

A Comparison of the Eigenstates of a Hydrogenic Impurity in Spherical and Parabolic Quantum Dots

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In previous papers we calculated the energy spectra of a hydrogen impurity located at the center of spherical and parabolic quantum dots. In this work, a comparison of the eigenstates of a hydrogenic impurity in spherical and parabolic quantum dots is discussed in detail. Moreover, the Stark effect on the parabolic quantum dots is investigated. Our calculated results reveal that for both spherical and parabolic quantum dots, the eigenenergies are just like those of a free-space hydrogenic atom, when the dot size is extremely small. On the other hand, the eigenenergies are also like those of a free-space hydrogenic atom when the dot size is extremely large, except that they are shifted by the confining potential. When the dot size is between these two extreme situations, the energy level splitting and degeneracy of the energy levels are quite different for these two cases. The theoretical results show that the energy plateau of the parabolic quantum dot is not obvious when compared to that of the spherical quantum dot.

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I. Introduction

Due to the high progress in scientific technology in the past few years, people can now make “artificial atoms” or “quantum dots”, as they are called [1, 2]. Since the scale of these nanostructures has approached to the size of an atom, physicists are trying to disclose the quantum mechanism behind them. The simplest model is a hydrogen atom located at the center of a spherical cavity with a discontinuous potential to simulate the quantum dot. The exact solutions for this model have been reported by Yang and several other researchers [3-6]. However, a spherical cavity is still not good enough for a real quantum dot. In a previous work we reported another model, a parabolic quantum dot [7].

In this paper we calculate the eigenstates of a spherical quantum dot (SQD) and a parabolic quantum dot (PQD) and make a detailed comparison between them. Moreover, the Stark effect on the parabolic quantum dots is investigated. In Sec. II, we present an exact solution for a SQD, which is simpler than that reported in our previous paper [5]. We also discuss how a SQD influences the impurity’s wave function. In Sec. III, we calculate the eigenstates of a PQD; some novel properties of this model are found and compared with those of a spherical dot. Moreover, we study the Stark effect on the parabolic quantum dots. The effects of dot size and external electric field are discussed. A summary of the results is presented in Sec. IV.

II. Spherical quantum dot

II-1. Formulation

The Hamiltonian of a hydrogenic impurity located at the center of a spherical quantum dot can be written as:

$$H = -\frac{\hbar^2}{2m^*} \nabla^2 - \frac{Ze^2}{\epsilon r} + V(r); \quad (1)$$

where

$$V(r) = \begin{cases} V_0 & r < R_0 \\ 0 & r \geq R_0 \end{cases} \quad (2)$$

and m^* , ϵ and Z are the effective mass, dielectric constant and core charge, V_0 and R_0 are the confining potential and the radius of the SQD, and they are all positive. The value of the confining potential V_0 ranges from zero to infinity. The solution of the Schrödinger equation, since it is a spherically symmetric potential field, can be written as:

$$\tilde{\psi}(r; \mu; \theta) = \frac{u(r)}{r} Y(\mu; \theta); \quad (3)$$

The radial solutions of the bound states can be expressed in terms of generalized hypergeometric functions [8] as follows:

Solution regular at $r = 0$:

$$u_{in}(r) \gg e^{-\kappa_{in} r} (2^{-\kappa_{in} r})^{l+1} {}_1F_1 \left(\mu; \frac{Z}{\epsilon_{in}} + l + 1; 2l + 2; 2^{-\kappa_{in} r} \right); \quad (4)$$

where

$$\kappa_{in} = \sqrt{2(E + V_0)}$$

Solutions regular at $r = R_0$:

$$u_{out}(r) \gg e^{-\kappa_{out} r} (2^{-\kappa_{out} r})^{Z/\epsilon_{out}} {}_2F_0 \left(\mu; \frac{Z}{\epsilon_{out}} + l + 1; 1; \frac{Z}{\epsilon_{out}}; \frac{1}{2^{-\kappa_{out} r}} \right); \quad (5)$$

