Energy and Shannon entropy for a hydrogen atom confined in a dielectric spherical microcavity

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Abstract. We calculate the energy and Shannon entropy for a hydrogen atom confined in a dielectric spherical microcavity for the fist time. In contrast to the hydrogen atom in the vacuum microcavity, some unexpected and interesting phenomena appear: First, the turning radius for the bound energy changes from positive to negative depends on the dielectric constant of the spherical microcavity sensitively. With the increase of the relative dielectric constant, the turning radius gets larger. Second, the dielectric spherical microcavity impacts the rearrangement of the excited state energy, and breaks the energy degeneracy of the excited states. At some given radius, there is energy crossover between different orbital. Third, the dielectric in the spherical microcavity affects the Shannon entropy for the confined hydrogen atom greatly. The Shannon entropy in the vacuum microcavity is the smallest and the Shannon entropy increases with the relative dielectric constant. For smaller size spherical microcavity, the Shannon entropy change is always negative, which suggests that the electron density is localized. With the increase of the radius of the microcavity, the Shannon entropy change becomes positive, and the confinement of the electron density gets delocalized. Our results show that we can control the confining effect of the spherical microcavity on the atom by changing the dielectric. This work can guide the future experimental studies for trapping and manipulating of atoms and molecules in the external environment and has some practical applications in metrology and quantum information processing.

Keywords: Shannon entropy；confinement; dielectric spherical microcavity

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1.Introduction

In the past several decades, study of the atoms and molecules confined in the quantum wells has attracted extensive attention. As we know, the classical and quantum behavior of free atoms or molecules are familiar. However, when the atoms or molecules are confined in micro-size domains, their physical characters will be completely different from those in the free case[1-3]. From the aspect of the quantum mechanics, the difference is caused by the modification of the boundary conditions when solving the Schrodinger equation. Spatially confined atoms appear in many basic and applied researches, such as optical traps [4,5], atom optic billiards [6–10], low dimensional nano-materials [11], quantum dot or quantum wires[12],etc. These confined systems have many physical applications. For example, the atom optic billiards can be considered as a rapidly scanning and tightly focused laser beam, which can create a time-averaged quasi-static potential for atoms[6-7]. The confined atom in the two-dimensional quantum wells has been widely used in the semiconductor micro-junction[13]. The confined quantum dot or quantum wire systems are applied to manufacture transistors because of their high mobility and carrier scattering suppression[14-15].

Pioneering studies of the confined system were dated back to 1930s. In order to study the polarizability of the hydrogen atom under high pressure, Michels et al put forward a theoretical model of a hydrogen atom confined by an impenetrable spherical microcavity [16-17]. It was found when the size of the spherical cavity is very small, the pressure acting on the hydrogen atom is very high. Therefore, this

model can be used to simulate the experimental study of hydrogen atom under high pressure condition. Ever since then, this model has been extended to study the atomic or molecular structures of quantum confined system by many researchers. Some typical researches are as follows: in 1976, Suryanarayana and Weil studied the hyperfine splitting of the hydrogen atom in a spherical box [18]. Aquino et al. studied some physical properties of the confined hydrogen atom in a spherical box with impenetrable walls using different methods[19-21]. Later, they calculated the Shannon and Fisher entropies for a hydrogen atom under soft spherical confinement[22]. Very recently, Garza et al. studied the Shannon entropy for a hydrogen atom confined by four different potentials[23]. Salazar calculated the Shannon-information entropy sum in the confined hydrogenic atom[24]. Ley-Koo studied the superintegrability and symmetry breakings in confined atoms and molecules[25], etc. In these previous studies, they all considered the atom confined in the external environment without dielectric. Then what will happen if the atom is confined in a dielectric spherical microcavity?

