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EXACT SOLUTION OF FINITE PARABOLIC POTENTIAL DISC-LIKE QUANTUM DOT WITH AND WITHOUT ELECTRIC FIELD

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The exact series solutions of finite parabolic potential disc-like quantum dot are given in the absence and presence of uniform applied electric field. We define some normalized parameters. From the complex eigenenergy $E = E_0 - i\Gamma/2$, due to the electric field, we calculate the resonance width Γ of a bounded state. The ground and the first excited state of the electron and the hole are obtained with and without the electric field. The corresponding envelope functions are presented as a function of the disc dimensionality, radius R and half-width L.

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Keywords: quantum dot, finite parabolic potential, uniform applied electric field, complex eigenenergy, resonance width, electron and the hole states

1. *Introduction*

Semiconductor quantum dots have attracted a lot of attention in recent years [1 – 5]. Due to their atomic-like spectra, they are interesting for future applications as well as for basic research activities. In quantum dots, the ultimate quantum confinement effects restrict the motion of optically excited electrons and holes in three spatial directions. As a consequence, the free particle energy levels are quantized. For the last ten years, it has been possible to process a new parabolic quantum dot disc.

GaAs and its lattice-matched heterojunction have received considerable attention in view of the efficient emission of coherent light. GaAs technology is quite mature and a large number of optoelectronic and electronic devices have been made using this material.

Up to now, theoretical studies that have been devoted to the parabolic potential in quantum dot disc are very rare. Most of these studies consider the spherical quantum dot [6 – 8]. Even the previous treatments of the quantum dot disc considered the infinite [9,10] and constant value [11] of the confinement potential inside the dot .

In the present paper, we find solutions of the Schrödinger equation for the electron and the hole, confined in a parabolic disc-like quantum dot, manufactured of GaAs semiconductor material. First, we determine the electron and the hole ground state without the electric field and we compare our results with those existing in the literature [11]. Then, we investigate the influence of a uniform electric field on the ground and the first excited states, and on the redistribution of the electron and the hole wavefunctions. The paper is organized as follows: in Section 2, we describe the essential features of the theory and some details of our series calculations, the results are given in Section 3 and in Section 4 we give our conclusion.

2. Theory

Consider an electron with charge $-|e|$ and effective mass m_e^* in a parabolic potential disc-like quantum dot of radius R, half-width L, and depth V_0 in the presence of a uniform electric field F along z-direction as shown in Fig. 1. The time-independent Schrödinger equation for such a system is given by

$$-\frac{\hbar^2}{2m_i^*}\nabla_i^2\psi(r_i) + V_0\left(\frac{r_i}{R}\right)^2\psi(r_i) = E^{\parallel}\psi(r_i)\,, \qquad |r_i| \le R\,, \tag{1}$$

and in the z-direction, we have

$$-\frac{\hbar^2}{2m_i^*}\frac{\mathrm{d}^2\psi(z_i)}{\mathrm{d}z_i^2} + \left[V_0\left(\frac{z_i}{L}\right)^2 + |e|Fz_i\right]\psi(z_i) = E^{\perp}\psi(z_i)\,, \qquad |z_i| \le L\,. \tag{2}$$

Schrödinger equations outside the dot in the in-plane and z-direction are given by

$$-\frac{\hbar^2}{2m_i^*}\nabla_i^2\psi(r_i) + V_0\psi(r_i) = E^{\parallel}\psi(r_i)\,, |r_i| > R\,, \tag{3}$$

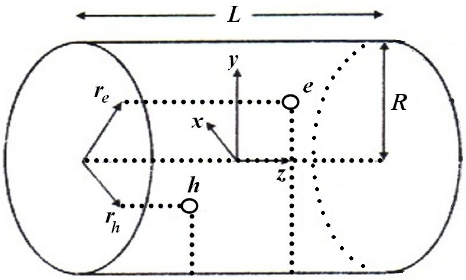

Fig. 1. The various coordinates in the quantum disc. The r's denote the in-plane coordinates and the z's denote the positions along the disc axis.

$$-\frac{\hbar^2}{2m_i^*}\frac{\mathrm{d}^2\psi(z_i)}{\mathrm{d}z_i^2} + \big[V_0 + |e|Fz_i\big]\psi(z_i) = E^{\perp}\psi(z_i)\,, \big|z_i\big| > L\,. \tag{4}$$

