Exact Numerical Solution of the Binding Energy of Hydrogenic Impurity in Quantum Circle and Dot

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Abstract

Exact numerical solution of the lower lying state binding energies of hydrogenic impurity located at the center of a GaAs-$Al_xGa_{1-x}As$ quantum circle and quantum dot. The eigenfunctions of the impurity can be expressed in terms of Whittaker functions and Coulomb wave functions. The ground state and lower lying state binding energies are expressed in terms of the circle and dot radius. For the single layer quantum circle, the ground state binding energy approaches 4 Ry as the radius approaches infinite and zero, like a hydrogenic impurity in 2-D. For the single layer quantum dot, the ground state binding energy approaches 1 Ry as the radius approaches infinite and zero, like a hydrogenic impurity in 3-D. For the multi-layer case, the ground state binding energy approaches the same value as the single layer case as the radius approaches infinite, but it approaches different value as the radius reduces to zero. Our results are in agreement with the prediction of He^8.

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1. Introduction

The development and improvement of semiconductor growth techniques such as chemical vapor deposition (CVD), liquid-phase epitaxy (LPE) and molecular beam epitaxy (MBE), have led to the possibility of controlling material composition and of incorporating impurity on the electronic de Broglie scale[1-5]. Impurity states in various confined systems, such as quantum-well wires (QWWs) and quantum dots (QDs), have been a subject of extensive investigations in basic and applied research. The GaAs- $Al_xGa_{1-x}As$ heterostructure system is potentially useful material for high-speed digital, high-frequency microwave, and electro-optic device applications[6].

A great number of studies concern the electronic bound states of impurity in semiconductor. Since Bastard's[7] pioneer works in the study of the binding energy of a hydrogenic impurity within an infinite potential-well structure, many theoretical works have been devoted to the study of the properties of impurity states in various confining systems. The binding energy of the lower lying state of a hydrogenic impurity E_b in D dimensions is given by[8] $E_b=[2/(2n+D-3)]^2$ Ry, where Ry is the effective Rydberg and n is the principal quantum number. In the 2-D case, the binding energy increases four times relative to the 3-D case, while in the 1-D case the increases is infinite. Bryant[9-10] improved the model calculation by assuming a finite barrier for the confining potential with the impurity on and off the axis of cylinder wire. The binding energies for the bound states of hydrogenic impurity in a quantum-well wire of GaAs-$Ga_{1-x}Al_xAs$ have been found to be 2-3 times larger than those of in comparable 2-D wells. In the calculation of the hydrogenic impurity states, a variational principle with a trial wave function which takes into account the confinement of the carriers in the quantum-well wire or the quantum dot was usually employed[9-23]. All of the calculations have shown that the binding energy of the impurity atom in a quantum well depends prominently on the barrier height V_0 and the well size. The physical properties of electrons in quantum dots are very different from those in the bulk. As a consequence of the confinement, energy levels are discrete. The existence of these atomic-like state may be utilized in future laser where laser properties can

be tailored by proper choices of well and barrier materials as well as sizes and shapes of the QDs. The change in impurity binding energies due to confinement effect has been observed in photoluminescence[24-27] and Raman-scattering[28,29] experiments on the impurities in the quantum wells.

The study of the impurity states in quantum dots is of physics interest because specific properties of the impurity in lower-dimensional structures can be achieved easily by varying the radius of the quantum dot. The properties of an impurity atom in a quantum dot may appear to be unaffected by the boundary when the radius is very large. For an impurity in a QD with infinite confining potential, as the radius is reduced, the electron can move only in a smaller space and spends closer to the impurity ion. However, spatial confinement will cause the kinetic energy of the electron to increase due to the uncertainty principle and eventually may make the electron to overcome the attractive potential. Therefore, the total energy of the impurity may change from negative to positive for certain dot radius 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. Thus, the effective strength of the Coulomb interaction in QDs can be adjusted by varying the dot radius. On the contrary, dramatic changes in the binding energies may serve as a clear signal for changes in the effective dimension of QDs.

Yafet et al. first discussed the bound states of hydrogen atom subjected to a magnetic field. They showed the ground-state electronic wave function contracts in all dimensions but elongates along the field direction as the field strength increases. The effect of a magnetic field on the 1s- and 2p-like states of an electron bound to a hydrogenic impurity in a quantum-well structure have been examined by Chauduri et al. They have shown that binding energy increases in response to larger magnetic fields directed along the growth axis of a quantum-well or as the width of the quantum-well becomes smaller. Smith et al. have reported oscillatory structure in

capacitance versus gate voltage in zero magnetic field and have attributed it to the discrete energy states of a quantum dot. Kumar et al. indicated that the energy levels are quite insensitive to the charge in the quantum dot at a fixed gate voltage, and that the evolution of levels with increasing magnetic field is similar to that for a parabolic potential. Liu et al. investigated theoretically and experimentally the energy levels and allowed optical transitions with ΔE of a qusi-zero-dimensional electron gas in a magnetic field.

Our system is constructed as a core made of GaAs surrounded by a shell of $Al_xGa_{1-x}As$ and then embedded in the bulk of $Al_yGa_{1-y}As$. The polarization and image charge effects [30-31] may be significant if there is a large dielectric discontinuity between the dot and the surrounding medium. However, this is not the case for the GaAs-$Al_xGa_{1-x}As$ quantum system; therefore we ignore such effects. The barrier height between GaAs and $Al_xGa_{1-x}As$ can be obtained from a fixed ratio Q=0.7 of the band-gap discontinuity[6] $\Delta E_g = 1.247x$ eV for $0 \le x \le 0.45$ and $\Delta E_g = 0.576 + 0.125x + 0.143x^2$ for $0.45 < x \le 1$. In this paper, the effective atomic units are used so that all energies are measured in the units of the effective Rydberg(Ry) and all distances are measured in the units of effective Bohr radius a_0^*. The Ry and a_0^*. can be determined by $\frac{\mu e^4}{2\hbar^2\varepsilon^2}$ and $\frac{\varepsilon\hbar^2}{\mu e^2}$, where μ and ε are, respectively, the electronic effective mass and the dielectric constant of GaAs material and equal to $0.067m_e$ and 13.18. Then the Ry and a_0^*. are equal to 5.2 meV and 104 $\overset{o}{A}$, respectively.

