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ELECTRON AND HOLE CONFINEMENT STATES IN QUANTUM DOT DISC

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The ground-state energies of an electron and of a hole in a finite-potential quantum dot disc of GaAs are calculated. Solving the Schrödinger equation for the two particles separately, we calculated the first two excited states for each one. To study the effect of the disc dimensionality on the eigen-energies, we considered different discs with different values of radius (R) and width (L). Discussing the potential effect, we examined the eigen-value behaviour at different values of the barrier heights. The corresponding wave functions are obtained.

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1. *Introduction*

Recent progress in crystal growth and process techniques has made it possible to realize zero-dimensional systems such as clusters and nano-crystallites. In these structures, ultimate quantum confinement effects restrict the motion in three spatial directionsof the optically excited electrons and holes. As a consequence, free-particle energy levels are quantized and Columbic correlation effects [1] are enhanced. For the last ten years, it has been possible to process a new class of spherical quantum dots (QDs) called quantum dot discs - quantum well or inhomogeneous quantum dots (IQDs) composed of two semiconductor materials. One of them, that with the smaller bulk band gap, is embedded between a core and outer shell of the material with the larger band gap. These structures can exhibit some remarkable and interesting phenomena associated with the redistribution of the electron and hole wave functions, such as an increase in the band-edge absorption when the shell material has a small band gap and a rapid change in the luminescence efficiency. The original characteristics of these structures are that their physical properties can be controlled and adjusted by changing the core diameter, the thickness of the well and the size of the outermost shell.

Self-assembled quantum dots have much to offer in theoretical studies of these structures. First, they are small with a lateral extent of ~ 20 nm [2], which cannot be realized lithographically. This small lateral size leads to large quantization energies, typically tens of meV. The Coulomb interaction energy between two particles confined in such a dot can be smaller than the quantization energy, which means that a quantum mechanical description of the Coulomb effects is important. Second, the dots are highly homogeneous, so that simultaneous charging of as many as 10^6 dots has been achieved [3,4]. This is ideal for optical experiments.

Recently, there has been a lot of work on obtaining analytic or semi-analytic results for various QD shapes. The latter is often done using an infinite barrier; this approximation is valid for electron states in large-radii QDs. One goal of the recent work is to obtain a better physical picture of the QD disc and explore the effect of both the disc dimensionality and finite-barrier potential on electron and hole energy levels, consequently, the optical properties of the QDs (to be discussed in our future paper). As a recent example of the latter methodology, Cantele et al. [5] discovered topological surface states in spheroidal QDs, while some of other shapes considered so far are spheres [6], cones [7] and rectangles [8].

In the present work, we study the excited states of an electron and of a hole in a quantum dot disc, using the effective-mass approximation with a finite confinement-potential model. Varying the radius (R) and width (L) of the quantum dot disc, the quantum disc arrangement allows one to systematically explore the various limiting situations of the quantum dot ($R < a_\mathrm{B}$ and $L < a_\mathrm{B}$, where a_B is the 3-D electron Bohr radius). Consequently, the corresponding wave functions are calculated.

2. *Theoretical model*

In the effective-mass approximation, we write Schrödinger equation for single particle in 2D as

$$\left(- \frac{\hbar^2}{2m^*} \nabla^2 + V_1(\boldsymbol{r}) \right) f(\boldsymbol{r}) \quad = \quad E_1 f(\boldsymbol{r}). \tag{1}$$

By 2D we mean the in-plane coordinates, i.e x and y. The z direction is considered separately as Schrödinger equation in 1D

$$\left(- \frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial z^2} + V_2(z) \right) g(z) \quad = \quad E_2 g(z). \tag{2}$$