If we name $V_1(r) = V_0(r/R)^2$ and $V_2(z) = V_0(z/L)^2$, the actual 3-D finite confinement potential is not straightforwardly the sum of $V_1 + V_2$. Using the perturbation approach suggested by Le Goff [13], we write the 3D finite parabolic confinement potential as $V = V_1(r) + V_2(z) + \delta V(r, z)$, which is treated as a perturbation potential. Here

$$\delta V \quad = \quad \begin{cases} V_1 + V_2, & \text{if } r < R \;\text{ and }\; |z| < L \\ \\ -V_0, & \text{otherwise} \end{cases} \,.$$

In the cylindrical coordinates, we used $\nabla^2 = \partial^2/\partial r_i^2 + (1/r_i)\partial/\partial r_i$, where i stands for electron or hole. Defining $r = r_i/R$ and $Z = z_i/L$, we can write the previous four equations in terms of r, Z, and the following normalized parameters, $\widetilde{V}^2 = 2m^*R^2V_0/\hbar^2$, $\widetilde{U}^2 = 2m^*R^2E^{\parallel}/\hbar^2$, as the follows:

The in-plane solution.

$$\Psi''(r) + \frac{1}{r}\Psi'(r) + (\widetilde{U}^2 - \widetilde{V}^2r^2)\Psi(r) = 0\,, \qquad |r| \le 1\,, \tag{5}$$

$$\Psi''(r) + \frac{1}{r}\Psi'(r) + (\widetilde{U}^2 - \widetilde{V}^2)\Psi(r) = 0\,, \qquad |r| > 1\,. \tag{6}$$

We use the substitution $\xi = \widetilde{V}r^2$, and assume that $\psi(\xi) = \exp\{-\xi/2\}\phi(\xi)$. Applying this substitution into Eq. (5), we obtain the following differential equation

$$\xi\frac{\mathrm{d}^2\phi}{\mathrm{d}\xi^2} + \big(1-\xi\big)\frac{\mathrm{d}\phi}{\mathrm{d}\xi} - \frac{1}{2}\left(1 - \frac{\widetilde{U}^2}{2\widetilde{V}}\right)\phi \quad = \quad 0\,. \tag{7}$$

Equation (7) has a solution in the form of the confluent hypergeometric function [14] $M(\alpha, \beta, \xi)$, with $\alpha = (1/2)[1 - \widetilde{U}^2/(2\widetilde{V})]$ and $\beta = 1$. The solution of Eq. (6) outside the dot is the modified second order Bessel function, $K_0(qr)$, where $q^2 = \widetilde{V}^2 - \widetilde{U}^2$. Thus we may write the solution inside and outside the quantum disc as

$$\psi(r) = \begin{cases} c_1 \exp\big\{-\dfrac{\widetilde{V}r^2}{2}\big\}M(\alpha,\beta,\widetilde{V}r^2), & |r| \le 1\,, \\ \\ c_2K_0(qr), & |r| > 1\,, \end{cases}$$

where $\phi(\xi)$ is the hypergeometric function $M(\alpha, \beta, \xi^2)$. Applying the boundary condition for the continuity of ψ and its first derivative, we get the following transcendental equation

$$2\phi'(\widetilde{V}) - \left(1 + \frac{qK_0'}{\widetilde{V}K_0(q)}\right)\phi(\widetilde{V}) = 0\,, \tag{8}$$

where K_0' is the negative of the second-order Bessel function with an argument 1. The roots of the in-plane eigenenergies are $E^{\parallel}$.