where

$$\kappa_{out} = \sqrt{2E}$$

II-2. Discussion

By imposing the boundary conditions on the solutions we can get a suitable E value for every state of the impurity. From it we can find the hydrogenic impurity's eigenenergies and wave functions. To make our results more understandable, we let the reduced mass and the dielectric constant be the same as for a free-space hydrogen, that is, the effective Rydberg energy R_y^a is equal to the Rydberg energy R_y (13.6 eV), and the effective Bohr radius a^a is equal to the Bohr radius a_0 (0.529 Å). Here we assume that the confining potential V_0 is 3 eV. For convenience, we

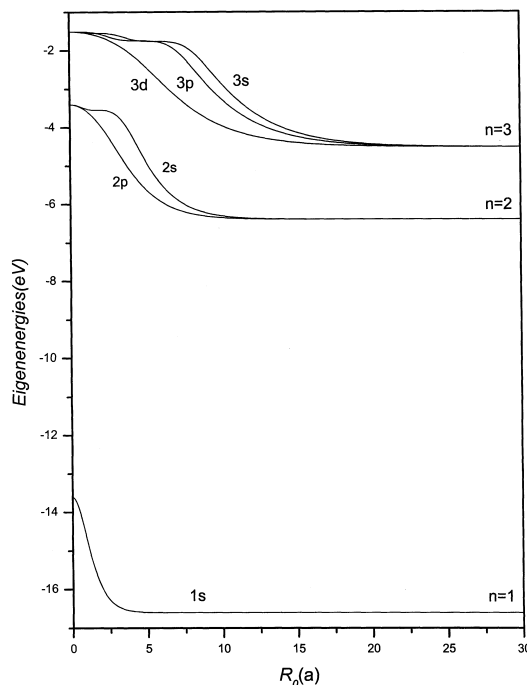


FIG. 1. The eigenenergies of a spherical quantum dot of 3 eV well depth, from the 1s to 3d states, as functions of R_0 .

still use the principal number n to represent the eigenstate in order to compare with the corresponding states of a free-space hydrogen.

In Fig. 1, we present the eigenenergies of the different n l states as functions of the dot radius. For each n state, the eigenenergy increases as the radius decreases. It is found that when the dot radius is extremely small, the eigenenergies of the impurity approach the corresponding energies of a free-space hydrogen: $E \cong -\frac{1}{2} R_0^{-2}$. On the other hand, when the dot radius is large enough, the eigenenergies approach a value which is equal to the confining potential plus the corresponding energy of a free-space hydrogen: $E \cong -\frac{1}{2} (Z^2 R_0^{-2} + V_0)$. In the mean time, when the dot radius is at these two extreme situations, the eigenenergies are in l degeneracy just as the degeneracy of a free-space hydrogen atom.

Between these two extreme situations, the l degeneracy disappears. For the same principal number, when the dot radius decreases, the smaller l states' eigenenergies increase more quickly than those of the bigger l states. This is due to the fact that, when the confining electron is in a small l state, it distributes itself at the more outer part of the impurity than the electron in a big l state, most of the time. While the dot radius is decreasing, the margin of the confining potential pushes the small l state first. Hence, its eigenenergy is influenced earlier than the big l state. That is why the small l state's eigenenergies increase more quickly than those of the big l state as the dot radius decreases.

The number of times that the energy increases is equal to the bump number of the electron radial probability distribution function. For example, since there are two bumps in the radial

probability distribution function of the 3p state, the 3p state's eigenenergy has two increasing times as the dot radius decreases from $30 a_0$ to zero. The reason is that, when the margin of the well meets the outer bump, it will push the bump into the inner part of the impurity. During this time the influence of the well is apparent, and hence the eigenenergy increases more quickly. When the outer bump has penetrated the well, then the node of the function is near the well's margin. During this time the eigenenergy increases slowly, and the changes of the dot radius seem to have little influence on the impurity. However, when the margin meets the inner bump and begins to push the bump, the eigenenergy increases quickly again. It is found that not every dot radius influences the eigenenergy. It depends on which state the confining electron is in and what the value of the dot radius is.