Before we proceed, we should mention that the electron and the hole confined states in QD were solved recently by Willatzen et al. [9]. He used parabolic cylinder coordinates and solved Schrödinger equation for QD in such coordination system, but for the infinite barrier. Considering the confinement potentials V_1 and V_2 (defined by Eq. (5)), the solutions of Eqs. (1) and (2) are of the form [10]

$$F(r) = \begin{cases} J_0(\theta r) & \text{for} \quad r \le R \\ BK_0(\beta r) & \text{for} \quad r > R \end{cases}, \tag{3}$$

and

$$g(z) = \begin{cases} \cos(Mz) & \text{for} \quad |z| \le L/2[4] \\ A\exp(-q|z|) & \text{for} \quad |z| > L/2. \end{cases} . \tag{4}$$

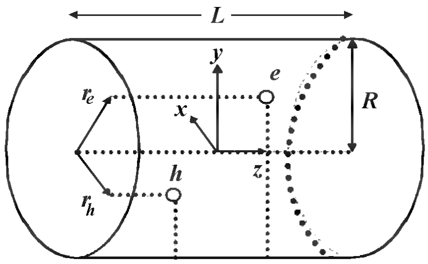

Fig. 1. The various coordinates in the quantum disc. The r's denote the in-plane coordinates, and the z's denote the positions along the disc axis.

Figure 1 describes the quantum dot disc and its dimensions R and L. Considering the cylindrical coordinates in which ∇^2 is given by

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}.$$

Therefore, Eq. (1) becomes

$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + D\right) f(r) = 0,$$

where, $D = \theta^2$ (if $r \le R$) and $D = \beta^2$ (if $r > R$), where β is a complex quantity, and it is the argument of second-order modified Bessel function K_0, ($\beta^2 = (2m^*/\hbar^2)(V_0 - E_1)$). Here, we define J_0 as the zero order Bessel function with the argument $\theta^2 = (2m^* E_1/\hbar^2)$. A and B are constants and will be determined from the continuity of the first derivatives of the wave functions at the boundaries, $M^2 = (2m^* E_2/\hbar^2)$, and $q^2 = (2m^*/\hbar^2)(V_0 - E_2)$.

The confinement potentials in QDs can possess various shapes depending on their origin and on the QDs structures [11]. The confining potential in self-assembled QDs, where stems from the band offsets and can be modified by both the alloying [12] and the strain effects [13]. Therefore, we used the rectangular potential well

$$V = \begin{cases} 0 & \text{if} \quad r < R \quad \text{and} \quad |z| < L/2 \\ V_0 & \text{otherwise} \end{cases} . \qquad (5)$$

As proposed in Ref. [10], for the full 3D motion the product of the two functions given by Eqs. (3) and (4) is no longer a solution of the 3D effective-mass Schrödinger equation since the actual 3D finite confinement potential is not the sum of V_1 and V_2, but

$$V = V_1(\boldsymbol{r}) + V_2(z) + \delta V(\boldsymbol{r}, z),$$

where, δV equals zero inside the well, and has the value $-V_0$ outside. It follows that the ground-state energy of a confined particle in QD disc with finite potential can be

$$E = E_1 + E_2 - \langle \delta V \rangle .$$

Applying the boundary conditions, we obtain the following transcendental equation

$$J_0(\theta R) K_0'(\beta R) - J_0'(\theta R) K_0(\beta R) = 0, \qquad (6)$$

where $J_0'(\theta r) = -\theta J_1(\theta r)$, but for $K_0'(\beta r)$ we use the derivation of the series formula for $K_0(\beta r)$. The numerical solutions of Eq. (6) were evaluated using our own computer programs in the Matlab language, to obtain the electron or the hole eigen-energy (E_1) in the plane direction. The corresponding transcendental equation along the disc axis (z) is given by

$$M \sin(ML) - q \cos(ML) = 0. \qquad (7)$$

The first solutions of Eqs. (6) and (7) represent the ground-state energies of the particle in the in-plane (E_1) and along the disc axis (z) directions (E_2), respectively. The higher solutions correspond to the excited energies.