The z-direction solution. For z-direction equation, when the electric field is equal to zero, we apply the same method as with the r-direction equation and we get the following differential equation

$$\xi\frac{\mathrm{d}^2\phi}{\mathrm{d}\xi^2} + \left(\frac{1}{2} - \xi\right)\frac{\mathrm{d}\phi}{\mathrm{d}\xi} - \frac{1}{4}\left(1 - \frac{\widetilde{W}^2}{\widetilde{N}}\right)\phi \quad = \quad 0\,. \tag{9}$$

Here the arguments of the hypergeometric function $M(\alpha', \beta', \xi)$ are $\xi = \widetilde{N}Z^2$, $\beta' = 1/2$ and $\alpha' = (1/4)(1 - \widetilde{W}^2/\widetilde{N})$, and we can write the solution of Eq. (9) as

$$\psi(Z) \quad = \quad \begin{cases} c' \exp\left\{-\dfrac{\widetilde{N}Z^2}{2}\right\} M(\alpha', \beta', \widetilde{N}Z^2)\,, & |Z| \le 1\,, \\[2ex] c'' \exp\{-k|Z|\}\,, & |Z| > 1\,, \end{cases}$$

where $\widetilde{W}^2 = 2m^*L^2E^{\perp}/\hbar^2$, $\widetilde{N}^2 = 2m^*L^2V_0/\hbar^2$ and $k^2 = \widetilde{N}^2 - \widetilde{W}^2$. Considering the boundary conditions, we get the following transcendental equation

$$2\phi'(\widetilde{N}) - \left(1 - \frac{k}{\widetilde{N}}\right)\phi(\widetilde{N}) = 0\,. \tag{10}$$

Solving Eq. (10) numerically, we obtained the particle eigenenergies in the z-direction without the electric field. In the case when $F\neq 0$, we make series expansion of the envelope wavefunction in Eqs. (2) and (4). Before we proceed, we rewrite Eqs. (2) and (4) as

$$\psi''(Z) + \left[\gamma^2 - \widetilde{N}^2(Z + Z_0)^2\right]\psi(Z) = 0\,, \qquad |Z| \le 1\,, \tag{11}$$

$$\psi''(Z) + \left(\widetilde{W}^2 - \widetilde{F}Z - \widetilde{N}^2\right)\psi(Z) = 0\,, \qquad |Z| > 1\,, \tag{12}$$

where

$$\gamma^2 = \widetilde{W}^2 + \frac{\widetilde{F}^2}{4\widetilde{N}^2}\,, \quad Z_0 = \frac{\widetilde{F}}{2\widetilde{N}^2}\,, \quad \widetilde{F} = \frac{2m^*|e|FL^3}{\hbar^2}\,.$$

Let $\psi(Z)$ be of the form $\psi(Z) = \sum_{n=0}^{\infty} a_n x^n$, where $x = Z + Z_0$.

Substituting into Eq. (11), we get

$$\sum_{n=0}^{\infty} \left[(n+2)(n+1)a_{n+2} + \gamma^2 a_n - \widetilde{N}^2 a_{n-2}\right] x^n = 0\,,$$

and we can write a_{n+2} as

$$a_{n+2} = \frac{\widetilde{N}^2 a_{n-2} - \gamma^2 a_n}{(n+2)(n+1)}\,.$$

The general solution of Eq. (11) can be written in terms of $\psi_{\rm even}$ and $\psi_{\rm odd}$ as

$$\psi(Z) = A\psi_{\rm even} + B\psi_{\rm odd}\,.$$

For the even coefficients, we put $a_0 = 1$ and $a_1 = 0$, then $a_2 = -\gamma^2 a_0/2$ and $a_4 = (\widetilde{N}^2 a_0 - \gamma^2 a_2)/12$.

For the odd coefficients, we have $a_1 = 1$ and $a_3 = -\gamma^2 a_1/6$. Thus, the envelope wavefunction in the z-direction, at the left, inside and the right of the parabolic potential disc-like quantum dot is represented by

$$\psi(Z) = \begin{cases} C\big[Bi(\eta) + {\rm i}Ai(\eta)\big]\,, & Z < -1\,, \\ A\psi_{\rm even}(Z) + B\psi_{\rm odd}(Z)\,, & |Z| \le 1\,, \\ D{\rm Ai}(\eta)\,, & Z > 1\,, \end{cases}$$

where $\eta = \widetilde{F}^{1/3}[(Z+Z_0)+k^2/\widetilde{F}]$, and Ai and Bi are the independent Airy and Bairy functions, respectively. Applying the boundary conditions, we get the following secular equation