In this paper, we study the confinement effect of the dielectric spherical microcavity on the physical properties of the hydrogen atom for the first time. We assume that the hydrogen atom is at the center of a spherical microcavity filled with dielectric. This system represents a physically more realistic model to simulate the atom immersed in a dielectric environment. By solving the Schrodinger equation with suitable boundary condition, we obtain the eigen-energy and wave function of this system analytically. Since the Shannon entropy in the configuration space is a good

indicator to measure the localization or delocalization of the electron density for the confined system[22], we also calculate the Shannon entropy for the hydrogen atom confined in a dielectric spherical microcavity. Our calculation suggests, compared to the confined hydrogen atom in a spherical microcavity without dielectric, some unexpected phenomenon appear. The energy and Shannon entropy of this system depend on the size and the relative dielectric constant of the spherical microcavity sensitively. For a given dielectric spherical microcavity, the variation of the ground state energy and Shannon entropy as a function of the radius of the microcavity is analyzed. If the radius of the microcavity is very large, the spatially confinement effect on the electron is small, the energy is negative and the electron density is delocalized, as a result, the Shannon entropy change becomes positive. However, as the radius of the microcavity decreases, the electron energy changes from negative to positive due to the strong confinement effect induced by the microcavity, which cannot happen in a free hydrogen atom. The Shannon entropy change changes from positive to negative, which suggest that the electron density is localized and the electron has little possibilities to escape from the spherical microcavity. For the excited states, the energy degeneracy is broken. For example, at given principal quantum number n, the energy varies with the orbit angular momentum, $E_{np} \neq E_{ns}$. There are energy crossings among some excited states. The energy of E_{np} state can be larger than the $E_{(n+1)p}$ state. This is another unexpected result for the confinement hydrogen atom. In addition, we also discuss the influence of the relative dielectric constant of the spherical microcavity on the energy and Shannon entropy of this

system. Our work suggests that we can use a dielectric spherical microcavity to simulate the experimental study of hydrogen atom under different environments. Since the dielectric spherical microcavity is accessible for laboratory experiment, then the classical dynamics of this system is a real physical system instead of an abstract theoretical model. From this work it is evident that the investigation of a rather simple system, like the hydrogen atom confined in a microcavtiy leads to a variety of interesting and complicated properties. We hope that our results can guide the future researches about the atomic or molecular structures confined in the micro-size domains.

2. The wave function and Shannon entropy for the hydrogen atom confined by a dielectric spherical microcavity

Consider a hydrogen atom located at the center of a dielectric spherical microcavity with impenetrable surfaces, the relative dielectric constant is ε and the radius is r_d. The Hamiltonian of this system can be described as (in atomic unit):

$$H = -\frac{1}{2}\nabla^2 + V(r),\tag{1}$$

where $V(r)$ is the confining potential:

$$V(r) = \begin{cases} -\dfrac{1}{\varepsilon r} & r < r_d \\ +\infty & r \geq r_d \end{cases}\tag{2}$$

2.1 The analytic solution of the energy and wave function of this system

The Schrodinger equation associated to the hydrogen atom in the dielectric spherical microcavity has the following expression (in spherical coordinates):

$$-\frac{1}{2}\left\{ \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta \frac{\partial}{\partial\theta} \right] + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial\varphi^2} - \frac{1}{\varepsilon r} \right\}\psi(r,\theta,\varphi) = E\psi(r,\theta,\varphi)$$

$$\tag{3}$$

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Here, $\psi(r,\theta,\varphi)$ $(r < r_d)$ is the wave function of the hydrogen atom inside the dielectric spherical microcavity. Outside of the microcavity, $\psi(r \geq r_d,\theta,\varphi) = 0$.

As in the case of the hydrogen atom in the free space, the wave function $\psi(r,\theta,\varphi)$ in the spherical microcavity can be divided into the product of two parts: $\psi(r,\theta,\varphi) = R(r)Y_{lm}(\theta,\varphi)$. Here $R(r)$ is radial function and $Y_{lm}(\theta,\varphi)$ is the familiar spherical harmonic function. The radial function $R(r)$ satisfies the following equation:

$$-\frac{1}{2}\left\{\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2} - \frac{1}{\varepsilon r}\right\}R(r) = ER(r) \qquad (4)$$

with the boundary condition $R(r_d) = 0$.

As we know, for the case of the free hydrogen atom, the energy of the electron is always negative. However, if the hydrogen atom is confined in a microcavity, the surface of the microcavity will put a pressure on the atomic electron, which makes the energy of the electron can be positive. Therefore, for the case of the confined hydrogen atom, the energy of the electron can be positive or negative due to the confinement of the dielectric spherical microcavity[12]. In the following, we find the solution of the radial Schrodinger equation in two cases.