3. Results and discussion

The calculations in this work consider a self-assembled artificial atom confined in a cylindrical disc manufactured of the semiconductor material GaAs. In further calculations, we apply the material parameters of GaAs embedded in $Al_{0.4}Ga_{0.6}As$. That implies that $V_0 = 0.324$ eV in the case of an electron with effective mass $m_e^* = 0.0665$, and hole-confinment potential equal to 0.1746 eV with the effective hole mass of $m_h^* = 0.34$. The dielectric constant is $\varepsilon = 13.18$.

The numerical solution of the transcendental equation (6) is shown in Fig. 2. In the figure, we plot the ground-state energy of the electron as a function of the QD

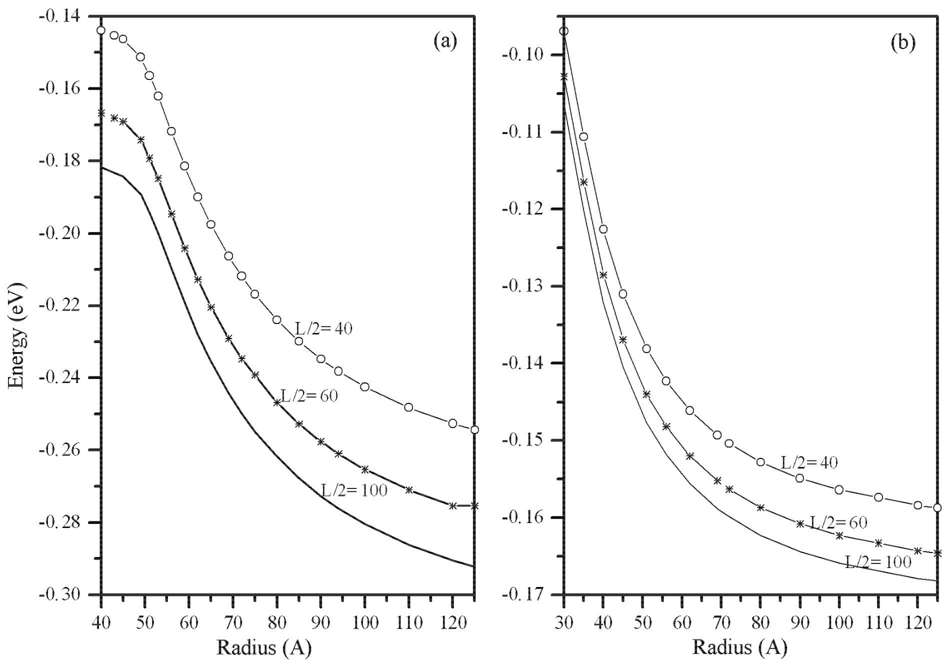

Fig. 2. (a) The electron ground-state energy (eV) *vs. disc radius R for three values of disc width,* $L/2 = 40$*, 60 and 100* Å. (b) The hole ground-state energy for the same three values of $L/2$.

radius (R) in Å. These values are calculated at three different values of the disc width $L/2 = 40$, 60 and 100 Å. As we see in Fig. 2(a), the ground-state energy of the confined particle in QD has large values at small radius and width. That is to say, in the range R and $L <$ effective Bohr radius ($a_{\rm B} = 125.4$ Å), a large value of the ground-state energy is obtained.

The eigen-values of Eq. (7) give the carrier's ground-state energy along the z-direction. The results are displayed in Fig. 3. We further applied different value of the potential V_0. Fig. 3(a) represents the electron ground-state energy at $V_0 = 0.324$ and 0.3566 eV. We notice that the electrons become more confined when the Al concentration is increased in the QDs. Similarly, it is also the case for the hole (see Fig. 3b).