$$\begin{vmatrix} Bi(\bar\eta) + {\rm i}\,Ai(\bar\eta) & -\psi_{\rm even}(Z_0-1) & -\psi_{\rm odd}(Z_0-1) & 0 \\ \dfrac{\widetilde{F}^{\frac13}}{L}\left[Bi'(\bar\eta) + {\rm i}Ai'(\bar\eta)\right] & -\psi'_{\rm even}(Z_0-1) & -\psi'_{\rm odd}(Z_0-1) & 0 \\ 0 & \psi_{\rm even}(1+Z_0) & \psi_{\rm odd}(1+Z_0) & -Ai(\eta^+) \\ 0 & \psi'_{\rm even}(1+Z_0) & \psi'_{\rm odd}(1+Z_0) & -\dfrac{\widetilde{F}^{\frac13}}{L}Ai'(\eta^+) \end{vmatrix} = 0. \tag{13}$$

By solving Eq. (13), we determine the eigenenergy of the particle in the presence of the electric field in the z-direction. The total ground state energy of a particle in the parabolic potential disc-like quantum dot can be approximated by

$$E = E^{\|} + E^{\perp} - \langle\delta V\rangle.$$

Note that the normalized parameters defined above are used to express all our solutions. Thus the obtained results are universal for both electrons and holes in all cases.

3. Results and discussion

We applied the above solutions to a finite parabolic potential disc-like quantum dot in the GaAs semiconductor. We used the electron and the hole effective masses $m_e^* = 0.0665m_0$ and $m_h^* = 0.34m_0$, respectively. The energy gap offset was taken as 65% and 35%, with the energy gap $E_g = 1.247x$, which implies the confinement potentials of the electron and the hole $V_e = 0.65E_g$, and $V_h = 0.35E_g$, respectively. x represents the Al concentration in the barrier material $Al_xGa_{1-x}As$.

Figure 2 displays the variation of the particle total ground energy for both the electron and the hole, with the structure parameter $\widetilde{V}$. The total carriers ground energy is calculated at two different values of Al content, but for the same half-width $L = 7$ nm. We see the higher potential confinement, the higher ground state energy.

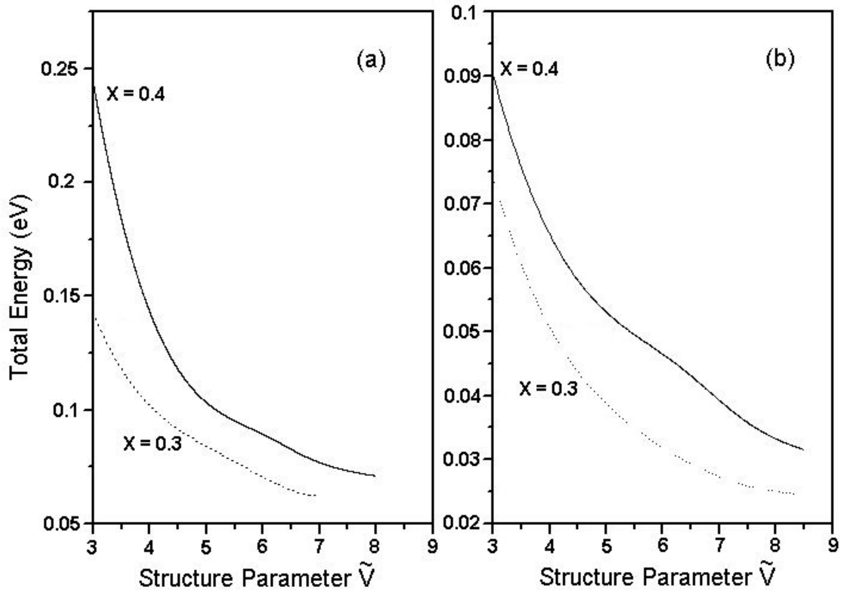

Fig. 2. The variation of the partical total energy with the structure parameter $\widetilde{V}$ at two different values of Al *concentration x: (a) represents the electron and (b) represents the hole.*

To examine the effect of the electric field on the ground state of a finite parabolic potential disc-like quantum dot, we display in Fig. 3a the variation of both the ground and the first excited states for the electron with the applied electric field. The results for the hole are shown in of Fig. 3b. Both the excited and the ground state energies are calculated for the same two previous values of x, where the disc dimensions are $R = 6$ nm, and $L = 7$ nm. The energies of the levels decrease when increasing the electric field, while their values increase with the structure parameter $\widetilde{V}$.