2. Theory

A. 2D-impurity confined in the multi-layer quantum circle

Consider an impurity located at the center of circle confined by circle potential wells. The confining potential V_1 is assumed to be zero inside the dot (ρ<a), and V_2 inside the shell(a≦ρ<b), V_3 outside the shell (ρ≧b), where a is the core circle

radius and b is the total circle (core plus shell) radius, therefore b-a is the thickness of the shell. According to the effective-mass approximation, the Hamiltonian of the system can be written as

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

where

$$V(\rho) = \begin{cases} 0, if\ \rho < a \\ V_2, if\ a \le \rho < b \\ V_3, if\ \rho \ge b \end{cases}$$

and $V(\rho)$ is the confining potential, μ and ε are the electronic effective mass and the dielectric constant of the material. The Schrödinger equation expressed in polar coordinates (ρ, θ)

$$H\Psi(\rho, \theta) = E\Psi(\rho, \theta) \tag{1}$$

can be written as:

$$-\frac{\hbar^2}{2\mu}\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}\right]\Psi - \frac{e^2}{\varepsilon\rho}\Psi + V(\rho)\Psi = E\Psi \tag{2}$$

Separate $\Psi(\rho, \theta)$ into a product of three terms $R(\rho)\Theta(\theta)$. Where $\Theta(\theta)$ can be expressed as $\Phi(\varphi) = e^{im\varphi}$, m=0, ±1, ±2.... The equation for the radial part $R(\rho)$ can be obtained as follows:

$$-\frac{\hbar^2}{2\mu}\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} - \frac{m^2}{\rho^2}\right]R(\rho) - \frac{e^2}{\varepsilon\rho}R(\rho) + V(\rho)R(\rho) = ER(\rho) \tag{3}$$

This equation can be solved in two different situations:

(I). For $\rho < a$, $V(\rho) = 0$

Eq. (2) can be rewritten as

$$-\frac{\hbar^2}{2\mu}\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} - \frac{m^2}{\rho^2}\right]R(\rho) - \frac{e^2}{\varepsilon\rho}R(\rho) = ER(\rho) \tag{4}$$

As the electron is confined inside the core dot, the existence of positive energy bound states is possible, therefore, solutions of the Schrödinger equation can be studied in two regions:

(a). For negative-energy, E<0

Define $\alpha_{1a}^2 = -\frac{8\mu E}{\hbar^2} > 0, \xi = \alpha_{1a}\rho$ and $\lambda_1 = \frac{2\mu e^2}{\varepsilon\hbar^2\alpha_{1a}}$, then Eq. (4) can be expressed as:

$$\frac{\partial^2 R}{\partial\xi^2} + \frac{1}{\xi}\frac{\partial R}{\partial\xi} + \left[-\frac{1}{4} + \frac{\lambda_1}{\xi} - \frac{m^2}{\xi^2}\right]R = 0 \tag{5}$$

If we further write $R(\xi) = \xi^{-1/2}W(\xi)$, then Eq. (5) becomes

$$\frac{\partial^2 W}{\partial\xi^2} + \left[-\frac{1}{4} + \frac{\lambda_1}{\xi} - \frac{\frac{1}{4} - m^2}{\xi^2}\right]W = 0 \tag{6}$$

Eq. (6) is the Whittaker equation [32,33] which has two linearly independent solutions. Since the wave function has to be finite everywhere, the solution of the radial part in the ρ <a region can be expressed as:

: $$R(\xi) = \xi^{-\frac{1}{2}}W_{\lambda_1,m}(\xi) = e^{-\frac{\xi}{2}}\xi^m\Phi(m+\frac{1}{2}-\lambda_1, 2m+1, \xi) \tag{7}$$

where Φ is the confluent hypergeometric function

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

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

$$R_1(\alpha_{1a}\rho) = C_{1a}e^{-\frac{\alpha_{1a}\rho}{2}}(\alpha_{1a}\rho)^m\Phi(m+\frac{1}{2}-\lambda_1, 2m+1, \alpha_{1a}\rho) \tag{8}$$

where C_{1a} is the normalization constant.

(b). For positive-energy, E>0

Define $\alpha_{1b}^2 = \frac{2\mu E}{\hbar^2} > 0, \xi = \alpha_{1b}\rho$ and $\beta_1 = -\frac{\mu e^2}{\varepsilon\hbar^2\alpha_{1b}}$, then Eq. (4) can be expressed as:

$$\frac{\partial^2 R}{\partial\xi^2} + \frac{1}{\xi}\frac{\partial R}{\partial\xi} + \left[1 + \frac{2\beta_1}{\xi} - \frac{m^2}{\xi^2}\right]R = 0 \tag{9}$$

If we further write $R(\xi) = \xi^{-1/2}F(\xi)$, then Eq. (9) becomes

$$\frac{\partial^2 F}{\partial \xi^2}+\left[1+\frac{2\beta_1}{\xi}-\frac{m^2-\frac{1}{4}}{\xi^2}\right]F=0 \tag{10}$$

Eq. (10) is the Coulomb wave equation[34] which has two linearly independent solutions $F_{\beta_1,m}(\xi)$ and $G_{\beta_1,m}(\xi)$, where

$$F_{\beta_1,m}(\xi)=\xi^{m+\frac{1}{2}}\Phi_{\beta_1,m}(\xi).\,, \tag{11a}$$

$$G_{\beta_1,m}(\xi)=F_{\beta_1,m}(\xi)\left[\ln(2\xi)+\frac{q_m(\beta_1)}{p_m(\beta_1)}\right]+\theta_{\beta_1,m}(\xi) \tag{11b}$$

and

$$\Phi_{\beta_1,m}(\xi)=\sum_{k=0}^{\infty}A_k^m(\beta_1)\xi^{k-\frac{1}{2}}$$

The recurrence relation can be expressed as:

$$A_m^m(\beta_1)=1$$

$$A_{m+1}^m(\beta_1)=-\frac{2\beta_1}{1+2|m|}$$

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

$G_{\beta_1,L}(\xi)$ is singular at ξ=0, hence the wave function of the radial part in the region E>0 can be expressed as

$$R_1(\alpha_{1b}r)=C_{1b}\sum_{k=0}^{\infty}A_k^m(\beta_1)(\alpha_{1b}\rho)^{k+|m|}. \tag{12}$$

where C_{1b} is the normalization constant.

(Ⅱ). For $a\leqq\rho<b$, $V(\rho)=V_2$

The differential equation for the radial part $R(\rho)$ can be expressed as:

$$-\frac{\hbar^2}{2\mu}\left[\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{m^2}{\rho^2}\right]R(\rho)-\frac{e^2}{\varepsilon\rho}R(\rho)+V_2R(\rho)=ER(\rho) \tag{13}$$

Define $\alpha_2^2=-\frac{8\mu(E-V_2)}{\hbar^2}>0$, $\xi=\alpha_2\rho$, $\lambda_2=\frac{2\mu e^2}{\varepsilon\hbar^2\alpha_2}$ and $R(\xi)=\xi^{-1/2}W(\xi)$, then Eq. (13)

can be rewritten as:

$$\frac{\partial^2 W}{\partial \xi^2}+\left[-\frac{1}{4}+\frac{\lambda_2}{\xi}-\frac{\frac{1}{4}-m^2}{\xi^2}\right]W=0 \tag{14}$$

This is the Whittaker equation. Thus, the solution can be written as:

$$\begin{aligned}R_2(\alpha_2\rho)&=C_{21}e^{-\frac{\alpha_2\rho}{2}}(\alpha_2\rho)^{|m|}\Phi(|m|+\frac{1}{2}-\lambda_2,2|m|+1,\alpha_2\rho)\\&+C_{22}e^{-\frac{\alpha_2\rho}{2}}(\alpha_2\rho)^{|m|}\Big\{\Phi(|m|+\frac{1}{2}-\lambda_2,2|m|+1,\alpha_2\rho)\ln(\alpha_2\rho)\\&+\sum_{k=0}^{\infty}\frac{(|m|+\frac{1}{2}-\lambda_2)_k}{(2|m|+1)_k}\frac{(\alpha_2\rho)^k}{k!}\times\Big[\phi(|m|+\frac{1}{2}-\lambda_2+k)-\phi(2|m|+1+k)-\phi(1+k)\Big]+\\&+\frac{\Gamma(2|m|)\Gamma(2|m|+1)\Gamma(-|m|+\frac{1}{2}-\lambda_2)(-1)^{2|m|+1}}{\Gamma(|m|+\frac{1}{2}-\lambda_2)}\times\sum_{k=0}^{2L}\frac{(-|m|+\frac{1}{2}-\lambda_2)_k}{(-2|m|-1)_k}\frac{(\alpha_2\rho)^{k-2|m|}}{k!}\Big\}\end{aligned} \tag{15}$$

where C_{21}, C_{22} are normalization constants.