III. Parabolic quantum dot

III-1. Formulation

To study the interesting properties of a parabolic quantum dot, we use parabolic coordinate system. First we transform the coordinate system from spherical coordinates $(r; \theta; \phi)$ to parabolic coordinates $(\xi; \eta; \phi)$ [9]. Taking the coordinate system as equal-potential surface on the boundary, we can simulate a parabolic cavity [7]. Let us consider a hydrogen impurity located at the center of a parabolic cavity. The Hamiltonian of a hydrogen impurity inside such a cavity is

$$H = -\frac{\hbar^2}{2m} \nabla^2 - \frac{Ze^2}{r} + V; \quad (6)$$

where

$$V = \begin{cases} -V_0; & \xi \leq R_0; \eta \leq R_0 \\ 0; & \text{otherwise:} \end{cases}$$

The exact solution can be expressed as follows:

$$\psi(\xi; \eta; \phi) = u(\xi)v(\eta)e^{im\phi}; \quad (7)$$

Inside the cavity $u(\xi)$ is:

$$u_{in}(\xi) \propto e^{-\sqrt{2} \xi} {}_1F_1(j - n_1; j + 1; -2\sqrt{2} \xi); \quad (8)$$

where

$$\sqrt{2} \xi = \frac{p}{\hbar} \sqrt{E + V_0};$$

$$n_1 = \frac{Z_1}{2} - \frac{1}{2}(jm + 1);$$

Outside the cavity $u(\xi)$ is:

$$u_{out}(\xi) \propto e^{-\sqrt{2} \xi} {}_2F_0 \left(\begin{matrix} - \\ \mu \end{matrix} ; -n_1^0; -jm; - \right) \sqrt{\frac{1}{2 - \mu}}; \quad (9)$$

where

$$r_0 = \frac{r}{\frac{1}{2}E},$$

$$n_1^0 = \frac{Z_1}{2} + \frac{1}{2}(jm_j - 1);$$

Equations (8) and (9) may be applied to $\psi(r)$ if the parameter Z_1 is replaced by Z_2 and the variable r is replaced by r' , respectively.

When $R_0 = 0$ or 1 , we find that the expectation values of r and Z can be expressed in analytically closed forms, which are given as follows:

$$\langle r \rangle = \frac{\mu}{n^2} \left[\frac{3}{2} z_1 z_2 + \frac{1}{4} \frac{m^2}{Z} \right] = Z; \quad (10)$$

$$\langle z \rangle = \frac{\mu}{2} n^2 (z_1 + z_2) = Z; \quad (11)$$

where $z_j = Z_j = Z$.

The parabolic coordinate separation is the best method for studying the Stark effect of hydrogen and the PQD. We assume that the external electric field is a constant vector directed along the Z axis. Suppose that the electric field strength F is weak, so that the perturbation method is applicable. The Hamiltonian can be written as $H = H_0 + H^0$. The unperturbed Hamiltonian H_0 is the same as that shown in Eq. (6). The perturbation H^0 is given as $H^0 = eFz$. Any energy level of the PQD is degenerate except for the ground-state. The first order perturbation matrix for these degenerate states is diagonal. The matrix element is given by

$$H_{ij}^0 = \langle n; m_i; Z_j | H^0 | n; m_j; Z_j \rangle = eF \langle z \rangle_{ij};$$

independent of degeneracy. The corrected energy is

$$E_{nmZ_1} = E_{nmZ_1}^0 + eF \langle z \rangle_{nmZ_1}; \quad (12)$$

III-2. Discussion

For comparison, V_0 is chosen to be 3 eV and the nuclear charge Z is equal to 1. Different values of V_0 and Z can be used when needed. From Fig. 2, we find that:

- (1) At $R_0 = 0$ and 1 , it has the correct limit. When the dot size is extremely small, the eigenenergies E of the impurity approach the corresponding energy of a free-space hydrogen: $E \approx -\frac{1}{2} R_0^2 = -n^2$. When the radius of the dot is large enough, the eigenenergies approach values which are equal to the confining potential plus the corresponding energy of a free-space hydrogen: $E \approx -\frac{1}{2} (Z^2 R_0^2 = n^2 + V_0)$. The results are the same as those for the spherical quantum dot.
- (2) The model shows level crossing for the $n = 2$ and $n = 3$ states, just like a spherical quantum dot does. But the energy plateaus of this model is not so obvious as the ones in spherical quantum dot. The results for principal quantum numbers $n = 1, 2, 3$ are shown in Fig. 2 for demonstration.

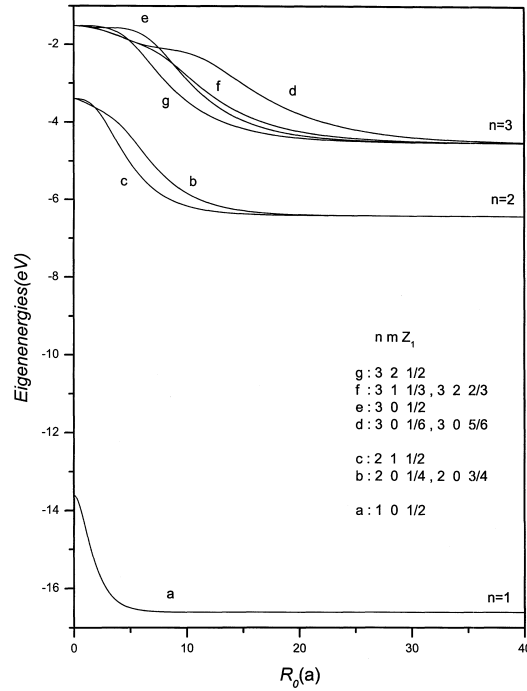


FIG. 2. The eigenenergies of a parabolic quantum dot in the low excited states $n = 1, 2, 3$ as functions of R_0 . Compared with a spherical quantum dot, the energy plateaus are not obvious.

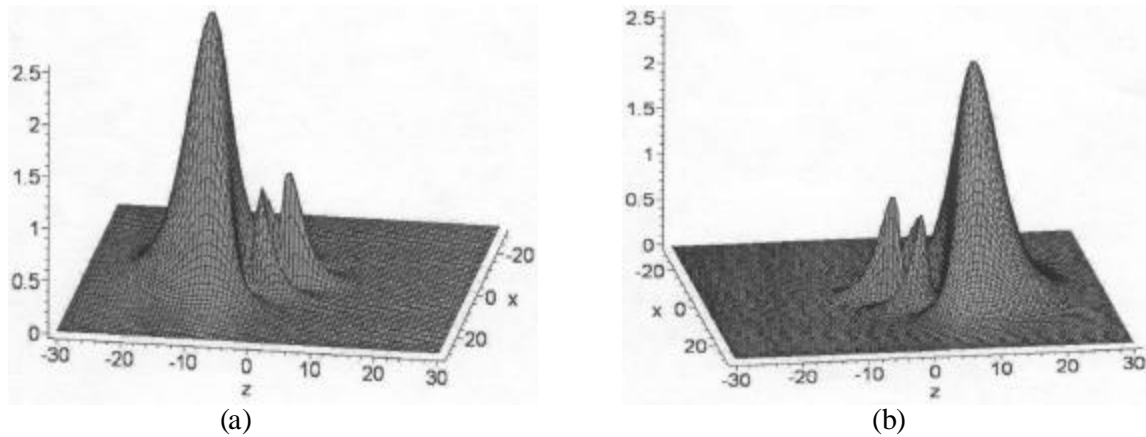


FIG. 3. (a) The electron probability distribution of a PQD for the state $n = 3, m = 0, Z_1 = 1/6$, when R_0 equals 0 or infinity. (b) The electron probability distribution of a PQD for the state $n = 3, m = 0, Z_1 = 5/6$, when R_0 equals 0 or infinity.