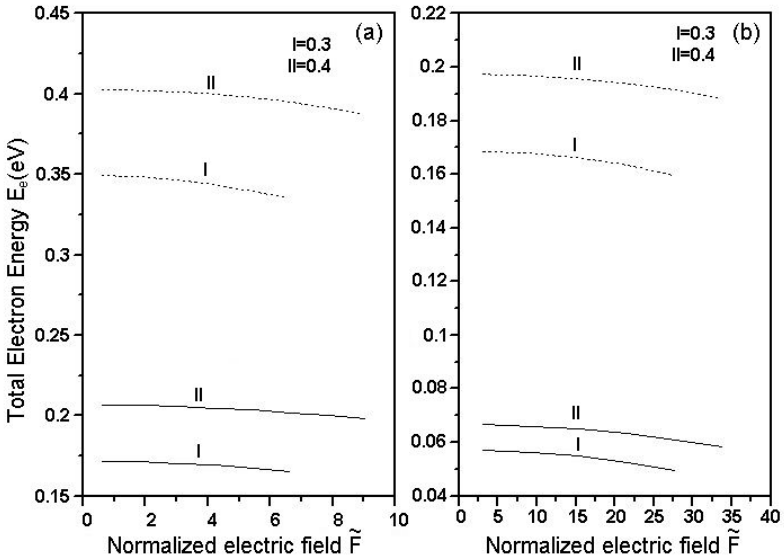

Fig. 3. The total particle energy as a function of the applied normalized electric field ($\widetilde{F}$). The solid lines represent the ground state energy, and the dashed lines represent the first excited state for the same values of x: (a) stands for the electron and (b) stands for the hole. Here $R = 6$ nm and $L = 7$ nm.

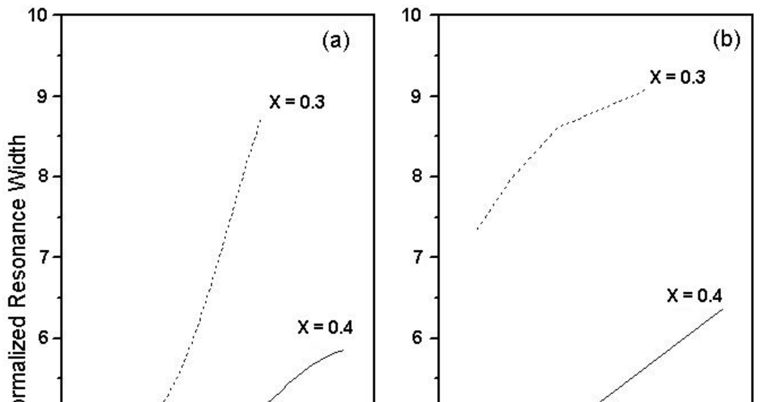

Fig. 4. The change of the normalized width of the electron ground state (a) and the first excited state (b), with the normalized electric field $\widetilde{F}$ for $R = 6$ nm, $L = 7$ nm and two different values of x.

The normalized resonance width $\widetilde{\Gamma} = \Gamma/V_0$ as a function of the normalized electric field $\widetilde{F}$ is plotted in Fig. 4. Examining Fig. 4a (electron ground state) and Fig. 4b (electron first excited state), we notice that the normalized resonance width $\widetilde{\Gamma}$ increases rapidly with the electric field, which means that the particle lifetime τ, which is defined as $\tau = \hbar/\Gamma$, decreases rapidly with the electric field. Also, as the structure parameter $\widetilde{V}$ increases, the rate of $\widetilde{\Gamma}$ decreases, while $\widetilde{F}$ value becomes smaller. We find that the $\widetilde{\Gamma}$ values of the ground state are much smaller than those of the first excited state, especially at small values of $\widetilde{V}$. This is due to the fact that the effect of the barrier for the ground state is much greater than for the first excited state.

