氫雜質在量子點中的束縛能

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摘要

以有效質量近似法來計算氫雜質位於量子點(QD)中心的電子能階與束縛能，所得的特徵函數分別以懷泰克函數及庫侖波函數表示之。在無限高的位阱中，基態的束縛能的大小隨量子點半徑的縮減而增加,甚至增加至無限大。而在有限高的位阱中，基態的束縛能的大小隨量子點半徑的縮減而增加；但當到達一最大值後，隨即下降；並於半徑縮減至零時，束縛能減小至一特定值。對於被束縛在具有無限高位勢的量子點中的氫雜質的數個較低能階的能量我們也計算求得。

Binding Energy of Hydrogenic Impurity in Quantum Dots

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Abstract

The electronic state energies and the binding energies of a hydrogenic impurity located at the center of quantum dot (QD) are calculated within the effective-mass approximation. The eigenfunctions are expressed in term of Whittaker functions and Coulomb wave functions. For the infinite confining potential well, the binding energy of ground state is found to become infinite when the dot radius vanishes. For the finite confining potential well, the binding energy is found to approach a maximum value first as the dot radius decreases from larger value, and then it decreases to a characteristic value as the dot radius approach zero. The state energies for several lower lying excited states of the hydrogenic impurity confined within an infinite potential well QD are also calculated.

1.Introduction

Recently, the development of experimental crystal growth techniques such as chemical vapor deposition (CVD)[1], liquid-phase epitaxy (LPE), and molecular beam epitaxy (MBE) makes the fabrication of semiconductor structures of dimensions comparable to electronic de Broglie wavelength become possible[2-5]. Such structures are the so-called quantum wells(QW), quantum well wires(QWW) and quantum dot(QD). In the past ten years, impurity states in various confined systems, such as QWW, and QD have become a subject of extensive investigations in basic and applied researches. Altered by their size, the electronic[4,5] and optical [6-9]properties of the constituent semiconductor materials could be very different. For example, enhanced exciton binding energies and very high electronic mobilities have been reported for modulation doped quantum well layers of $GaAs/Ga_{1-x}Al_xAs$ [10-21].

Studies of quantum dots are very interesting problems because specific properties of these lower-dimensional structures can be easily achieved by varying the radius of the quantum dot. The properties of quantum dot may appear to be unaffected by the boundary when the radius of the quantum dot is very large. As the radius of the quantum dot become smaller, it behaves very much like an impurity atom in the three-dimensional case. For a QD with infinite confining potential, as the radius is reduced, an electron can move only in a smaller space and spends most of its time close to the impurity ion. However, spatial confinement begins to cause the kinetic energy of the electron to increase due to the uncertainty principle and eventually it may overcome the attractive potential between the electron and the impurity atom. The total energy may change from negative to positive at a certain radius of the confining system and finally diverges to infinity as the radius approaches zero. Moreover, the effective strength of the Coulomb interaction between the electron and the impurity atom depends on the geometric dimension of the system and is enhanced as the size of the system is reduced. All of the calculations have shown that the confinement and binding energy of impurity atom in a quantum well depend on the barrier V_0, the well size and sharp. The physical properties of electrons in quantum dots are very different from those in the bulk[4-21].

In this paper we calculate the electronic state energies and the binding energies of a hydrogenic impurity located at the center of quantum dot by using of effective-mass approximation. The impurity eigenfunctions are expressed in term of Whittaker functions and Coulomb wave functions.

2. Theory

A. hydrogenic impurity confined in the quantum dot

The calculation is based on the effective-mass approximation. Consider a hydrogenic impurity located at the center of a spherical dot which is confined by a spherical potential well with radius a. According to effective-mass theory, the Hamiltonian of this system can be written as

$$H = -\frac{\eta^2}{2\mu}\nabla^2 - \frac{e^2}{\varepsilon r} + V(r)$$

where

$$V(r) = \begin{cases} 0 \ , if\ r < a \\ V_0 \ , if\ r \geq a \end{cases}$$

and μ , ε are the effective mass, dielectric constant. V(r) is the confining potential. The Schrödinger equation for our system can be expressed as :

$$\mathbf{H}\ \Psi\ (r,\ \theta\ ,\ \varphi\ ) = E\ \Psi\ (r,\ \theta\ ,\ \varphi\ ) \quad (1)$$

In spherical coordinates (r, θ, φ), the above equation can be written as

$$-\frac{\eta^2}{2\mu}\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]\Psi - \frac{e^2}{\varepsilon r}\Psi + V(r)\Psi = E\Psi \quad (2)$$