(Ⅲ). For $\rho \geqq b$, $V(\rho)=V_3$

The differential equation for the radial part $R(\rho)$ can be expressed as:

$$-\frac{\hbar^2}{2\mu}\left[\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\frac{m^2}{\rho^2}\right]R(\rho)-\frac{e^2}{\varepsilon\rho}R(\rho)+V_3R(\rho)=ER(\rho) \tag{16}$$

Define $\alpha_3^2=-\frac{8\mu(E-V_3)}{\hbar^2}>0$, $\xi=\alpha_3\rho$, $\lambda_3=\frac{2\mu e^2}{\varepsilon\hbar^2\alpha_3}$, and $R(\xi)=\xi^{-1/2}W(\xi)$, then Eq. (16) becomes

$$\frac{\partial^2 W}{\partial \xi^2}+\left[-\frac{1}{4}+\frac{\lambda_3}{\xi}-\frac{\frac{1}{4}-m^2}{\xi^2}\right]W=0 \tag{17}$$

This is the Whittaker equation. The Whittaker functions expressed in Eq. (15) is not well behaved as ξ becomes very large, we thus turn to use the integral representation of Whittaker function

$$W_{\lambda_3,L}(\xi) = C_3 e^{-\frac{\xi}{2}} \xi^{\lambda_3} \int_{0^+}^{\infty} e^{-t} t^{-\lambda_3+m-\frac{1}{2}} (1+\frac{t}{\xi})^{\lambda_3+m-\frac{1}{2}} dt \tag{18}$$

in our calculation. Hence the radial part wave function in the $\rho > b$ region can be written as

$$R_3(\alpha_3\rho) = C_3 e^{-\frac{\alpha_3 r}{2}} (\alpha_3\rho)^{\lambda_3-\frac{1}{2}} \int_0^{\infty} e^{-t} t^{-\lambda_3+m-\frac{1}{2}} (1+\frac{t}{\alpha_3\rho})^{\lambda_3+m-\frac{1}{2}} dt \tag{19}$$

The boundary conditions require:

$$\frac{R_1'(\alpha_1 a)}{R_1(\alpha_1 a)} = \frac{R_2'(\alpha_2 a)}{R_2(\alpha_2 a)} \tag{20}$$

$$\frac{R_2'(\alpha_2 b)}{R_2(\alpha_2 b)} = \frac{R_3'(\alpha_3 b)}{R_3(\alpha_3 b)} \tag{21}$$

Using above two equations, one can obtain the eigenvalue E.

B. electron confined in the multi-layer quantum circle

The Hamiltonian of an electron confined in the multi-layer quantum circle can be written as:

$$H = -\frac{\hbar^2}{2\mu}\nabla^2 + V(\rho) \tag{22}$$

where

$$V(\rho) = \begin{cases} 0, if\ \rho < a \\ V_2, if\ a \le \rho < b \\ V_3, if\ \rho \ge b \end{cases}$$

Schrödinger equation for the radial part R(ρ) can be expressed in spherical coordinate as:

$$-\frac{\hbar^2}{2\mu}\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} - \frac{m^2}{\rho^2}\right] R(\rho) + V(\rho)R(\rho) = ER(\rho) \tag{23}$$

(I). For $\rho < a$, V(ρ)=0

The Eq. (23) can be written as

$$\frac{d^2R}{d\rho^2}+\frac{1}{\rho}\frac{dR}{d\rho}+(\frac{2\mu E}{\hbar^2}-\frac{m^2}{\rho^2})R=0 \tag{24}$$

Comparing with the modified Bessel equation, the wave function of the radial part can be expressed as

$$R_1(\rho)=C_1J_m(\sqrt{\frac{2\mu E}{\hbar^2}}\rho) \tag{25}$$

(Ⅱ). For $a\leqq\rho<b$, $V(\rho)=V_2$

Set $\alpha_2^2=-\frac{8\mu(E-V_2)}{\hbar^2}>0$, $\xi=\alpha_2\rho$, and $R(\xi)=\xi^{-1/2}W(\xi)$, then Eq. (23) becomes

$$\frac{\partial^2W}{\partial\xi^2}+\left[-\frac{1}{4}+\frac{\frac{1}{4}-m^2}{\xi^2}\right]W=0 \tag{26}$$

This is the Whittaker equation. Thus, the solution of the system can be written as

$$R_2(\alpha_2\rho)=C_{21}e^{-\frac{\alpha_2\rho}{2}}(\alpha_2\rho)^m\Phi(m+\frac{1}{2},2m+1,\alpha_2\rho)$$

$$+C_{22}e^{-\frac{\alpha_2\rho}{2}}(\alpha_2\rho)^{-m}\Phi(-m+\frac{1}{2},-2m+1,\alpha_2\rho) \tag{27}$$

(Ⅲ). For $\rho\geqq b$, $V(\rho)=V_3$

Let $\alpha_3^2=-\frac{8\mu(E-V_3)}{\hbar^2}>0$, $\xi=\alpha_3\rho$, and $R(\xi)=\xi^{-1/2}W(\xi)$, then Eq. (23) becomes

$$\frac{\partial^2W}{\partial\xi^2}+\left[-\frac{1}{4}+\frac{\frac{1}{4}-m^2}{\xi^2}\right]W=0 \tag{28}$$

which is the Whittaker equation, and the solution of the system can be written as

$$R_3(\alpha_3\rho)=C_3e^{-\frac{\alpha_3\rho}{2}}\int_{0^+}^{\infty}e^{-t}t^{m-\frac{1}{2}}(1+\frac{t}{\alpha_3\rho})^{m-\frac{1}{2}}dt \tag{29}$$

Using boundary conditions

$$\frac{R_1'(\alpha_1a)}{R_1(\alpha_1a)}=\frac{R_2'(\alpha_2a)}{R_2(\alpha_2a)} \tag{30}$$

$$\frac{R_2'(\alpha_2 b)}{R_2(\alpha_2 b)} = \frac{R_3'(\alpha_3 b)}{R_3(\alpha_3 b)} \tag{31}$$

one can obtain the eigenvalue E.

