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Energy levels and states of parabolic cylindrical lens shaped quantum dots

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The parabolic cylindrical lens shaped quantum dot is investigated theoretically. The Schrödinger equation for an electron confined in this structure is solved in the parabolic cylindrical coordinate system. The wavefunctions for the electron are presented in terms of confluent hypergeometric functions, and the electron energy spectra are also obtained.

Keywords: quantum dot, artificial atom, energy level, wavefunction
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Quantum dots or artificial atoms[1−3] have attracted great interest due to their potential applications in a wide variety of optoelectronic and microelectronic devices. Quite different from that in bulk materials, electrons in the quantum dots have significant quantum effects, since they are completely confined in a small space by the band gap difference between two types of materials. To calculate the electron structure, quantum dots are usually treated as sphere,[4,5] cylindrical,[6,7] pyramid, and truncated pyramid[8−11] shapes. However, it is most widely observed in experiments that quantum dots are typically lens-shaped.[12−15] Pei *et al* investigated the elastic fields in the self-assembled lens-shaped quantum dots arrays by three-dimensional finite element analysis.[16] Recently, we presented a solvable lens-shaped quantum dot model that is formed by two co-focus paraboloids of revolution, and provided the wavefunctions and energy spectrum for electron confined in this system.[17]

According to the experiment results obtained by Mui *et al*,[12] quantum dots with a shape more closely approximate to a parabolic cylindrical lens can be made. Moreover, the nano-ribbons produced by Meng *et al*[18] can also be considered approximately as they have parabolic cylindrical lens shape or elliptic cylinder structure. Recently, we have just investigated the elliptic cylindrical quantum dot theoretically.[19] In this paper, we present a model for parabolic cylindrical lens shaped quantum dot, of which boundary layers are of two co-focus parabolic cylinders. In our model, the electron is confined in a parabolic cylinder. We want to give the wave functions and the energy levels of the electron in this structure. We make an attempt to solve the Schrödinger equation with an infinite well potential in parabolic cylindrical coordinate system, since it is difficult to work out in Cartesian coordinate system for its complicate boundary conditions.

We introduce the parabolic cylindrical coordinates λ, μ, and z, which have the following relations to Cartesian coordinates:[20]

$$x = \frac{1}{2}(\lambda - \mu), \quad y = \sqrt{\lambda\mu}, \quad z = z. \tag{1}$$

In this parabolic cylindrical coordinate system, the Laplacian is[20]

$$\nabla^2 = \frac{4}{\lambda+\mu}\left[\sqrt{\lambda}\frac{\partial}{\partial\lambda}\left(\sqrt{\lambda}\frac{\partial}{\partial\lambda}\right) + \sqrt{\mu}\frac{\partial}{\partial\mu}\left(\sqrt{\mu}\frac{\partial}{\partial\mu}\right)\right] + \frac{\partial^2}{\partial z^2}. \tag{2}$$

Our purpose is to solve the Schrödinger equation

$$\left\{\frac{4}{\lambda+\mu}\left[\sqrt{\lambda}\frac{\partial}{\partial\lambda}\left(\sqrt{\lambda}\frac{\partial}{\partial\lambda}\right) + \sqrt{\mu}\frac{\partial}{\partial\mu}\left(\sqrt{\mu}\frac{\partial}{\partial\mu}\right)\right] + \frac{\partial^2}{\partial z^2} + \frac{2m\left[E - V(\lambda,\mu,z)\right]}{\hbar^2}\right\}\psi = 0, \tag{3}$$

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where $V=0$, when $0 \le \lambda < a$, $0 \le \mu < b$, $0 < z < L$, and $V=\infty$, in other regions; m is the mass of electron; a, b, and L are three constants which are related to the size and shape of the quantum dot (see Fig.1.).

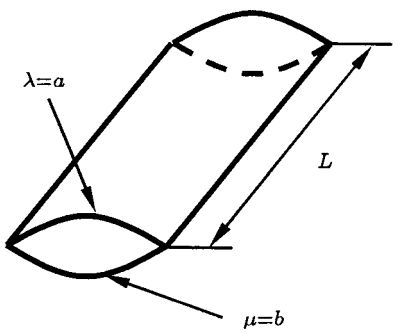


Fig.1. The geometry of the parabolic cylindrical lens shaped quantum dot.