For each $Z_1 \in 1=2$ state with fixed n and m , there exists a degenerate state with $Z_1^0 = 1_j Z_1$. For fixed quantum number $n = 3, m = 0$, we plot the electron probability distribution of the states with $Z_1 = 1/6$ and $5/6$, respectively, in Figs. 3a and 3b. The results show that: (1) the probability

distribution is not symmetric in the $z = 0$ plane; (2) the smaller probability distribution concentrates in the upper part of the dot for the smaller Z_1 ; (3) they are mutually symmetric in the $z = 0$ plane (for the $Z_1 = 1/6$ state, with z changed to $-z$, the probability distribution is the same as that for $Z_1 = 5/6$). Therefore, the degeneracy of this pair can not be destroyed by the size of the dot.

TABLE I. Results of the theoretical calculation. Different dot size, quantum number of the states, expectation value of z , and eigenenergy are respectively listed in columns 1 to 4. The last column shows the energy level splitting caused by the Stark effect with electric field strength $F = 5 \times 10^{14}$ a.u.^a

R_0/a	n	jm_j	Z_1	$\langle z \rangle$	E_{NF} (eV)	E_F (eV)	
0	2	0	1/4 ; 3/4	-3 ; 3	-3.4014	-3.4422 ; -3.3606	
		1	1/2	0		-3.4014	
	3	0	1/6 ; 5/6	-9 ; 9	-1.5117	-1.6342 ; -1.3892	
		0	1/2	0		-1.5117	
		1	1/3 ; 2/3	-4.5 ; 4.5		-1.5729 ; -1.4505	
	4	0	2	1/2	0	-0.8504	-1.5117
			0	1/8 ; 7/8	-18 ; 18		-1.0953 ; -0.6055
		0	0	3/8 ; 5/8	-6 ; 6	-0.9320	-0.9320 ; -0.7688
			1	1/4 ; 3/4	-12 ; 12		-1.0137 ; -0.6871
			1	1/2	0		-0.8504
			2	3/8 ; 5/8	-6 ; 6		-0.9320 ; -0.7688
	4	2	0	1/4 ; 3/4	-2.5428 ; 2.5428	-4.3038	-4.3388 ; -4.2692
1			1/2	0	-4.5824		
3		0	1/6 ; 5/6	-8.2017 ; 8.2017	-1.7747	-1.8863 ; -1.6631	
		0	1/2	0		-1.5726	
1		1	1/3 ; 2/3	-4.5555 ; 4.5555	-1.7822	-1.8442 ; -1.7202	
		2	1/2	0		-1.6976	
4		0	0	1/8 ; 7/8	-16.8867 ; 16.8867	-0.9789	-1.2087 ; -0.7491
			0	3/8 ; 5/8	-5.6008 ; 5.6008		-0.8830
		1	1	1/4 ; 3/4	-12.0783 ; 12.0783	-0.9526	-1.1169 ; -7883
			1	1/2	0		-0.9504
		2	3/8 ; 5/8	-5.8015 ; 5.8015	-0.9210	-0.9999 ; -0.8421	
			3	1/2		0	-0.8633