Case 1: the energy of the electron is positive, $E>0$. Let $\xi = \alpha r$, where $\alpha^2 = 2E$. Then Eq.(4) becomes:

$$\frac{\partial^2 R(\xi)}{\partial \xi^2} + \frac{2}{\xi}\frac{\partial R(\xi)}{\partial \xi} + [1 - \frac{2\eta}{\xi} - \frac{l(l+1)}{\xi^2}]R(\xi) = 0 \qquad (5)$$

where $\eta = -\frac{1}{\varepsilon\alpha}$. The boundary condition becomes $R(\alpha r_0) = 0$. Furthermore, we set $R(\xi) = \xi^{-1}F(\xi)$, then we get:

$$\frac{\partial^2 F(\xi)}{\partial \xi^2} + [1 - \frac{2\eta}{\xi} - \frac{l(l+1)}{\xi^2}]F(\xi) = 0 \qquad (6)$$

The above equation is a Coulomb equation. Considering the boundary condition, its solution can be expressed as:

$$F(\xi) \propto F(l,\eta,\xi), \tag{7}$$

with $F(l,\eta,\xi)$ is the regular Coulomb wave function. Therefore, the solution of Eq.(5) becomes:

$$R(r) = A(\alpha r)^{-1} F(l,-\frac{1}{\varepsilon\alpha},\alpha r), \tag{8}$$

here A is a normalization constant. The value of α can be determined from the boundary condition:

$$F(l,-\frac{1}{\varepsilon\alpha},\alpha r_d) = 0 \tag{9}$$

Therefore, the total energy of the system can be obtained:

$$E = \frac{\alpha^2}{2}. \tag{10}$$

Case 2: the energy of the electron is negative, $E<0$. Set $\varsigma = \beta r$, where $\beta^2 = -8E$. Then Eq.(4) becomes:

$$\frac{\partial^2 R(\varsigma)}{\partial \varsigma^2} + \frac{2}{\varsigma}\frac{\partial R(\varsigma)}{\partial \varsigma} + [-\frac{1}{4} + \frac{\lambda}{\varsigma} - \frac{l(l+1)}{\varsigma^2}]R(\varsigma) = 0 \tag{11}$$

where $\lambda = \dfrac{2}{\varepsilon\beta}$. The boundary condition becomes $R(\beta r_d) = 0$. Furthermore, we set $R(\varsigma) = \varsigma^{-1} F(\varsigma)$, then the above equation can be written as:

$$\frac{\partial^2 F(\varsigma)}{\partial \varsigma^2} + [-\frac{1}{4} + \frac{\lambda}{\varsigma} + \frac{\frac{1}{4} - (l+\frac{1}{2})^2}{\varsigma^2}]F(\varsigma) = 0 \tag{12}$$

The above equation is a Whittaker equation[]. Its solution can be written as:

$$F_{\lambda,l}(\varsigma) \propto e^{-\varsigma/2}\varsigma^{l+1} K(l+1-\lambda, 2l+2, \varsigma), \tag{13}$$

here $K(l+1-\lambda, 2(l+1), \varsigma)$ is the Kummer function[12].

Therefore, the solution of Eq.(11) can be expressed as:

$$R(r) = Be^{-\beta r/2}(\beta r)^l \, \mathrm{K}(l+1-\frac{2}{\varepsilon\beta}, 2l+2, \beta r). \tag{14}$$

Where B is a normalization constant. The value of β can be determined from the boundary condition:

$$\mathrm{K}(l+1-\frac{2}{\varepsilon\beta}, 2l+2, \beta r_d) = 0 \tag{15}$$

The total energy of this system can be given as:

$$E = -\frac{\beta^2}{8}. \tag{16}$$

As discussed above, the energy of the electron in the dielectric spherical microcavity can be positive or negative. Then what is the turning point for the bound state energy changes from positive to negative? This problem can be obtained by setting $E=0$ in Eq.(4):

$$-\frac{1}{2}\left\{ \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2} - \frac{1}{\varepsilon r} \right\} R(r) = 0 \tag{17}$$

The solution of the above equation is dependent on the value of the orbital angular momentum l and can be expressed as[12]:

$$R_l(r) = \frac{1}{\sqrt{r}} J_{2l+1}(\sqrt{8r/\varepsilon}), \tag{18}$$

where J_{2l+1} is the Bessel function.