$\Psi(r, \theta, \varphi)$ may be separated into the product $\mathbf{R}(r)\Theta(\theta)\,\Phi(\varphi)$, as in the case of the hydrogen atom, $\Theta(\theta)$ is the associated Legendre polynomial, and $\Phi(\varphi)=e^{im\varphi}$, m=0, ±1, ±2.... The differential equation for the radial part R(r) can be obtained as follows:

$$-\frac{\eta^2}{2\mu}\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{L(L+1)}{r^2}\right]R(r) - \frac{e^2}{\varepsilon r}R(r) + V(r)R(r) = ER(r) \quad (3)$$

(I). for r < a , V(r)=0, the eq. (2) can be written as

$$-\frac{\eta^2}{2\mu}\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{L(L+1)}{r^2}\right]R(r) - \frac{e^2}{\varepsilon r}R(r) = ER(r) \quad (4)$$

Since the motion of the electron is confined inside the dot, the existence of

positive bound states is possible. Therefore, one should study solutions of the Schrödinger equation in two regions. (a)For $E<0$, the solutions can be expressed in terms of Whittaker functions. (b)For $E>0$, the solutions can be expressed in terms of the Coulomb wave functions.

(a).Negative-energy region, $E<0$.

We set $\alpha_{1a}^2 = -\frac{8\mu E}{\eta^2} > 0, \xi = \alpha_{1a} r$ *and* $\lambda_1 = \frac{2\mu e^2}{\varepsilon \eta^2 \alpha_{1a}}$. Then Eq.(4) can be expressed as:

$$\frac{\partial^2 R}{\partial \xi^2} + \frac{2}{\xi}\frac{\partial R}{\partial \xi} + \left[-\frac{1}{4} + \frac{\lambda_1}{\xi} - \frac{L(L+1)}{\xi^2}\right] R = 0$$

(5)

If we further write $\mathbf{R}(\xi) = \xi^{-1}\mathbf{W}(\xi)$, then Eq.(5) becomes

$$\frac{\partial^2 W}{\partial \xi^2} + \left[-\frac{1}{4} + \frac{\lambda_1}{\xi} + \frac{\frac{1}{4} - (L+\frac{1}{2})^2}{\xi^2}\right] W = 0$$

(6)

Eq.(6) is the Whittaker equation [22,23] with the solutions as :

$$W_{\lambda_1, L}(\xi) = e^{-\frac{\xi}{2}} \xi^{L+1} \Phi(L+1-\lambda_1, 2L+2, \xi)$$

(7a)

or

$$W_{\lambda_1, -L}(\xi) = e^{-\frac{\xi}{2}} \xi^{-L+1} \Phi(-L+1-\lambda_1, -2L+2, \xi)$$

(7b)

where Φ is the confluent hypergeometric function

$$\Phi(a,b,x) = 1 + \frac{a}{b}\frac{x}{1} + \frac{a(a+1)}{b(b+1)}\frac{x^2}{2!} + \ldots + \frac{a(a+1)\ldots(a+k)}{b(b+1)\ldots(b+k)}\frac{x^k}{k!} + \ldots$$

$$= \sum_{k=0}^{\infty} \frac{(a)_k}{(b)_k}\frac{x^k}{k!}$$

The solution of Eq.(5) can be expressed as:

$$R(\xi) = \xi^{-1} W_{\lambda_1, L}(\xi) = e^{-\frac{\xi}{2}} \xi^{L} \Phi(L+1-\lambda_1, 2L+2, \xi)$$

(8a)

or

$$R(\xi) = \xi^{-1} W_{\lambda_1, -L}(\xi) = e^{-\frac{\xi}{2}} \xi^{-L} \Phi(-L+1-\lambda_1, -2L+2, \xi)$$

(8b)

Considering the wave function must be finite everywhere, we have to drop the solution of Eq.(8b). Then wave function of radial part in the r < a region, can be expressed as:

(b).Positive-energy region, E > 0.