^aelectric field strength in atomic unit a.u. = $0.51422082 \times 10^{12}$ V/m

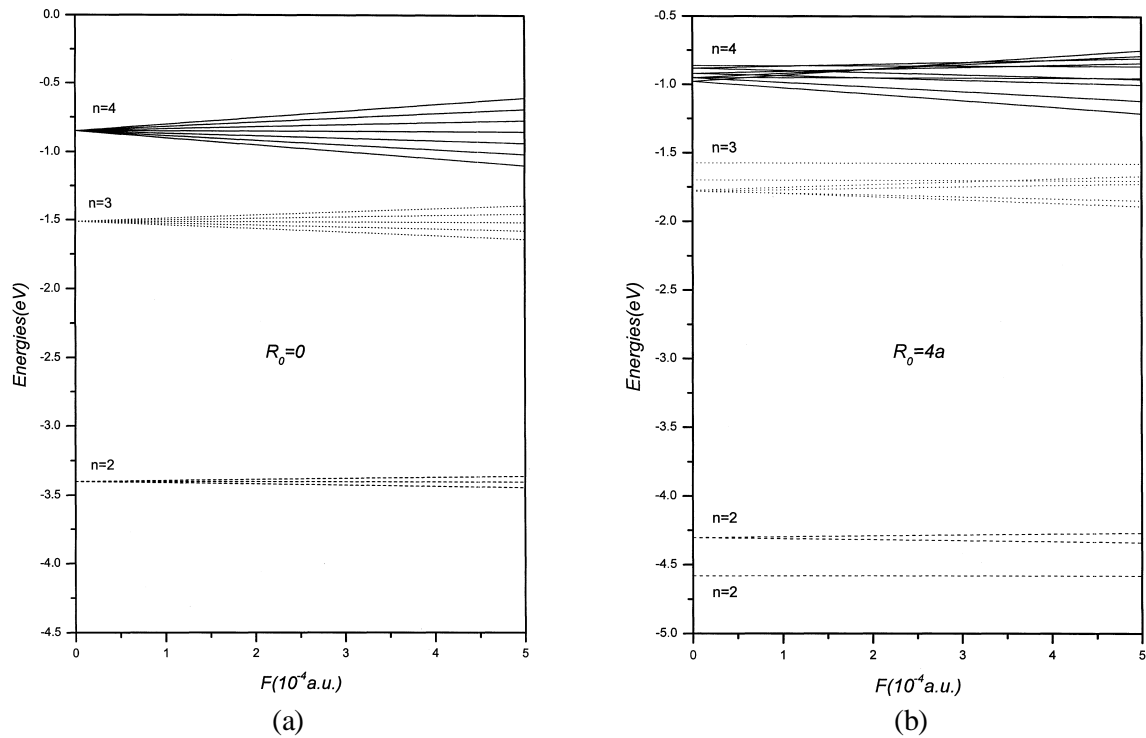


FIG. 4. (a) The energy splitting of the Stark effect as a function of the electric field strength for a PQD as R_0 equals 0. (b) The energy splitting of the Stark effect as a function of the electric field strength for a PQD as R_0 equals $4a$.

We also study the Stark effect on the parabolic quantum dots. In Table I, we list some results of the theoretical calculation. Specifically, different dot size, quantum number of the states, expectation value of Z , and eigenenergy are respectively listed in columns 1 to 4. The energy level splitting caused by the Stark effect with electric field strength $F = 5 \times 10^4 \text{ a.u.}$ is listed in the last column of Table I. From the results we note that the values of $\langle jhzi_j \rangle$ of a state at $R_0 = 0$ are larger than those at all other dot sizes. For $n = 2$ states there exists a minimum value at $R_0 = 4a$, where the margin of the dot meets the bumps and they are compressed most seriously. The expectation value of Z is a very important term for calculating the Stark effect for all states. By Eq. (12) we can compute the energy level splitting under a weak external electric field. In Fig. 4, we show the energy splitting of the Stark effect as a function of the electric field strength with two different dot sizes (R_0 equals 0 and $4a$). Figure 4a indicates that the energy splitting due to the Stark effect is most extreme as R_0 equals 0, because the value of $\langle jhzi_j \rangle$ is the largest in this situation. The number of the splitting levels is $2n - 1$ for any principal quantum number n . In Fig. 4b, for the $n = 2$ state, the effect of dot size is larger than the Stark effect. Figure 4 explicitly shows that the effect of a confining potential seriously competes with the Stark effect. These two effects result in a maximum number of splitting levels of $n(n + 1) = 2$.