C. Hydrogenic impurity confined in the MLQD

Consider a hydrogenic impurity located at the center of a multi-layer spherical dot confined by spherical potential wells. The confining potential V_1 is assumed to be zero inside the dot (r<a), and V_2 inside the shell(a≦r<b), V_3 outside the shell (r≧b), where a is the core radius and b is the total dot (core plus shell) radius, therefore b-a is the thickness of the shell. According to the effective-mass approximation, the Hamiltonian of the system can be written as

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

where

$$V(r) = \begin{cases} 0 \ , if\ r < a \\ V_2 \ , if\ a \le r < b \\ V_3 \ , if\ r \ge b \end{cases}$$

and V(r) is the confining potential, μ and ε are the electronic effective mass and the dielectric constant of the material. The Schrödinger equation expressed in spherical coordinates (r, θ, φ)

$$H\Psi(r, \theta, \varphi) = E\Psi(r, \theta, \varphi) \tag{32}$$

can be written as:

$$-\frac{\hbar^2}{2\mu}\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]\Psi - \frac{e^2}{\varepsilon r}\Psi + V(r)\Psi = E\Psi \tag{33}$$

Separate $\Psi(r, \theta, \varphi)$ into a product of three terms $R(r)\Theta(\theta)\Phi(\varphi)$. Where $\Theta(\theta)$ can be expressed in terms of the associated Legendre polynomial, and $\Phi(\varphi)=e^{im\varphi}$, m=0, ±1, ±2.... The equation for the radial part R(r) can be obtained as follows:

$$-\frac{\hbar^2}{2\mu}\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{L(L+1)}{r^2}\right]R(r) - \frac{e^2}{\varepsilon r}R(r) + V(r)R(r) = ER(r) \tag{34}$$

This equation can be solved in two different situations:

(I).For r<a , V(r)=0

Eq. (34) can be rewritten as

$$-\frac{\hbar^2}{2\mu}\left[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{L(L+1)}{r^2}\right]R(r)-\frac{e^2}{\varepsilon r}R(r)=ER(r) \tag{35}$$

As the electron is confined inside the core dot, the existence of positive energy bound states is possible, therefore, solutions of the Schrödinger equation can be studied in two regions:

(a).For negative-energy, E<0

Define $\alpha_{1a}^2=-\frac{8\mu E}{\hbar^2}>0$, $\xi=\alpha_{1a}r$ and $\lambda_1=\frac{2\mu e^2}{\varepsilon\hbar^2\alpha_{1a}}$, then Eq. (35) can be expressed as:

$$\frac{\partial^2 R}{\partial\xi^2}+\frac{2}{\xi}\frac{\partial R}{\partial\xi}+\left[-\frac{1}{4}+\frac{\lambda_1}{\xi}-\frac{L(L+1)}{\xi^2}\right]R=0 \tag{36}$$

If we further write R(ξ)= ξ^{-1}W(ξ), then Eq. (36) becomes

$$\frac{\partial^2 W}{\partial\xi^2}+\left[-\frac{1}{4}+\frac{\lambda_1}{\xi}+\frac{\frac{1}{4}-(L+\frac{1}{2})^2}{\xi^2}\right]W=0 \tag{37}$$

Since the wave function has to be finite everywhere, the solution of the radial part in the r<a region can be expressed as:

$$R_1(\alpha_{1a}r)=C_{1a}e^{-\frac{\alpha_{1a}r}{2}}(\alpha_{1a}r)^L\Phi(L+1-\lambda_1,2L+2,a_{1a}r) \tag{38}$$

where C_{1a} is the normalization constant.

(b).For positive-energy, E>0

Define $\alpha_{1b}^2=\frac{2\mu E}{\hbar^2}>0$, $\xi=\alpha_{1b}r$ and $\beta_1=-\frac{\mu e^2}{\varepsilon\hbar^2\alpha_{1b}}$, then Eq. (34) can be expressed as:

$$\frac{\partial^2 R}{\partial\xi^2}+\frac{2}{\xi}\frac{\partial R}{\partial\xi}+\left[1-\frac{2\beta_1}{\xi}-\frac{L(L+1)}{\xi^2}\right]R=0 \tag{39}$$

If we further write R(ξ)= ξ^{-1}F(ξ), then Eq. (39) becomes

$$\frac{\partial^2 F}{\partial \xi^2}+\left[1-\frac{2\beta_1}{\xi}-\frac{L(L+1)}{\xi^2}\right]F=0 \tag{40}$$

Eq. (40) is the Coulomb wave equation, hence the wave function of the radial part in the region E>0 can be expressed as:

$$R_1(\alpha_{1b}r)=C_{1b}\sum_{k=L+1}^{\infty}A_k^L(\beta_1)(\alpha_{1b}r)^{k-1} \tag{41}$$

where C_{1b} is the normalization constant.

(Ⅱ). For $a\leqq r<b$, $V(r)=V_2$

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

$$-\frac{\hbar^2}{2\mu}\left[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{L(L+1)}{r^2}\right]R(r)-\frac{e^2}{\varepsilon r}R(r)+V_2R(r)=ER(r) \tag{42}$$

Define $\alpha_2^2=-\frac{8\mu(E-V_2)}{\hbar^2}>0$, $\xi=\alpha_2 r$, $\lambda_2=\frac{2\mu e^2}{\varepsilon\hbar^2\alpha_2}$ and $R(\xi)=\xi^{-1}W(\xi)$, then Eq. (42) can be rewritten as:

$$\frac{\partial^2 W}{\partial \xi^2}+\left[-\frac{1}{4}+\frac{\lambda_2}{\xi}+\frac{\frac{1}{4}-(L+\frac{1}{2})^2}{\xi^2}\right]W=0 \tag{43}$$

This is the Whittaker equation. Thus, the solution can be written as:

$$\begin{aligned}R_2(\alpha_2 r)=&C_{21}e^{-\frac{\alpha_2 r}{2}}(\alpha_2 r)^L\Phi(L+1-\lambda_2,2L+2,\alpha_2 r)\\&+C_{22}e^{-\frac{\alpha_2 r}{2}}(\alpha_2 r)^L\{\Phi(L+1-\lambda_2,2L+2,\alpha_2 r)\ln(\alpha_2 r)\\&+\sum_{k=0}^{\infty}\frac{(L+1-\lambda_2)_k}{(2L+2)_k}\frac{(\alpha_2 r)^k}{k!}\times[\phi(L+1-\lambda_2+k)-\phi(2L+2+k)-\phi(1+k)]+\\&+\frac{\Gamma(2L+1)\Gamma(2L+2)\Gamma(-L-\lambda_2)(-1)^{2L+2}}{\Gamma(L+1-\lambda_2)}\times\sum_{k=0}^{2L}\frac{(-L-\lambda_2)_k}{(-2L)_k}\frac{(\alpha_2 r)^{k-2L-1}}{k!}\}\end{aligned} \tag{44}$$

where C_{21}, C_{22} are normalization constants.