Considering the bound state boundary condition, $R_l(r_c) = 0$, which means $J_{2l+1}(\sqrt{8r_c/\varepsilon}) = 0$. Assuming $\sqrt{8r_c/\varepsilon} = x_i$, with x_i are the roots of the Bessel function J_{2l+1}, we can obtain the turning radius r_c for the bound state energy changes from positive to negative. The turning radius for the first several s, p states corresponding

to different dielectric constant are shown in Table 1. For example, if we assume that the hydrogen atom is confined in the GaAs dielectric spherical microcavity, then the relative dielectric constant ε =13.13. For the 1s bound state, the turning radius r_c=24.0968a.u. If the radius of the dielectric spherical microcavity is less than this value, $r < r_c$, the energy is positive, however, if the radius $r>r_c$, the energy is negative. For the 2p bound state, the energy changes from positive to negative when the radius is larger than 66.8095a.u. From this table, we find at a given bound state, the value of the turning radius gets larger with the increase of the relative dielectric constant, which suggests that the confinement effect of the spherical microcavity on the atom can be varied by the dielectric constant.

2.2 The Shannon entropy for the confined hydrogen atom

In the above section, we have delineated the method to solve the Schrodinger equation for the confined hydrogen atom in a dielectric spherical microcavity. It is found that the wave function has exact analytic solution: $\psi(r,\theta,\varphi) = R(r)Y_{lm}(\theta,\varphi)$. Here $R(r)$ is the radial function. If the energy of the bound state is positive, it is given by Eq.(8) ; otherwise, it is given by Eq.(14). The normalization constant A or B is determined by: $<\psi(r,\theta,\varphi)|\psi(r,\theta,\varphi)>=1$. Once the wave function is obtained, the electron density can be expressed as:

$$\rho(r,\theta,\varphi) =|\psi(r,\theta,\varphi)|^2 \tag{19}$$

The Shannon entropy is an important indicator to measure the delocalization or localization of the electron density for the confinement system. In the position space, the Shannon entropy is defined as[22,23]:

$$S_r = -\iiint \rho(r,\theta,\varphi)\ln[\rho(r,\theta,\varphi)]r^2 \sin\theta \, dr \, d\theta \, d\varphi \qquad (20)$$

In comparison to the free atom, the Shannon entropy change is given as:

$$\Delta S_r = S_r(r_d) - S_r^{free}. \qquad (21)$$

In this work, $S_r(r_d)$ denotes the Shannon entropy for the hydrogen atom confined by a dielectric spherical microcavity, and S_r^{free} is the Shannon entropy for the free hydrogen atom.

3. Results and discussion

From Sec.2, we find that the energy and Shannon entropy for the hydrogen atom confined by a dielectric spherical microcavity depend on the relative dielectric constant ε sensitively. Firstly, we consider the case that the hydrogen atom is confined in the GaAs dielectric spherical microcavity (ε =13.13). In Fig.1, we analyze the variation of the ground state energy E_{1s} as a function of the radius of the spherical microcavity. It is found when the radius of the GaAs dielectric spherical microcavity is very small, the energy is positive and very large. With the increase of the radius, the energy is decreased. At approximately $r \approx 24$ a.u., the energy changes from positive to negative, and such value coincides with the one given in Table 1. When the radius of the GaAs microcavity is very large, $r > 100$ a.u., the energy approaches to a given value: $E_{1s} \to -\dfrac{1}{2\varepsilon^2} = -0.0029$ a.u. The reason can be analyzed on the basis of the pressure imposed by the spherical microcavity on the electron. The pressure acting on the electron is expressed as follows[19]: $P = -\dfrac{1}{4\pi r_d^2}\dfrac{dE}{dr}\Big|_{r=r_d}$. For small confinement radius, the ground state energy decreases very fast with the radius of the spherical microcavity, the slope of the E-r curve shown in Fig.1(a) is large, so the pressure

imposed by the spherical microcavity on the electron is very big, which causes the kinetic energy of the electron get very large and finally it overcomes the attractive potential between the electron and the nucleus. So the total energy is positive and very large. For large confinement radius, the ground state energy changes very slowly with the radius, the slope of the E-r curve is very small. As a consequence, the pressure on the electron becomes decreased, and the energy gets small. For comparison, we compare the ground state energy for the hydrogen atom confined in the GaAs dielectric spherical microcavity and in the vacuum spherical microcavity. From this figure, we find that the ground state energy in the dielectric spherical microcavity is larger than the case in the vacuum spherical microcavity.