The variations of the ground-state energy as a function of the disc width (L) are depicted in Figs. 4a and b for both particles. Here we can say the same as for Fig. 2, the particle ground-state energies in QD disc increase at small values of both the radius R and the width L. Before we proceed, we notice from Figs. 2 and 4 that doubling the value of R causes an approximate decrease by 96 meV in the ground-state energy of the electron, while doubling the value of L results in a decrease by 35 meV, i.e., the electron ground-state energy does not depend

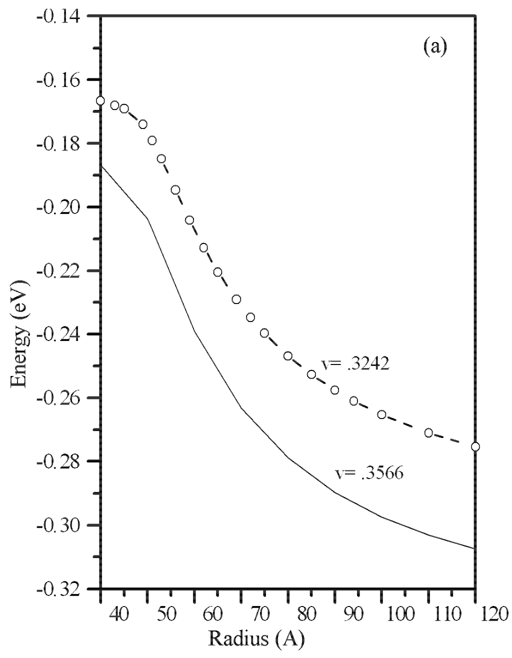

Fig. 3. (a) The electron ground-state energy as a function of radius R, for two values of the confinement potential V = 0.3242 and 0.3566 eV*, where* $L/2 = 60$ Å. (b) The same for the hole but at $V = 0.1746$ and 0.192 eV, and also $L/2 = 60$ Å.

strongly on the value of L. Here, we would like to add that the ground-state energy of the electron remains fairly constant for different values of $R > 80$ Å, and for $R > 60$ Åin case of the hole (Fig. 2). Similarly, in Fig. 4, the ground-state energy of both almost remains constant for values of $L > 100$ Å. Fig. 5a displays the energies of the ground-state and the first two excited states of the electron. The three curves were calculated for $L/2 = 90$ Å and $V_0 = 0.324$ eV. Figure 5b shows the hole ground and excited states for $V_0 = 0.1746$ eV and the same value of L. The qualitative behaviour of the excited-state energy levels is similar to that of the ground-state energy. We notice from Fig. 5a that for the QD disc with a small radius $R < 50$ Å, some excited states cease to be bound. Figure 5b shows that the hole excited states cease to be bound for $R < 30$ Å.

From Figs. 5 we notice the presence of bumps in the excited-state energy plot. We may refer these bumps to the following two reasons: First, due to the quantum-size effect because they appear at very small values of R (at $R < 50$ Å). In such geometrical constraints, carriers (electron or hole) feel the presence of the particle boundaries and respond to change their energy. Secondly, the e-h recombination energy is not released as a photon but is transferred to a third particle (an electron or a hole) that is re-excited to a higher energy state. Lastly, we display the ground-

