:

$$\Delta E = E_{bp}(n,\ell) - E_b(n,\ell), \tag{4}$$

where $E_{bp}(n,\ell)$ is the binding energy when the confining potential due to the electrons is included and $E_b(n,\ell)$ is the binding energy without it.

We show ΔE as a function of R in Figure 3 for $1s$ and $2s$ states for $\gamma_p = 0.4$, and in Figure 4 for the $2p$ state for $\gamma_p = 0.4$.

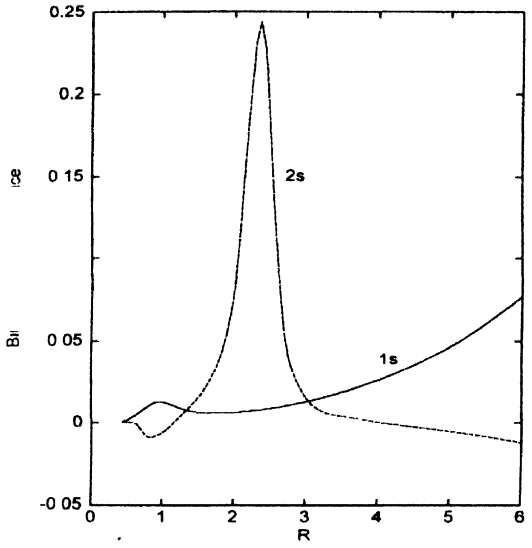

Figure 3. Binding energy difference ΔE for the $1s$ and $2s$ states as a function of R for $\gamma_p = 0.4$. The curve for the $2s$ state has been drawn with broken lines for the sake of clarity.

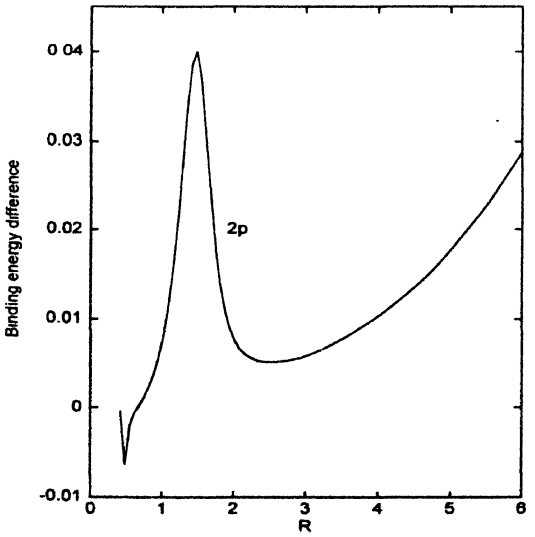

Figure 4. Binding energy difference ΔE for the $2p$ state as a function of R for $\gamma_p = 0.4$.

It will be noticed from Figure 3 that $1s$ state shows a small maximum at $R \simeq 1$ and then ΔE continues to increase with R. In the case of $2s$ state, ΔE at first, shows a shallow minimum at $R \simeq 0.9$ followed by a sharp peak and then it continues to decrease. Figure 4 shows that for $2p$ state, ΔE shows a sharp and narrow minimum, followed by a sharp peak at $R \simeq 1.5$ and then it continues to increase. Thus, we see that the effect of the parabolic potential depends very much on the state and is quite complex. The results for $\gamma_p = 0.8$ qualitatively show a very similar behaviour; quantitatively they are of course different.

4. Conclusions

We have investigated the effect of the parabolic confinement potential due to electrons on the binding energies of $1s$, $2s$ and $2p$ states of a donor impurity centered in a double-step potential barrier quantum dot within the effective mass approximation, as a function of the dot radius. The results show that as the dot radius increases, the effect of the parabolic potential depends very much on the state and is quite complex.

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