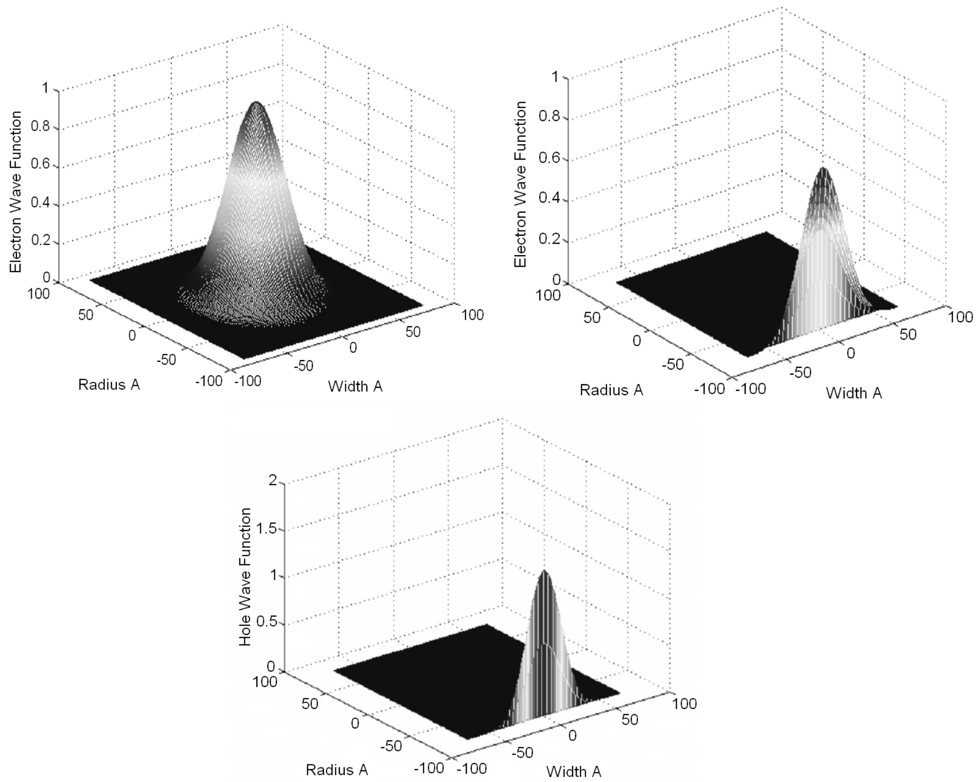

Fig. 5. Square of the wavefunction amplitude for the electron ground state as a function of radius for $R = 6$ nm and half-width $L = 7$ nm: (a) without field and (b) for $F = 70$ kV/cm. (c) Square of the wave function amplitude for the hole ground state at $F = 70$ kV/cm.

In Fig. 5a we display the absolute value of the wavefunction of the electron with the disc dimensions R and L, when the electric field $F = 0$. In Figs. 5b and 5c we show the absolute value of the wavefunction for the applied electric field

$F = 70$ kV/cm. Here we notice the deflection of the wavefunction to the right in the z-direction, which is the direction of the applied field.

4. Conclusion

In this paper, we have derived exact analytical solutions for the finite parabolic potential disc-like quantum dot without electric field. When the applied electric field is switched on, we derived the series solution inside and outside the quantum dot in the z-direction. The first excited state of the electron and the hole is investigated. The normalized resonance width of the ground state is smaller than of the first excited state. The corresponding electron and hole distributed wavefunctions are obtained. Since the finite parabolic quantum dot structure has wide applications, the study given here should be valuable for the understanding and for the design of structures involving quantum dots.

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EGZAKTNO RJEŠENJE ZA VALJKASTU KVANTNU TOČKU S KONAČNIM PARABOLNIM POTENCIJALOM BEZ POLJA I S ELEKTRIČNIM POLJEM

Izveli smo egzaktna rješenja u vidu nizova za kvantnu točku s parabolnim potencijalom, bez polja i s vanjskim električnim poljem. Definirali smo normirajuće parametre. Pomoću kompleksne svojstvene energije $E = E_0 - \mathrm{i}\Gamma/2$, uzrokovane električnim poljem, izračunali smo rezonantnu širinu Γ za vezana stanja. Osnovno i prvo više stanje elektrona i šupljine izveli smo bez polja i s električnim poljem. Odgovarajuće anvelopne funkcije predstavljamo u ovisnosti o veličini kvantne točke, polumjera R i poluširine L.