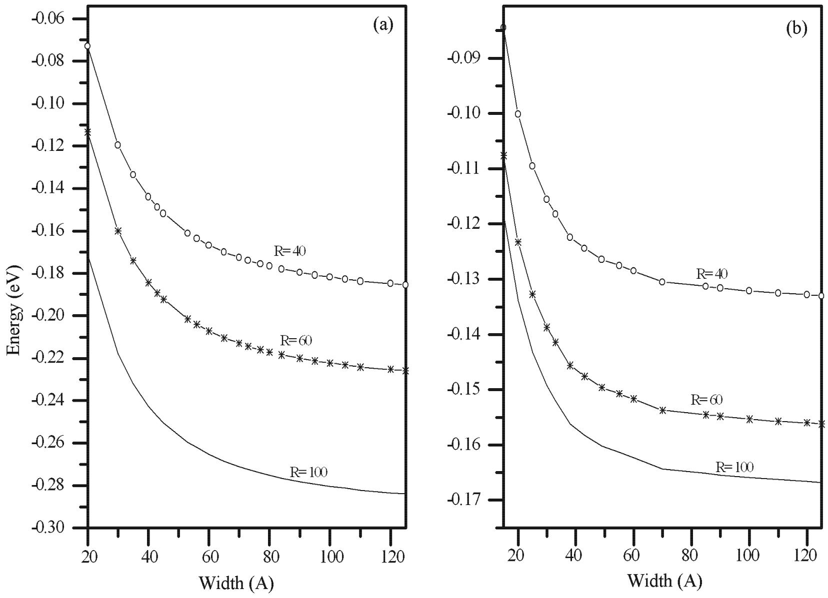

Fig. 4. (a) The electron ground-state energy as a function of the disc width $L/2$ *for three values of radius* $R =$ *40, 60 and 100* Å. (b) The hole ground-state energy for the same three values of R.

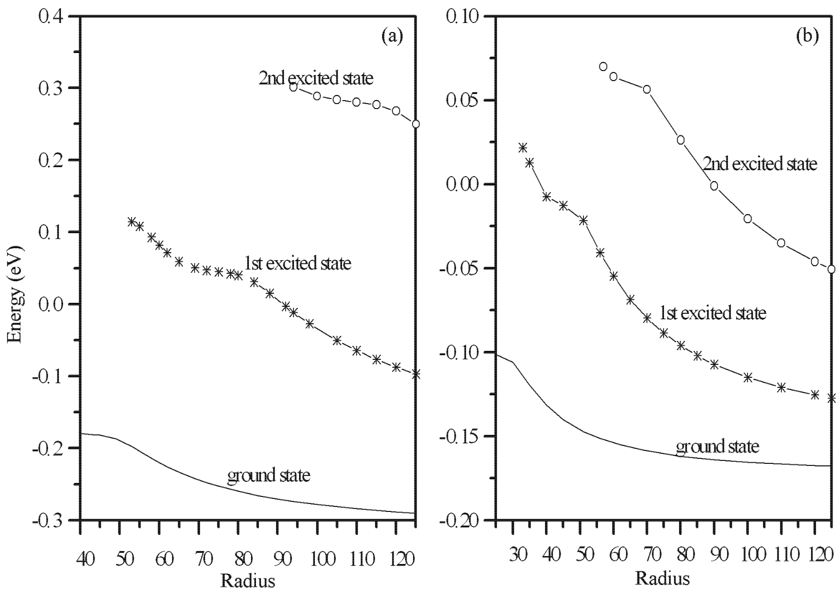

Fig. 5. (a) The electron ground and the first two excited states as a function of R *for* $L/2 =$ *90* Åand $V = 0.3242$ eV. (b) The hole ground and the first two excited states for the same values of $L/2$ and $V = 0.1746$ eV.

state and the first-excited-state of the electron wave function amplitudes squared, $(|f(r)g(z)|^2)$, in Fig. 6 as functions of R and z.