Equation (3) can be solved by the method of variables separation, now we discuss the solutions for $0 \le \lambda < a$, $0 \le \mu < b$, $0 < z < L$. The insertion of

$$\psi = A(\lambda) B(\mu) Z(z) \tag{4}$$

into Eq.(3) yields

$$Z'' + \frac{2mE_z}{\hbar^2} Z = 0, \tag{5}$$

$$\lambda \frac{A''}{A} + \frac{1}{2}\frac{A'}{A} + \mu \frac{B''}{B} + \frac{1}{2}\frac{B'}{B} + \frac{m(E-E_z)}{2\hbar^2}(\lambda+\mu) = 0. \tag{6}$$

The solution for Eq.(5) that satisfies the boundary conditions of $Z(0)=0$ and $Z(L)=0$ can be given by

$$Z = \sin\left(\frac{\sqrt{2mE_z}}{\hbar} z\right) \tag{7}$$

with

$$E_z = \frac{n_3^2 \pi^2 \hbar^2}{2mL^2}, \quad n_3 = 1,\ 2,\ 3, \cdots \tag{8}$$

From Eq.(6) we have

$$\lambda A'' + \frac{1}{2}A' + \left(k^2\lambda - \beta\right) A = 0, \tag{9a}$$

$$\mu B'' + \frac{1}{2}B' + \left(k^2\mu + \beta\right) B = 0, \tag{9b}$$

where β is a constant to be determined, $k = \sqrt{m(E-E_z)/2}/\hbar$. Using the transformations $A = \mathrm{e}^{\mathrm{i}k\lambda} G(\lambda)$ and $B = \mathrm{e}^{\mathrm{i}k\mu} H(\mu)$, we obtain

$$\lambda G'' + \left(2\mathrm{i}k\lambda + \frac{1}{2}\right) G' + \left(\frac{1}{2}\mathrm{i}k - \beta\right) G = 0, \tag{10a}$$

$$\mu H'' + \left(2\mathrm{i}k\mu + \frac{1}{2}\right) H' + \left(\frac{1}{2}\mathrm{i}k + \beta\right) H = 0. \tag{10b}$$

Introducing new variables $\xi = -2\mathrm{i}k\lambda$ and $\eta = -2\mathrm{i}k\mu$, Eqs.(10a) and (10b) can be changed into

$$\xi \frac{\mathrm{d}^2 G}{\mathrm{d}\xi^2} + \left(\frac{1}{2} - \xi\right) \frac{\mathrm{d}G}{\mathrm{d}\xi} - \left(\frac{1}{4} + \frac{\mathrm{i}\beta}{2k}\right) G = 0, \tag{11a}$$

$$\eta \frac{\mathrm{d}^2 H}{\mathrm{d}\eta^2} + \left(\frac{1}{2} - \eta\right) \frac{\mathrm{d}H}{\mathrm{d}\eta} - \left(\frac{1}{4} - \frac{\mathrm{i}\beta}{2k}\right) H = 0. \tag{11b}$$

Equations (11a) and (11b) are Kummer's standard form of confluent hypergeometric equation, and have the following solutions:

$$G_1 = F\left(\frac{1}{4} + \frac{\mathrm{i}\beta}{2k},\ \frac{1}{2},\ \xi\right), \tag{12a}$$

$$H_1 = F\left(\frac{1}{4} - \frac{\mathrm{i}\beta}{2k},\ \frac{1}{2},\ \eta\right). \tag{12b}$$

So the wavefunctions can be written as

$$\psi = \mathrm{e}^{\mathrm{i}k(\lambda+\mu)} F\left(\frac{1}{4} + \frac{\mathrm{i}\beta}{2k},\ \frac{1}{2},\ -2\mathrm{i}k\lambda\right) \times F\left(\frac{1}{4} - \frac{\mathrm{i}\beta}{2k},\ \frac{1}{2},\ -2\mathrm{i}k\mu\right) \times \sin\left(\frac{\sqrt{2mE_z}}{\hbar} z\right). \tag{13}$$