We set $\alpha_{1b}^2 = -\frac{2\mu E}{\eta^2} > 0$, $\xi = \alpha_{1b} r$ *and* $\beta_1 = -\frac{\mu e^2}{\varepsilon \eta^2 \alpha_{1b}}$. Then Eq.(4) can be expressed as:

$$\frac{\partial^2 R}{\partial \xi^2} + \frac{2}{\xi}\frac{\partial R}{\partial \xi} + \left[-\frac{1}{4} - \frac{2\beta_1}{\xi} - \frac{L(L+1)}{\xi^2}\right] R = 0$$

(10)

If we further write $\mathbf{R}(\xi) = \xi^{-1}\mathbf{F}(\xi)$, then Eq.(5) becomes

$$\frac{\partial^2 F}{\partial \xi^2} + \left[-\frac{1}{4} - \frac{2\beta_1}{\xi} - \frac{L(L+1)}{\xi^2}\right] F = 0$$

(11)

Eq.(11) is the Coulomb wave equation[24] which has two linearly independent solutions,
$F_{\beta_1,L}(\xi)$ *and* $G_{\beta_1,L}(\xi)$.

$$F_{\beta_1,L}(\xi) = \xi^{L+1}\Phi_{\beta_1,L}(\xi).$$

(12a)

$$G_{\beta_1,L}(\xi) = F_{\beta_1,L}(\xi)\left[\ln(2\xi) + \frac{q_L(\beta_1)}{p_L(\beta_1)}\right] + \theta_{\beta_1,L}(\xi)$$

(12b)

where $\Phi_{\beta_1,L}(\xi) = \sum_{k=L+1}^{\infty} A_k^L(\beta_1)\xi^{k-L-1}$

with recurrence relation:

$$A_{L+1}^L(\beta_1) = 1$$

$$A_{L+2}^L(\beta_1) = \frac{\beta_1}{L+1}$$

$$A_k^L(\beta_1) = \frac{2\beta_1 A_{k-1}^L(\beta_1) - A_{k-2}^L(\beta_1)}{(k+L)(k-L-1)} \quad for\ k > L+2$$

Since $G_{\beta_1,L}(\xi)$ is singular at $\xi = 0$. Hence the wave function of radial part in the E > 0 should be written as

$$R_1(\alpha_{1b}r) = C_{1b}\sum_{k=L+1}^{\infty} A_k^L(\beta_1)(\alpha_{1b}r)^{k-L}$$

(13)

where C_{1b} is the normalization constant.

(c). The turning point E=0

In this case, the bound- state energy changes from positive to negative. Substituting E=0 into Eq.(4) and arranging , we can get the equation as:

$$r^2\frac{\partial^2 R(r)}{\partial r^2} + 2r\frac{\partial R(r)}{\partial r} + \left[-L(L+1) + \frac{2\mu e^2}{\varepsilon\eta^2}r\right]R(r) = 0$$

(14)

Comparing with the modified Bessel equation

$$r^2\frac{\partial^2 u(r)}{\partial r^2} + (1-2\omega)r\frac{\partial u(r)}{\partial r} + (\omega^2 - \nu^2\gamma^2 + \alpha^2\gamma^2 r^{2\gamma})u(r) = 0$$

(15)

The solution of eq.(15) can express as :

$$u(r) = r^{\omega}\left[C_1' J_{\nu}(\alpha r^{\gamma}) + C_1' N_{\nu}(\alpha r^{\gamma})\right]$$

where $J_{\nu}(\alpha r^{\gamma})$:Bessel function

$N_{\nu}(\alpha r^{\gamma})$:Neumann function

We can get the following relations: ω=-1/2, γ =1/2, ν =2L+1, and $\alpha^2 = \frac{8\mu e^2}{\varepsilon\eta^2}$.

Since the radial function must be finite for L=0, the wave function of radial part we can write as

$$R_1(r) = C_{1c}J_{2L+1}\left(\sqrt{\frac{8\mu e^2}{\varepsilon\eta^2}}r^{\frac{1}{2}}\right)$$

(16)

(Ⅱ). for r > a , $V(r)=V_0$

The differential equation for the radial part R(r) can be expressed as:

$$-\frac{\eta^2}{2\mu}\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{L(L+1)}{r^2}\right]R(r) - \frac{e^2}{\varepsilon r}R(r) + V_0 R(r) = ER(r)$$

(17)

We set $\alpha_2^2 = -\frac{8\mu(E-V_0)}{\eta^2} > 0, \xi = \alpha_2 r$, $\lambda_2 = \frac{2\mu e^2}{\varepsilon\eta^2\alpha_2}$ and $\mathbf{R}(\xi) = \xi^{-1}\mathbf{W}(\xi)$. Then Eq.(17) becomes

$$\frac{\partial^2 W}{\partial \xi^2} + \left[-\frac{1}{4} + \frac{\lambda_2}{\xi} + \frac{\frac{1}{4} - (L+\frac{1}{2})^2}{\xi^2} \right] W = 0$$