III-3. Comparison between the SQD and PQD

Inside the SQD and PQD the wave functions are all in the form of the generalized hypergeometric function ${}_1F_1$, while outside the dots they are all in the form of ${}_2F_0$. But the ${}_iF_j$ of the PQD are more complicated than those of the SQD. The wave functions of the SQD are symmetric in the x y plane, but those of the PQD are not (if $z_1 \neq 1/2$). For each state of the SQD or PQD, the eigenenergy increases from $\frac{1}{2}(Z^2R_y^2=n^2 + V_0)$ to $\frac{1}{2}Z^2R_y^2=n^2$ as the dot size decreases. But the degeneracy and energy splitting are very different for these two quantum dots. When R_0 equals to zero, each $|j, m; z_1\rangle$ state of the PQD is a linear combination of the $|j, l; m\rangle$ states with different l in the SQD. The state of any principal quantum number n and the $\frac{1}{2}$ maximum $|m|$ with $z_1 = 1/2$ in the parabolic coordinate representation corresponds to the maximum orbital angular momentum l in the spherical coordinate representation. The corresponding relation is

$$|j, \frac{1}{2} |m|_{\max}; z_1 = 1/2\rangle = |j, l_{\max}; \frac{1}{2} |m|_{\max}\rangle \quad (13)$$

For example, for $n = 6$, $m = \frac{1}{2} 5$, $z_1 = z_2 = 1/2$, we obtain $\langle l | = 39 = Z$ from Eq. (10). This result can also be obtained for the $l = 5$ state from the following formula [10] in spherical coordinate space:

$$\langle l | = \frac{1}{2} 3n^2 - \frac{1}{2} (l + 1)^2 = Z \quad (14)$$

At $R_0 = 0$ and 1 the eigenenergies are in n^2 -degeneracy like the degeneracy of a free-space hydrogen atom. Between these two extreme situations, the n^2 -degeneracy disappears. For any specific n , it is found that the maximum number of the splitting levels is $[(n + 1)/2]^2$ if n is odd, and $n(n + 2)/4$ if n is even. This phenomenon is very different from the spherical quantum dot, where the number of the maximum splitting levels is n for any principal quantum number n .

The calculation of Stark effects for the SQD is much more difficult than that for the PQD. For the SQD, the perturbation matrix is non-diagonal. Moreover, every matrix element is complicated when calculated. When R_0 equals to zero, the SQD is the same as the PQD. They both become a hydrogenic atom in this specific situation. In spherical coordinates, the first order perturbation matrices for the degenerate states are not diagonal. Hence, the calculation of each matrix element is quite tedious. However, it is much easier to calculate the matrix elements in parabolic coordinates. When R_0 equals to zero, combining Eqs. (11) and (12), we get an analytic closed form:

$$E_{nmz_1} = E_n^0 + eF \frac{3}{2} n^2 (z_1 - z_2) = Z \quad (15)$$

This equation is in fact identical to that derived by Scharzschild and Epstein [9] on the base of the old quantum theory, which thus justifies the derivation of the equations discussed in this paper.

V. Conclusion

This article contains new results on different types of quantum dots. We apply different coordinates to study the characteristics of a hydrogen impurity in different cavities, and make detailed comparison between the two quantum dots under study. We solve the Schrödinger equation to obtain the system wavefunctions, eigenvalues, and their degeneracy analytically. We find that

the parabolic quantum dot has several features different from those of a spherical quantum dot. The competition of the dot size effect and the Stark effect are also studied. Since many researchers are now working on the electronic states in a quantum dot, these results would be helpful for people to understand quantum dots and manufacture an artificial atom.

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