According to the boundary conditions $\psi|_{\lambda=a} = 0$ and $\psi|_{\mu=b} = 0$, we can know that β and k should satisfy

$$F\left(\frac{1}{4} + \frac{\mathrm{i}\beta}{2k},\ \frac{1}{2},\ -2\mathrm{i}ka\right) = 0 \tag{14a}$$

and

$$F\left(\frac{1}{4} - \frac{\mathrm{i}\beta}{2k},\ \frac{1}{2},\ -2\mathrm{i}kb\right) = 0. \tag{14b}$$

From Eqs.(14a) and (14b), in principle, the parameter β and the energy E of the electron confined in the quantum dot can be obtained. In some particular cases, expressions (14a) and (14b) can be reduced to explicit forms.

When $-3\pi/2 < \arg z < \pi/2$, the confluent hypergeometric function can be given by[20]

$$F(\alpha,\gamma,z) \sim \frac{\Gamma(\gamma)}{\Gamma(\gamma-\alpha)} \mathrm{e}^{-\mathrm{i}\alpha\pi} z^{-\alpha} \times \left[1 + \sum_{n=1}^{\infty} (-1)^n \frac{(\alpha)_n (1-\gamma+\alpha)_n}{n! z^n}\right] + \frac{\Gamma(\gamma)}{\Gamma(\alpha)} \mathrm{e}^{z} z^{\alpha-\gamma} \times \left[1 + \sum_{n=1}^{\infty} \frac{(\gamma-\alpha)_n (1-\alpha)_n}{n! z^n}\right]. \tag{15}$$

For pure imaginary variable z, and when $|z|$ are large, the formula (15) can be simplified as[21,22]

$$F(\alpha,\gamma,z) \sim \frac{\Gamma(\gamma)}{\Gamma(\gamma-\alpha)}|z|^{-\alpha} \times \exp\left(-\mathrm{i}\frac{\pi}{2}\alpha\right) + \frac{\Gamma(\gamma)}{\Gamma(\alpha)}|z|^{\alpha-\gamma}\mathrm{e}^{z} \times \exp\left[-\mathrm{i}\frac{\pi}{2}(\alpha-\gamma)\right]. \tag{16}$$

According to the expression (16), when k is large, we have

$$\begin{aligned} & F\left(\frac{1}{4}+\frac{\mathrm{i}\beta}{2k},\ \frac{1}{2},\ -2\mathrm{i}ka\right) \\ \sim & \frac{\Gamma(1/2)}{\Gamma\left(\frac{1}{4}-\frac{\mathrm{i}\beta}{2k}\right)}(2ka)^{-(1+2\mathrm{i}\beta/k)/4} \\ & \times \exp\left(\frac{\pi\beta}{4k}-\mathrm{i}\frac{\pi}{8}\right) \\ & + \frac{\Gamma(1/2)}{\Gamma\left(\frac{1}{4}+\frac{\mathrm{i}\beta}{2k}\right)}(2ka)^{-(1-2\mathrm{i}\beta/k)/4} \\ & \times \exp\left(\frac{\pi\beta}{4k}-2\mathrm{i}ka+\mathrm{i}\frac{\pi}{8}\right). \end{aligned} \tag{17}$$

If we write

$$\Gamma\left(\frac{1}{4}+\frac{\mathrm{i}\beta}{2k}\right) = \left|\Gamma\left(\frac{1}{4}+\frac{\mathrm{i}\beta}{2k}\right)\right|\exp(\mathrm{i}\theta), \tag{18}$$

where

$$\theta = \arg\left(\Gamma\left(\frac{1}{4}+\frac{\mathrm{i}\beta}{2k}\right)\right), \tag{19}$$

we will know

$$\Gamma\left(\frac{1}{4}-\frac{\mathrm{i}\beta}{2k}\right) = \left|\Gamma\left(\frac{1}{4}+\frac{\mathrm{i}\beta}{2k}\right)\right|\exp(-\mathrm{i}\theta). \tag{20}$$