(18)

We obtain the Whittaker equation once again, but both Eq.(7a) and Eq.(7b) are not well behaved when ξ becomes large. The integral representation of Whittaker function is used as the solution of the system[25].

$$W_{\lambda_2,L}(\xi) = C_2 e^{-\frac{\xi}{2}} \xi^{\lambda_2} \int_0^\infty e^{-t} t^{-\lambda_2+L} (1+\frac{t}{\xi})^{\lambda_2+L} dt$$

(19)

Hence the wave function of radial part in the r > b should be written as

$$R_2(\alpha_2 r) = C_2 e^{-\frac{(\alpha_2 r)}{2}} (\alpha_2 r)^{\lambda_2 - 1} \int_0^\infty e^{-t} t^{-\lambda_2+L} (1+\frac{t}{\alpha_2 r})^{\lambda_2+L} dt$$

(20)

The boundary conditions require that the wave functions and its derivative should be continuous at the boundary. Thus one can get the following equation.

$$\frac{R_1'(\alpha_1 a)}{R_1(\alpha_1 a)} = \frac{R_2'(\alpha_2 a)}{R_2(\alpha_2 a)}$$

(21)

Solving Eq.(21), we obtain the eigenvalue E.

B. electron confined in the quantum dot

The Hamiltonian of this system can be written as

$$H = -\frac{\eta^2}{2\mu}\nabla^2 + V(r)$$

(22)

where $V(r) = \begin{cases} 0, & if\ r < a \\ V_0, & if\ r \geq a \end{cases}$

In the spherical coordinate, the Schrödinger equation for the radial part R(r) can be obtained as follows:

$$r^2\frac{\partial^2 R(r)}{\partial r^2}+2r\frac{\partial R(r)}{\partial r}+\left[-L(L+1)-\frac{2\mu V(r)}{\eta^2}\right]R(r)=-\frac{2\mu}{\eta^2}ER(r)$$

(23)

(I). for r < a , V(r)=0, the Eq. (23) can be written as

$$r^2\frac{\partial^2 R(r)}{\partial r^2}+2r\frac{\partial R(r)}{\partial r}+\left[-L(L+1)+\frac{2\mu E}{\eta^2}\right]R(r)=0$$

(24)

Comparing with the modified Bessel equation(Eq.(15)), the wave function of the radial part can be expressed as

$$R_1(r)=C_1 r^{-\frac{1}{2}}J_{L+\frac{1}{2}}(\sqrt{\frac{2\mu E}{\eta^2}})$$

(25)

(II). for r ≧ a , V(r)=V_0

Let $\alpha_2^2=-\frac{8\mu(E-V_2)}{\eta^2}>0$, $\xi=\alpha_2 r$, and $\mathbf{R}(\xi)=\xi^{-1}\mathbf{W}(\xi)$. Then eq.(27) becomes

$$\frac{\partial^2 W}{\partial\xi^2}+\left[-\frac{1}{4}+\frac{\frac{1}{4}-(L+\frac{1}{2})^2}{\xi^2}\right]W=0$$

(26)

We obtain the Whittaker equation once again, then the solution of the system written as

$$R_2(\alpha_2 r)=C_3 e^{-\frac{(\alpha_3 r)}{2}}(\alpha_2 r)^{-1}\int_0^\infty e^{-t}t^L(1+\frac{t}{\alpha_2 r})^L dt$$

(27)

The boundary conditions require that the wave functions and its derivative should be continuous at the boundary. Thus one can get the following equation.

$$\frac{R_1'(\alpha_1 a)}{R_1(\alpha_1 a)}=\frac{R_2'(\alpha_2 a)}{R_2(\alpha_2 a)}$$

(28)

Solving Eq.(28), we obtain the eigenvalue E.