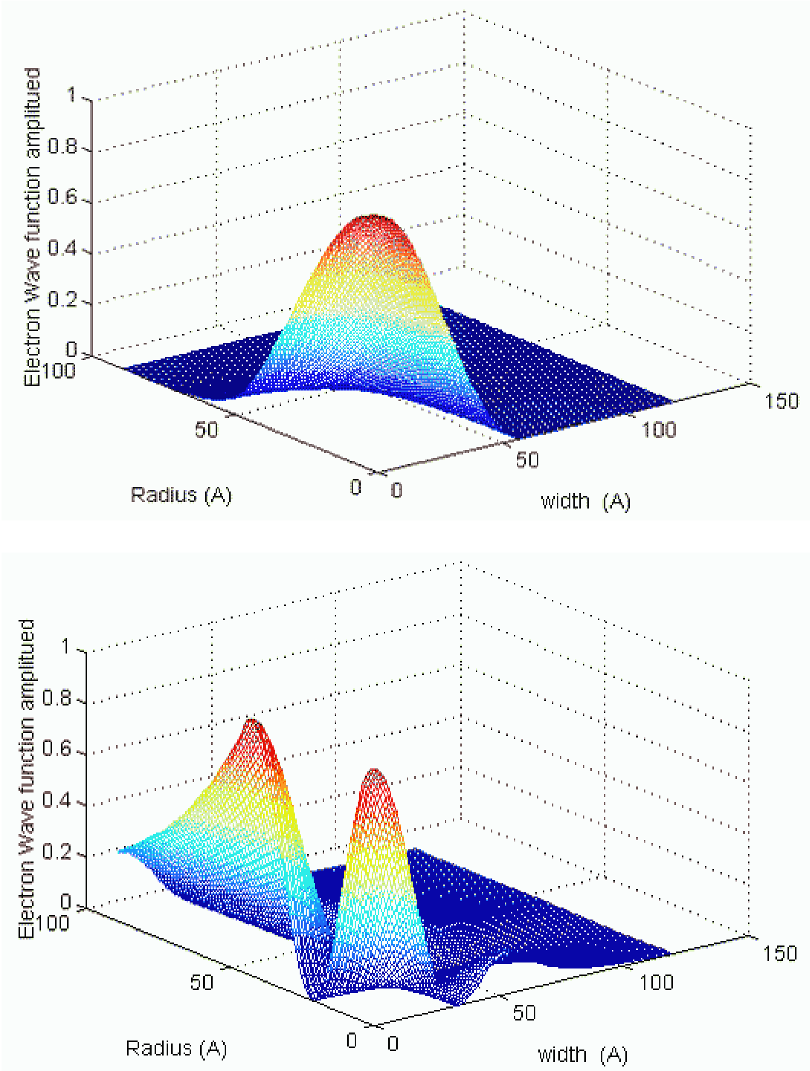

Fig. 6. (a, top) The electron ground-state wave function amplitude squared as a function of R and z. (b) The same as in (a) but of the electron first excited state.

3.1. Comparing our results with recent data

We carried out our calculation for the similar QD as in Ref. [14] where Ciurla et al. proposed a modeling of the confinement potentials in QDs as a power exponential potential, given by $V = V_0 \exp\{-(r/R)^p - (|z|/L)^p\}$. When the parameter "$p$" tends to infinity, the confinement potential in Ciurla's model is $V = V_0$ outside the well (at the boundaries) as in our model. We obtained a reasonable result, in agreement with the results of Ciurla et al. The deviation between our results and Ciurla's model does not exceed 3% for the ground states, and we also obtained reasonable agreement for the excited states. We refer that deviation to his limit of the parameter p at $p = 100$. For higher values of p (i.e., more than 100), the deviation would be smaller.

4. Conclusion

The ground and excited states for an electron confined in QD disc made of GaAs and embedded in $Al_{0.4}Ga_{0.6}As$ material, with finite potential, have been calculated numerically. Similar calculations were carried for the hole. The ground and the excited-state energies depend on the dimensions of the quantum dot and the confinement potential. We find a strong dependence on the quantum dot disc width (L), but weaker dependence on the radius (R). Both the ground and excited states show qualitatively the same behaviour. The eigen-states of the two particles are determined as a function of the disc radius and width. A good agreement between our results and that of Ref. [14] model has been obtained.

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VEZANA STANJA ELEKTRONA I ŠUPLJINE U VALJKASTOJ KVANTNOJ TOČKI

Izračunali smo energije osnovnih stanja elektrona i šupljine u konačnom potencijalu valjkaste kvantne točke u GaAs. Rješavanjem Schrödingerove jednadžbe posebno za svaku od čestica, izračunali smo prvo i dva viša stanja za svaku česticu. Radi proučavanja učinka veličine valjka na svojstvene energije, razmatrali smo valjke različitih polumjera i duljine. Razmatrali smo utjecaj potencijala ispitivanjem ovisnosti svojstvenih vrijednosti za tri vrijednosti visine barijere. Izveli smo odgovarajuće valne funkcije.