(Ⅲ). For $r\geqq b$, $V(r)=V_3$

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

$$-\frac{\hbar^2}{2\mu}\left[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{L(L+1)}{r^2}\right]R(r)-\frac{e^2}{\varepsilon r}R(r)+V_3R(r)=ER(r) \tag{45}$$

Define $\alpha_3^2=-\frac{8\mu(E-V_3)}{\hbar^2}>0$, $\xi=\alpha_3 r$, $\lambda_3=\frac{2\mu e^2}{\varepsilon\hbar^2\alpha_3}$, and R(ξ)= ξ^{-1}W(ξ), then Eq. (45) becomes

$$\frac{\partial^2 W}{\partial\xi^2}+\left[-\frac{1}{4}+\frac{\lambda_3}{\xi}+\frac{\frac{1}{4}-(L+\frac{1}{2})^2}{\xi^2}\right]W=0 \tag{46}$$

This is the Whittaker equation. The Whittaker functions expressed in Eq. (44) are not well behaved as ξ becomes very large, we thus turn to use the integral representation of Whittaker function

$$W_{\lambda_3,L}(\xi)=C_3e^{-\frac{\xi}{2}}\xi^{\lambda_3}\int_0^\infty e^{-t}t^{-\lambda_3+L}(1+\frac{t}{\xi})^{\lambda_3+L}dt \tag{47}$$

in our calculation. Hence the radial part wave function in the r>b region can be written as

$$R_3(\alpha_3 r)=C_3e^{-\frac{\alpha_3 r}{2}}(\alpha_3 r)^{\lambda_3-1}\int_0^\infty e^{-t}t^{-\lambda_3+L}(1+\frac{t}{\alpha_3 r})^{\lambda_3+L}dt \tag{48}$$

The boundary conditions require:

$$\frac{R_1'(\alpha_1 a)}{R_1(\alpha_1 a)}=\frac{R_2'(\alpha_2 a)}{R_2(\alpha_2 a)} \tag{49}$$

$$\frac{R_2'(\alpha_2 b)}{R_2(\alpha_2 b)}=\frac{R_3'(\alpha_3 b)}{R_3(\alpha_3 b)} \tag{50}$$

Using above two equations, one can obtain the eigenvalue E.

D. electron confined in the MLQD

The Hamiltonian of an electron confined in the MLQD can be written as:

$$H=-\frac{\hbar^2}{2\mu}\nabla^2+V(r) \tag{51}$$

where

$$V(r)=\begin{cases}0\ ,if\ r<a\\ V_2\ ,if\ a\le r<b\\ V_3\ ,if\ r\ge b\end{cases}$$

Schrödinger equation for the radial part R(r) can be expressed in spherical coordinate as:

$$r^2\frac{\partial^2 R(r)}{\partial r^2}+2r\frac{\partial R(r)}{\partial r}+\left[-L(L+1)-\frac{2\mu V(r)}{\hbar^2}r^2\right]R(r)=-\frac{2\mu}{\hbar^2}Er^2R(r) \qquad (52)$$

(Ⅰ). For r<a , V(r)=0

The Eq. (52) can be written as

$$r^2\frac{\partial^2 R(r)}{\partial r^2}+2r\frac{\partial R(r)}{\partial r}+\left[-L(L+1)+\frac{2\mu E}{\hbar^2}r^2\right]R(r)=0 \qquad (53)$$

Comparing with the modified Bessel equation, the wave function of the radial part can be expressed as

$$R_1(r)=C_1r^{-\frac{1}{2}}J_{L+\frac{1}{2}}\left(\sqrt{\frac{2\mu E}{\hbar^2}}r\right) \qquad (54)$$

(Ⅱ). For a≦r<b, V(r)=V_2

Set $\alpha_2^2=-\frac{8\mu(E-V_2)}{\hbar^2}>0$, $\xi=\alpha_2 r$, and R(ξ)=ξ^{-1}W(ξ), then Eq. (52) becomes

$$\frac{\partial^2 W}{\partial\xi^2}+\left[-\frac{1}{4}+\frac{\frac{1}{4}-(L+\frac{1}{2})^2}{\xi^2}\right]W=0 \qquad (55)$$

This is the Whittaker equation. Thus, the solution of the system can be written as

$$R_2(\alpha_2 r)=C_{21}e^{-\frac{\alpha_2 r}{2}}(\alpha_2 r)^L\Phi(L+1,2L+2,\alpha_2 r)\ +C_{22}e^{-\frac{\alpha_2 r}{2}}(\alpha_2 r)^{-L-1}\Phi(-L,-2L,\alpha_2 r) \qquad (56)$$

(Ⅲ). For r≧b , V(r)=V_3

Let $\alpha_3^2=-\frac{8\mu(E-V_3)}{\hbar^2}>0$, $\xi=\alpha_3 r$, and R(ξ)=ξ^{-1}W(ξ), then Eq. (52) becomes

$$\frac{\partial^2 W}{\partial\xi^2}+\left[-\frac{1}{4}+\frac{\frac{1}{4}-(L+\frac{1}{2})^2}{\xi^2}\right]W=0 \qquad (57)$$

which is the Whittaker equation, and the solution of the system can be written as

$$R_3(\alpha_3 r) = C_3 e^{-\frac{\alpha_3 r}{2}} (\alpha_3 r)^{-1} \int_0^{\infty} e^{-t} t^L (1 + \frac{t}{\alpha_3 r})^L dt \tag{58}$$

Using boundary conditions

$$\frac{R_1'(\alpha_1 a)}{R_1(\alpha_1 a)} = \frac{R_2'(\alpha_2 a)}{R_2(\alpha_2 a)} \tag{59}$$

$$\frac{R_2'(\alpha_2 b)}{R_2(\alpha_2 b)} = \frac{R_3'(\alpha_3 b)}{R_3(\alpha_3 b)} \tag{60}$$

one can obtain the eigenvalue E.

3. Results and discussions

The binding energy E_b of the impurity is defined as the difference between the electron energy with and without the binding of the impurity atom[9-11, 19-23], i.e.

$$E_b = E_e - E_i$$

where E_i and E_e represent the state energies of electron in multi-layer quantum circle and QD with and without impurity. The binding energy is the difference of the subband and conduction band. The definition of binding energy is well defined in the quantum wire system. Since there is at least one spatial dimension along which carriers can move freely as the radius reduces to zero. On the other hand, in the QD system where the carriers are confined in all three dimensions the conduction bands associated with the subband loses its original meaning. In fact, the conduction bands in a true sense are associated with the subbands which are entirely extended over the surrounding medium. In this work, we calculate the low lying state binding energy of a hydrogenic impurity located at the center of GaAs-$Al_xGa_{1-x}As$ quantum circle and QD. In our figure, 1s(i) is the curve of ground state energy with impurity; 1s(w-i) is the curve of ground state energy without impurity; 1s(b) is the curve of ground state binding energy.

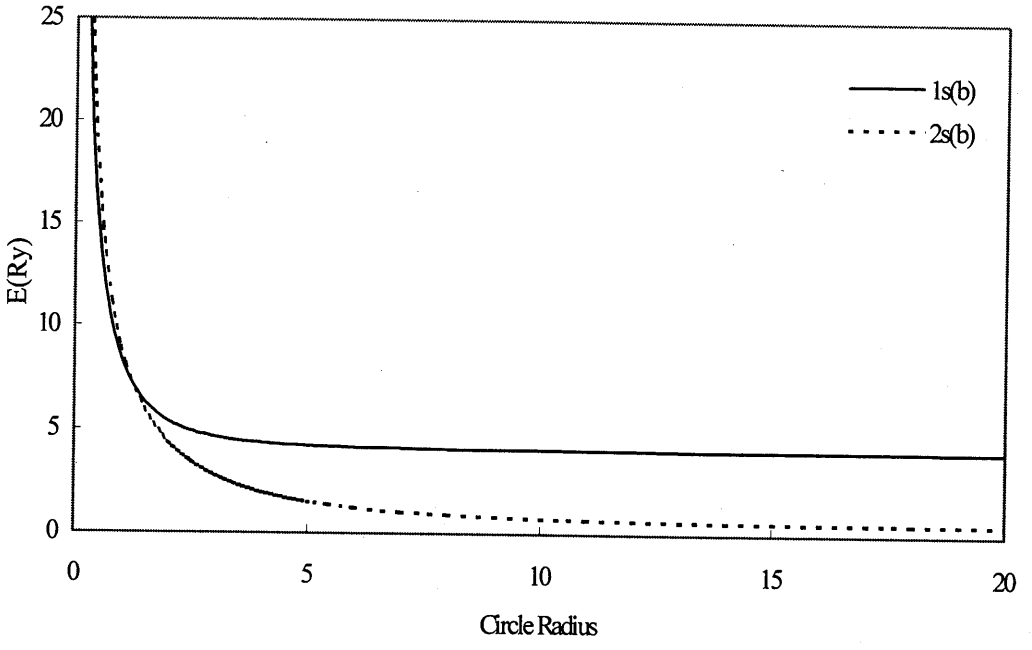

Fig. 1 The 1s- and 2s-like state binding energy of a 2-D impurity in single layer quantum circle as a function of circle radius with infinite potential barrier.