3.Results and discussions

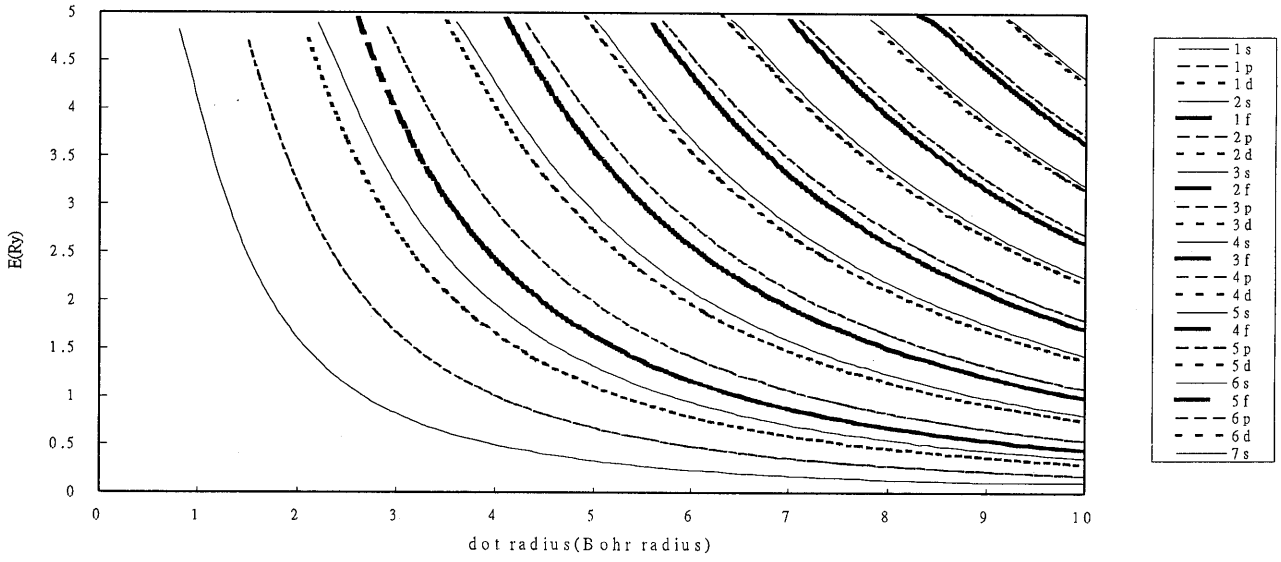

Fig 1:Spectrum of electron confined in the quantum dot with the potential well of V_0=5 Ry.

Fig.1. presents the spectrum of an impurity confined in the quantum dot with potential well of V_0=5. The radius is expressed in terms of the effective Bohr radius ($a_0^* = \varepsilon^2/(\mu e^2)$, and the energy is expressed in terms of the effective Rydberg($Ry=e^2/(2\varepsilon a_0^*)$. The order of En,l is the same as J.L. Zhu's[18,26]. In Fig.1, the bound-state energies for electronic states 1s 1p 1d 2s 1f 2p 2d 3s 2f 3p...in order sequence are presented as the functions of the dot radius. Table1 shows the calculated bound-state energies of a hydrogenic impurity confined in a QD, we compare our result with those of J.L. Zhu's.

Table1. Compare the bounded-state energy of electron in a QD with J.L. Zhu's, for R=1 a_0^* and

2.5 a_0^* and V_0=80Ry

$R(a_0^*)$	V_0 (Ry)	1s	1p	1d	2s	1f	2p	2d	3s	2f	3p	3d	4s	3f	4p	4d	5s	4f	
1	80	7.947	16.21	26.58	31.42	38.92	46.93	64.19	68.07										
1	80	7.957	16.23	26.59	31.43	38.92	47.02												J.L. Zhu'S
2.5	80	1.442	2.951	4.847	5.765	7.143	8.721	12.09	12.97	15.86	17.38	22.16	23.03	27.35	28.82	35.01	35.87	41.59	

2.5	80	1.446	2.958	4.866	5.781	7.151	8.735												J.L. Zhu·S

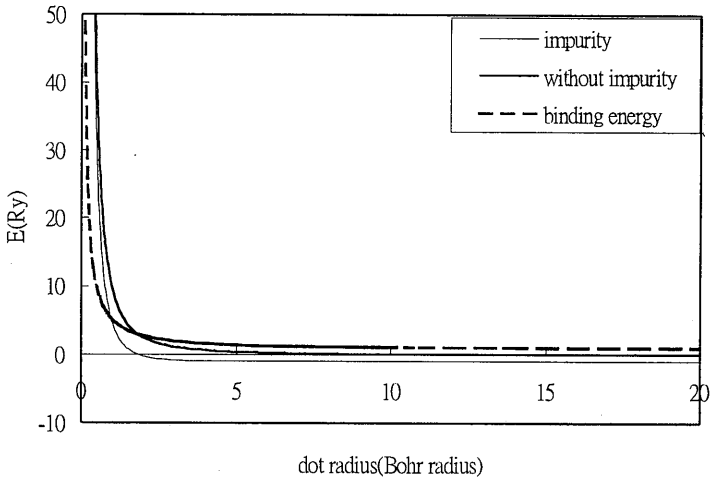

Fig.2a The ground state binding energy of a hydrogenic impurity in QD as a function of dot radius for the infinite barrier .