The substitution of expressions (18) and (20) into the expression (17) yields

$$\begin{aligned} & F\left(\frac{1}{4}+\frac{\mathrm{i}\beta}{2k},\ \frac{1}{2},\ -2\mathrm{i}ka\right) \\ \sim & \frac{\Gamma(1/2)}{\left|\Gamma\left(\frac{1}{4}+\frac{\mathrm{i}\beta}{2k}\right)\right|(2ka)^{1/4}}\exp\left(\frac{\pi\beta}{4k}-\mathrm{i}ka\right) \\ & \times\left\{\exp\left[\mathrm{i}ka-\frac{\mathrm{i}\beta}{2k}\ln(2ka)-\mathrm{i}\frac{\pi}{8}+\mathrm{i}\theta\right]\right. \\ & \left.+\exp\left[-\mathrm{i}ka+\frac{\mathrm{i}\beta}{2k}\ln(2ka)+\mathrm{i}\frac{\pi}{8}-\mathrm{i}\theta\right]\right\} \\ = & \frac{2\Gamma(1/2)}{\left|\Gamma\left(\frac{1}{4}+\frac{\mathrm{i}\beta}{2k}\right)\right|(2ka)^{1/4}}\exp\left(\frac{\pi\beta}{4k}-\mathrm{i}ka\right) \\ & \times\cos\left[ka-\frac{\beta}{2k}\ln(2ka)-\frac{\pi}{8}+\theta\right]. \end{aligned} \tag{21}$$

From Eq.(14a) and the above expression, we find

$$\cos\left[ka-\frac{\beta}{2k}\ln(2ka)-\frac{\pi}{8}+\theta\right]=0, \tag{22}$$

that is

$$ka-\frac{\beta}{2k}\ln(2ka)-\frac{\pi}{8}+\theta=\left(n_1+\frac{1}{2}\right)\pi. \tag{23a}$$

Similarly, from Eq.(14b) we can obtain

$$kb+\frac{\beta}{2k}\ln(2kb)-\frac{\pi}{8}-\theta=\left(n_2+\frac{1}{2}\right)\pi. \tag{23b}$$

Here, n_1 and n_2 should be large integers. Based on expressions (23a) and (23b), we know that the energy spectrum for high excited states can be given by

$$\begin{aligned} & \frac{a\sqrt{m(E-E_z)/2}}{\hbar}-\frac{\hbar\beta}{\sqrt{2m(E-E_z)}} \\ & \times\ln\left[a\sqrt{2m(E-E_z)}/\hbar\right]-\frac{\pi}{8} \\ & +\arg\left(\Gamma\left(\frac{1}{4}+\frac{\mathrm{i}\beta\hbar}{\sqrt{2m(E-E_z)}}\right)\right) \\ = & \left(n_1+\frac{1}{2}\right)\pi, \end{aligned} \tag{24a}$$

$$\begin{aligned} & \frac{b\sqrt{m(E-E_z)/2}}{\hbar}+\frac{\hbar\beta}{\sqrt{2m(E-E_z)}} \\ & \times\ln\left[b\sqrt{2m(E-E_z)}/\hbar\right]-\frac{\pi}{8} \\ & -\arg\left(\Gamma\left(\frac{1}{4}+\frac{\mathrm{i}\beta\hbar}{\sqrt{2m(E-E_z)}}\right)\right) \\ = & \left(n_2+\frac{1}{2}\right)\pi. \end{aligned} \tag{24b}$$

Particularly, in the case of $a=b$, that is, when the quantum dot has a symmetrical structure, we have

$$E-E_z=\frac{\pi^2\hbar^2}{2ma^2}\left(n_1+n_2+\frac{5}{4}\right)^2. \tag{25}$$

i.e.

$$\begin{aligned} E=&E_{n_1,n_2,n_3} \\ =&\frac{\pi^2\hbar^2}{2ma^2}\left(n_1+n_2+\frac{5}{4}\right)^2+\frac{\pi^2\hbar^2}{2mL^2}n_3^2. \end{aligned} \tag{26}$$