Fig. 1 shows the lower lying state binding energy of a 2-D impurity located at the center of quantum circle with infinite potential barrier. For infinite potential barrier, as the circle radius decreases from infinite to zero, the 1s-like state energy increases monotonically from 4 Ry to infinite and 2s-like state energy increases monotonically from 0.45 Ry to infinite. Fig. 2 and Fig. 3 show the ground state binding energy of a 2-D impurity located at the center of quantum circle with finite potential barrier V=5 Ry and V=10 Ry. For finite potential barrier, our calculated results show, as the circle radius decreases from infinite to zero, the ground state binding energy increases monotonically from 4 Ry to a maximum value for a circle radius, then decreases monotonically to 4 Ry finally. For infinite circle radius, the electron will be bounded in 2-D and the ground state binding energy will approach 4 Ry. As the circle radius decreases less and less, the confinement

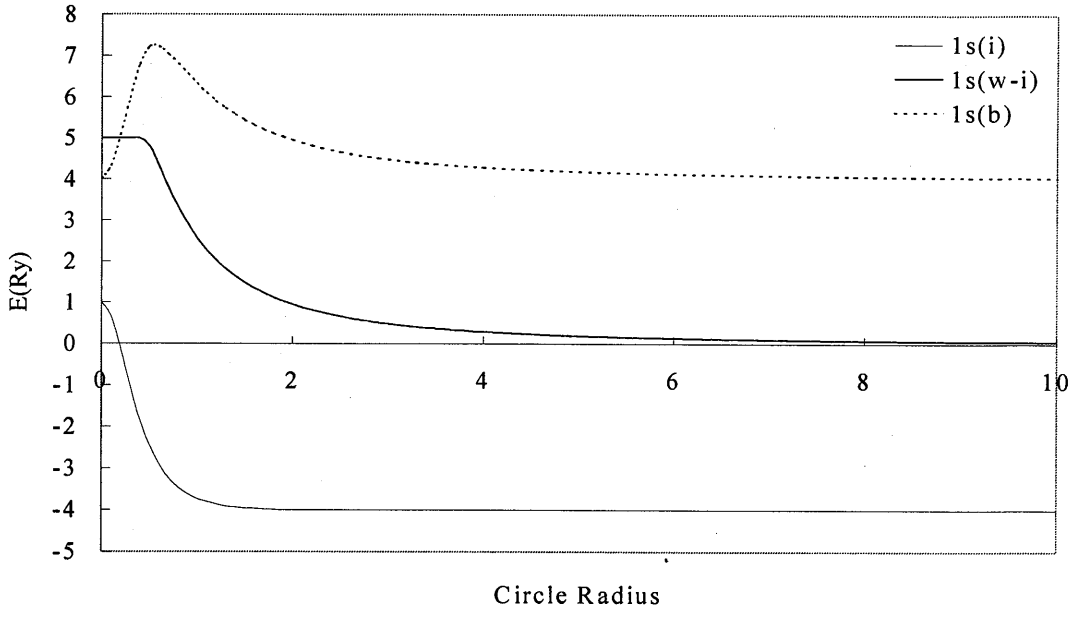

Fig. 2 The ground state binding energy of a 2-D impurity in single layer quantum circle as a function of circle radius with potential barrier V=5 Ry.

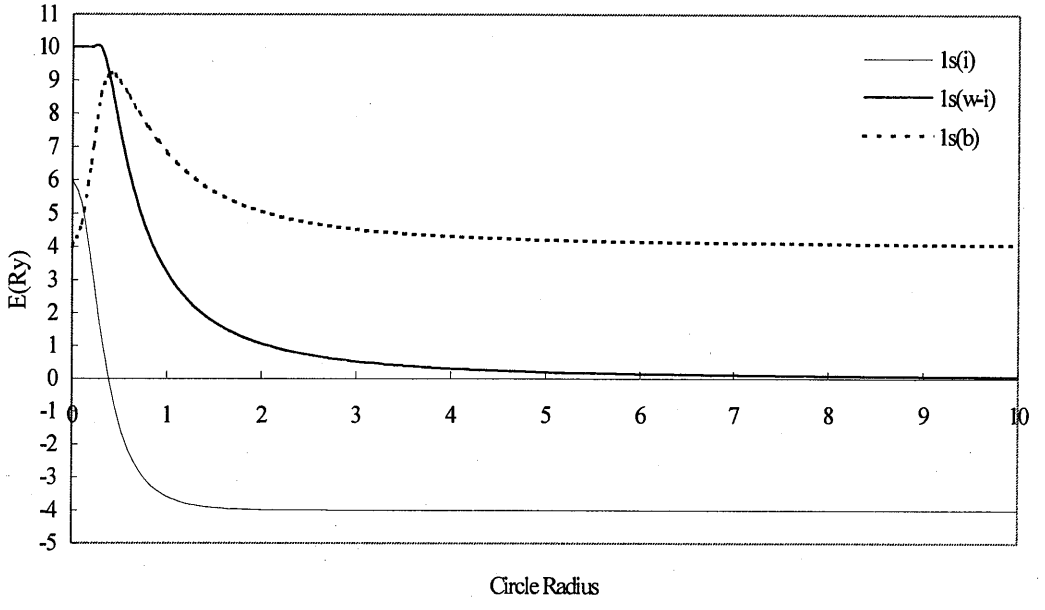

Fig. 3 The ground state binding energy of a 2-D impurity in single layer quantum circle as a function of circle radius with potential barrier V=10 Ry.