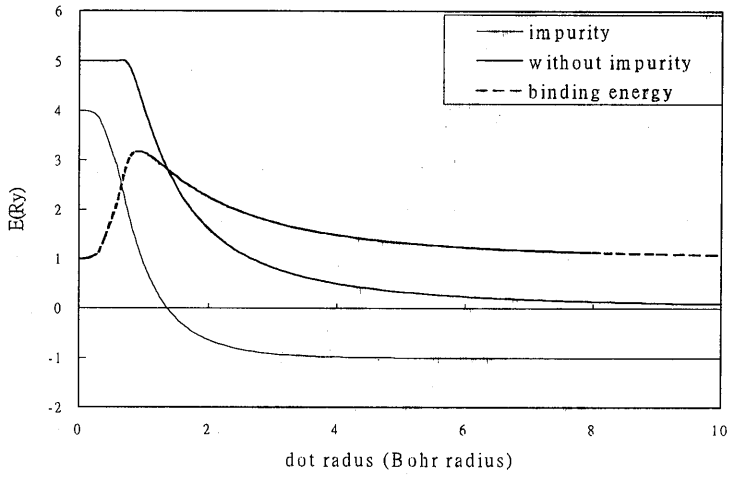

Fig.2b The ground state binding energy of a hydrogenic impurity in QD as a function of dot radius for the finite barrier V_0=5Ry.

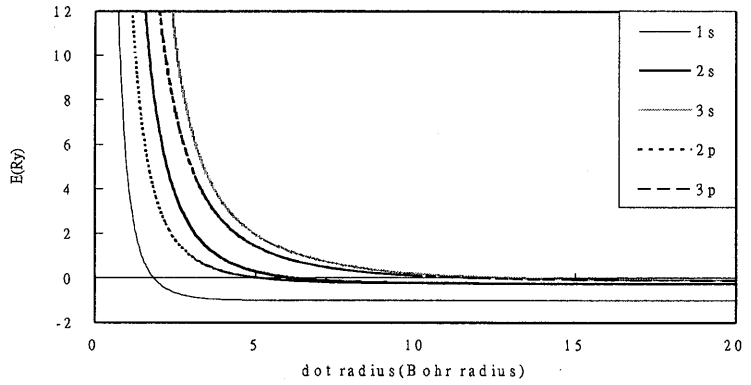

Fig.3 The excited state energy of hydrogenic impurity confined in the QD as a function of r for the infinite barrier .

In Fig.2a and Fig.2b, we plot the ground state binding energy of a hydrogenic impurity in QD as a function of dot radius for the infinite potential and finite potential cases. In the infinite potential case, the binding energy continuously increases and becomes to be infinite as the radius of the dot decreases to zero, our results are agree with those obtained by Chuu et al.[20]. While in the case of a finite potential well, the binding energy first approach to a maximum value as the dot radius decreases from a larger value and then decreases to a characteristic value. Fig.3 shows the excited state energy of a hydrogenic impurity confined in the QD as a function of the dot radius r. Our result shows that the energy of 1s state approaches to -1Ry, while both 2s and 2p states approach to -1/4Ry, and both 3s and 3p states approach to -1/9Ry as the dot radius becomes very large. The behavior is very similar with that of a free hydrogen atom. As the radius of dot decreases the degeneracy of 2s and 2p states is splitting. The degeneracy of the states 3s and 3p states behaves the same way too. Further, for small radii r, the energy of 2s state is larger than that of the 2p state.

4.Conclusion

We have solved the Schrodinger equation and obtained the exact solutions of the energy states a hydrogenic impurity confined e in a QD. The results are the same as that of J.L. Zhu's. The binding energy of hydrogenic impurity confined in a QD with a finite barrier potential is different from that with an infinite barrier potential. The binding energy continuously increases as the radius of the dot decreases while in the finite potential well case, the binding energy approaches a maximum value as the dot radius decreases and then decreases to a characteristic value. The excited state energy of a hydrogenic impurity confined with an

infinite potential in a QD is degenerate for large radii, and splits for small radii. For large radii, the energies of 1s,2s,2p,3s and 3p states approach to the energies of a free hydrogen atom.

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