Equations (11a) and (11b) also have another pair of solutions, which read

$$G_2=\xi^{1/2}F\left(\frac{3}{4}+\frac{\mathrm{i}\beta}{2k},\ \frac{3}{2},\ \xi\right), \tag{27a}$$

$$H_2=\eta^{1/2}F\left(\frac{3}{4}-\frac{\mathrm{i}\beta}{2k},\ \frac{3}{2},\ \eta\right), \tag{27b}$$

and lead to the following wavefunction:

$$\begin{aligned}\psi =&2\mathrm{i}k\mathrm{e}^{\mathrm{i}k(\lambda+\mu)}\left(\lambda\mu\right)^{1/2}\\&\times F\left(\frac{3}{4}+\frac{\mathrm{i}\beta}{2k},\ \frac{3}{2},\ -2\mathrm{i}k\lambda\right)\\&\times F\left(\frac{3}{4}-\frac{\mathrm{i}\beta}{2k},\ \frac{3}{2},\ -2\mathrm{i}k\mu\right)\sin\left(\frac{\sqrt{2mE_z}}{\hbar}z\right).\end{aligned}\tag{28}$$

In this case, the energy spectrum can be obtained by

$$F\left(\frac{3}{4}+\frac{\mathrm{i}\beta}{2k},\ \frac{3}{2},\ -2\mathrm{i}ka\right)=0,\tag{29a}$$

$$F\left(\frac{3}{4}-\frac{\mathrm{i}\beta}{2k},\ \frac{3}{2},\ -2\mathrm{i}kb\right)=0.\tag{29b}$$

Using the above-mentioned procedure, it can be deduced from Eqs.(29a) and (29b) that

$$ka-\frac{\beta}{2k}\ln\left(2ka\right)-\frac{3\pi}{8}+\phi=\left(n_1+\frac{1}{2}\right)\pi,\tag{30a}$$

$$kb+\frac{\beta}{2k}\ln\left(2kb\right)-\frac{3\pi}{8}-\phi=\left(n_2+\frac{1}{2}\right)\pi,\tag{30b}$$

where

$$\phi=\arg\left(\Gamma\left(\frac{3}{4}+\frac{\mathrm{i}\beta}{2k}\right)\right).\tag{31}$$

Similarly, we know that the energy spectrum for highly excited states in this case can be provided by

$$\begin{aligned}&\frac{a\sqrt{m\left(E-E_z\right)/2}}{\hbar}-\frac{\hbar\beta}{\sqrt{2m\left(E-E_z\right)}}\\&\times\ln\left[a\sqrt{2m\left(E-E_z\right)}/\hbar\right]-\frac{3\pi}{8}\\&+\arg\left(\Gamma\left(\frac{3}{4}+\frac{\mathrm{i}\beta\hbar}{\sqrt{2m\left(E-E_z\right)}}\right)\right)\\=&\left(n_1+\frac{1}{2}\right)\pi,\end{aligned}\tag{32a}$$

$$\begin{aligned}&\frac{b\sqrt{m\left(E-E_z\right)/2}}{\hbar}+\frac{\hbar\beta}{\sqrt{2m\left(E-E_z\right)}}\\&\times\ln\left[b\sqrt{2m\left(E-E_z\right)}/\hbar\right]-\frac{3\pi}{8}\\&-\arg\left(\Gamma\left(\frac{3}{4}+\frac{\mathrm{i}\beta\hbar}{\sqrt{2m\left(E-E_z\right)}}\right)\right)\\=&\left(n_2+\frac{1}{2}\right)\pi.\end{aligned}\tag{32b}$$

For a symmetrical parabolic cylindrical lens shaped quantum dot, i. e. when $a=b$, the energy spectrum for high excited states can be given by

$$\begin{aligned}E=&E_{n_1,n_2,n_3}\\=&\frac{\pi^2\hbar^2}{2ma^2}\left(n_1+n_2+\frac{7}{4}\right)^2+\frac{\pi^2\hbar^2}{2mL^2}n_3^2.\end{aligned}\tag{33}$$

In conclusion, we have presented a solvable theoretical model for parabolic cylindrical lens shaped quantum dots, and solved the Schrödinger equation for electron confined in this structure by adopting parabolic cylinder coordinate system. The wavefunctions are provided in terms of confluent hypergeometric functions, and the electron energy spectra are given through two pairs of equations. In particular, the energy spectra for highly excited states are also discussed in detail. The results we have obtained may be useful for the study of parabolic cylindrical lens shaped quantum dots.

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