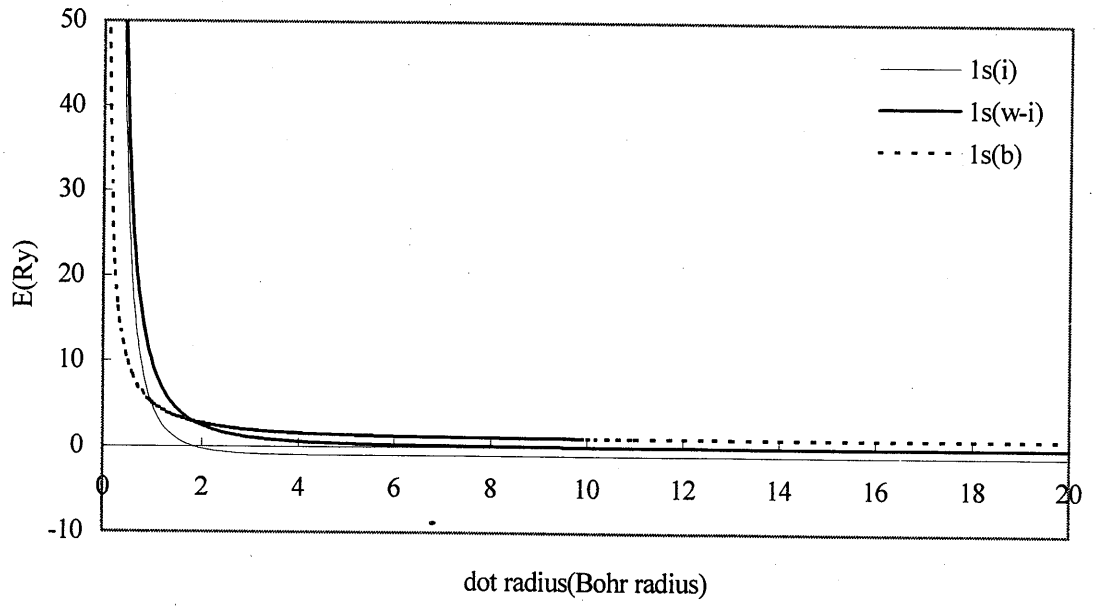

Fig. 4 The ground state binding energy of a hydrogenic impurity in single layer quantum dot as a function of dot radius with infinite potential barrier.

effect will push the binding energy larger and larger. Finally the electron leaks out the circle and the electron is bounded in 2-D, the ground state binding energy will approach 4 Ry.

Fig. 4 shows the ground state binding energy of a hydrogenic impurity located at the center of quantum dot with infinite potential barrier. For infinite potential barrier, as the dot radius decreases from infinite to zero, the ground state energy increases monotonically from 1 Ry to infinite. Fig. 5 shows the ground state binding energy of a hydrogenic impurity located at the center of quantum dot with finite potential barrier V=5 Ry. For finite potential barrier, our calculated results show, as the dot radius decreases from infinite to zero, the ground state binding energy increases monotonically from 1 Ry to a maximum value for a dot radius, then decreases monotonically to 1 Ry finally. For infinite dot radius, the electron will be bounded in 3-D and the ground state binding energy will approach 1 Ry. As the dot radius decreases gradually, the confinement effect will push the binding energy larger and

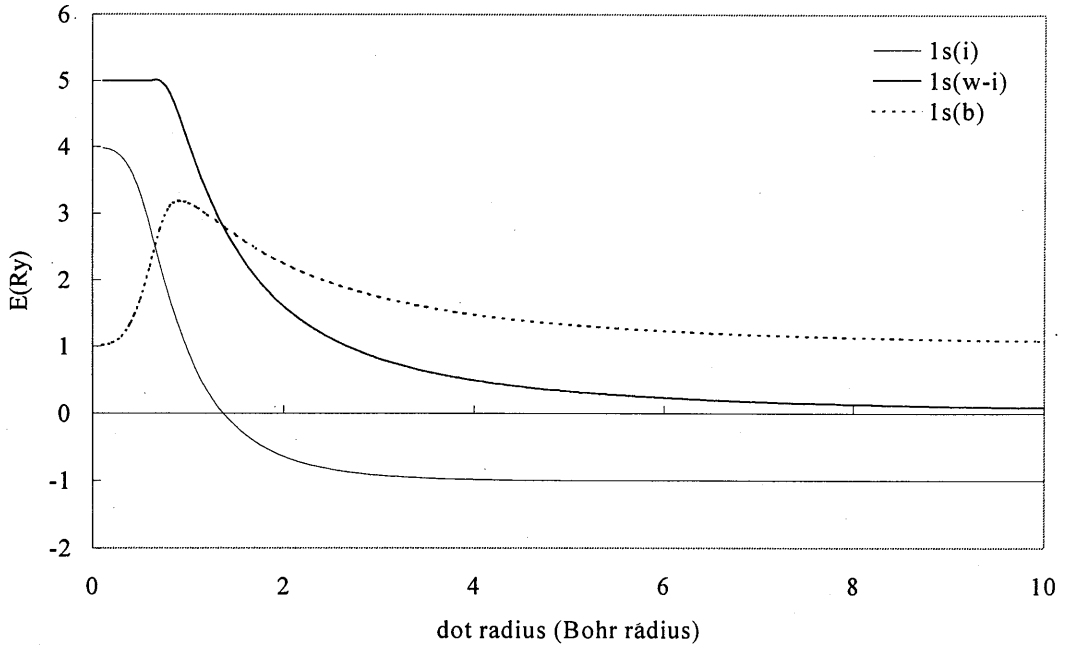

Fig. 5 The ground state binding energy of a hydrogenic impurity in single layer quantum dot as a function of dot radius with potential barrier V=5 Ry.

larger. Finally the electron leaks out the dot and the electron is bounded in 3-D, the ground state binding energy will approach 1 Ry. The binding energy of the lower lying state of a hydrogenic impurity E_b is given as[8]:

$$E_b = \left(\frac{2}{2n + D - 3} \right)^2 \text{ Ry}$$

where n=1, 2, 3...., is the principal quantum number and the D is the dimension of bound state. For 2-D, the binding energy of ground state and 2s-state of a hydrogenic impurity equals to 4 Ry and 0.44 Ry, respectively. And for 3-D the binding energy of ground state, 2s-state and 3s-state of a hydrogenic impurity equals to 1 Ry, 0.25 Ry and 0.11 Ry, respectively. Fig. 6 shows the lower lying state binding energy of a hydrogenic impurity in the center of single layer quantum circle and QD as a function of radius with the potential barrier V=5 Ry. Our results show the binding energy of ground state and 2s-state of a hydrogenic impurity in quantum circle equals to 4 Ry and 0.44 Ry, respectively, when the circle radius increases infinite. And the

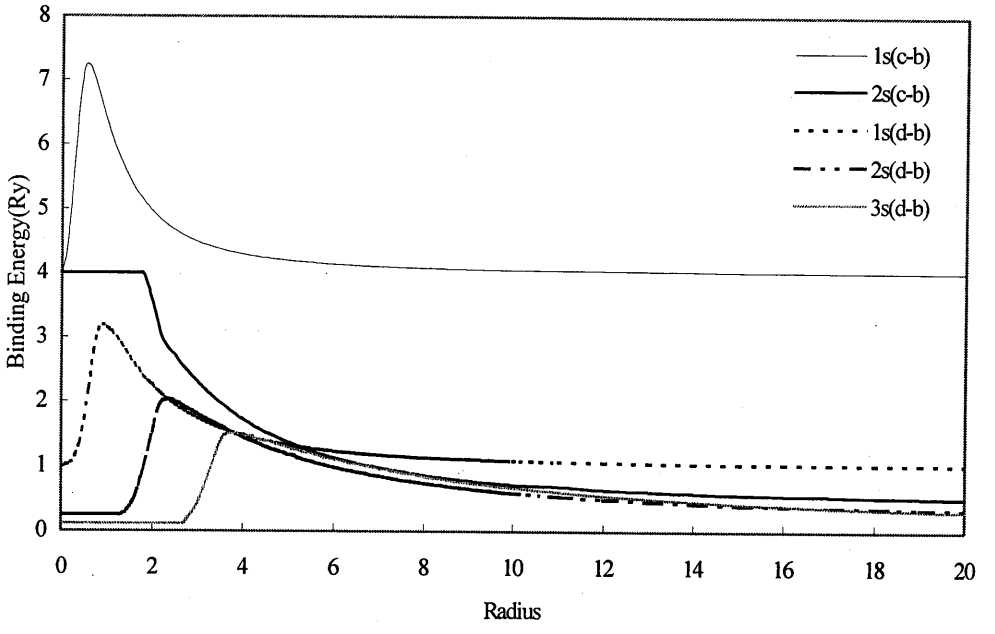

Fig. 6 The lower state binding energy of a hydrogenic impurity in the center of single layer quantum circle and QD as a function of radius with the potential barrier V=5 Ry .

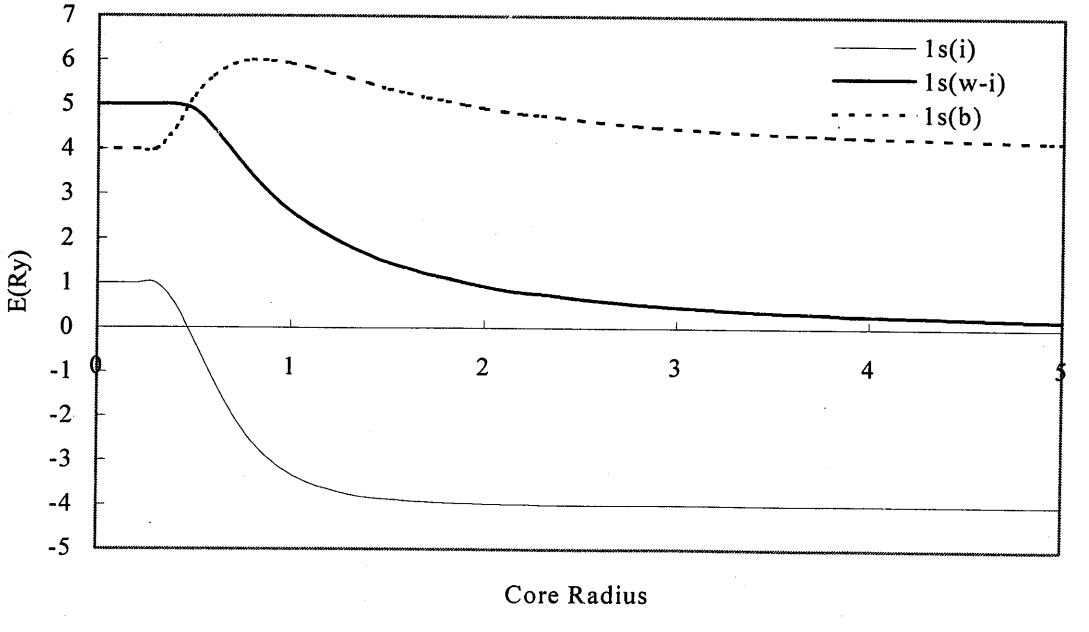

Fig. 7 The ground state binding energy of a 2-D impurity in multi-layer quantum circle as a function of core radius with V_2=10 Ry and V_3=5 Ry for b=10a_0^*.

binding energy of ground state, 2s-state and 3s-state of a hydrogenic impurity in QD equals to 1 Ry, 0.25 Ry and 0.11 Ry, respectively, when the dot radius increases infinite. For quantum circle and quantum dot, our calculated results is in agreement with He's predictions[8].

Fig. 7 shows the ground state binding energy of a 2-D impurity located at the center of multi-layer quantum circle with V_2=10 Ry and V_3=5 Ry. Fig. 8 shows the ground state binding energy of a hydrogenic impurity located at the center of multi-layer quantum dot with V_2=8 Ry and V_3=3 Ry. For infinite core radius, the ground state binding energy also will approach 4 Ry and 1Ry, like a free hydrogen atom in the 2-D and 3-D. For small core radius, the electron may be bounded in the shell region or bulk region, depending on the difference of shell potential and bulk potential, thus as the core radius reduces to zero the electron will get different binding energy.

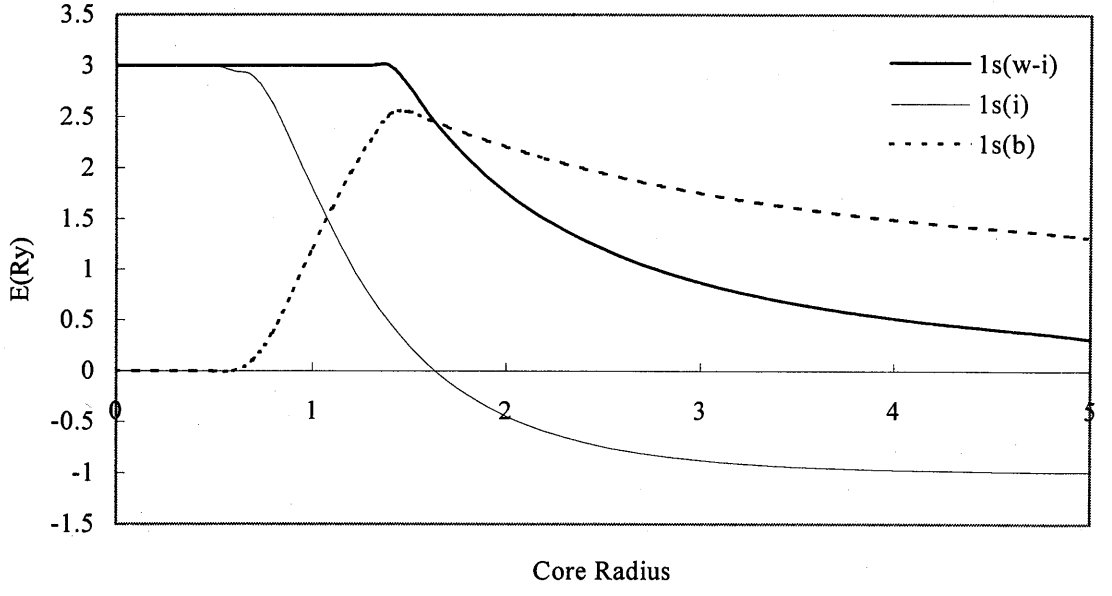

Fig. 8 The ground state binding energy of a hydrogenic impurity in multi-layer quantum dot as a function of core radius with V_2=8 Ry and V_3=3 Ry for b=10a_0^*.

4. Conclusion

We calculate the lower lying state energy of a hydrogenic impurity in a quantum circle and QD. For single layer quantum circle and QD, the ground state binding energy approaches 4 Ry and 1 Ry each, both as the radius increases infinite and reduces to zero, like a hydrogenic impurity in 2-D and 3-D. Our results are in agreement with the predictions of He[8]. For multi-layer quantum circle and QD, the ground state binding energy approaches 4 Ry and 1 Ry each, as the radius increases infinite only. For small core radius, the electron may be bounded in the shell region or bulk region, depending on the difference of shell potential and bulk potential, thus as the core radius reduces to zero the electron will get different binding energy.

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