In Fig.2, we show the distribution of the ground state electron density ρ_{1s} in the GaAs dielectric spherical microcavity at different radius. Fig.2(a) shows the electron density ρ_{1s} in the case of small radius of the GaAs microcavity, r_d=0.5a.u. It is found that the electron density decreases monotonically in the microcavity. When the radius of the GaAs microcavity increases, the electron density exhibits oscillations, and the number of nodes increases with the radius, as we show from Fig.2(b) to Fig.2(d). When the radius of the GaAs microcavity is very large, the node in the electron density disappears and the electron density decreases monotonically again.

Using Eq.(20), we calculate the Shannon entropy for the hydrogen atom in the dielectric spherical microcavity. In Fig.3(a), the black line is the ground state Shannon entropy for the hydrogen atom confined in the GaAs dielectric spherical microcavity. It can be seen that when the radius of the GaAs dielectric spherical microcavity is less

than 2.0 a.u., the Shannon entropy is negative. As we increase the radius of the spherical microcavity, the Shannon entropy changes from negative to positive. When the radius of the GaAs microcavity is larger than 100.0 a.u., the Shannon entropy changes very small, and approaches to a given value: $S_r(r_d)=11.8689$. Also in this figure, the red line denotes the Shannon entropy change ΔS_r relative to the free hydrogen atom. We found when the radius of the GaAs dielectric spherical microcavity $r_0 < 5.0$ a.u., the Shannon entropy change is negative. In this case, the electron density of the ground state is localized and the electron has no possibilities to escape from the GaAs spherical microcavity. However, when the radius of the microcavity $r_0 \geq 5.0$ a.u., the Shannon entropy change becomes positive, which suggests that the confinement of the electron density is delocalized. In Fig.3(b), we compare the ground state Shannon entropy for the hydrogen atom confined in the GaAs dielectric spherical microcavity with the case in the vacuum spherical microcavity. It is found when the radius of the spherical microcavity is very small, the difference between the two Shannon entropies is very small. With the increase of the radius of the spherical microcavity, their difference becomes obvious. The Shannon entropy confined by the GaAs dielectric spherical microcavity is larger than the case in the vacuum spherical microcavity.

In Fig.4, we show the variation of the excited state energies for the confined hydrogen atom with the radius of the GaAs dielectric spherical microcavity. It can be seen that the effect of the spherical microcavity breaks the degeneracy of the angular momentum. In a shell with the same principal quantum number *n*, the energy changes

for different angular momentum, $E_{np} \neq E_{ns}$. With the increase of the confinement

radius, the energy degeneracy is recovered.

In Fig.5, we show the excited state energy at a given radius of the spherical

microcavity. In Fig.5(a), the radius of the spherical microcavity is $r_d = 0.5$ a.u.. The

order of the excited state energies is: $E_{2p} < E_{2s} < E_{3p} < E_{3s} < E_{4p} < E_{4s} < E_{5p} < E_{5s}$.

With the increase of the radius of the spherical microcavity, the order of the excited

state energies will be changed. At some given radius, there are crossings among some

orbital energies. For example, as we show in Fig.5(d), $r_d = 50.0$ a.u., the order of the

excited state energies is: $E_{2p} < E_{2s} < E_{3p} < E_{3s} < E_{4s} < E_{5p} < E_{4p} < E_{5s}$. The energy

of the 4p orbit is larger than 5p orbit, which does not appear in the free hydrogen atom.

As the confinement radius is very large, some of the energy degeneracy is recovered

as in the free hydrogen atom. As we show in Fig.5(f), $r_d = 300.0$ a.u.,

$E_{2p} \approx E_{2s}, E_{3p} \approx E_{3s}$. In Table 2, we give the calculated values of the excited state

energy for the confined hydrogen atom with the radius of the GaAs dielectric

spherical microcavity.

In Fig.6, we show the variation of the excited state Shannon entropy for the

hydrogen atom confined in the GaAs dielectric spherical microcavity. It can be seen at

small radius, the difference of the Shannon entropy corresponds to different excited

state is small. With the increase of the size of the spherical microcavity, the difference

becomes apparent. In general, the Shannon entropy for a given excited state gets

larger with the increase of the radius, such as the 2s, 2p, 3s, 4s, 5p state. However,

there are some exceptions. The Shannon entropy corresponds to 4p state decreases

when the radius is larger than 200a.u. The reason can be analyzed as follows: From

Table 1, we found for the GaAs dielectric spherical microcavity, the turning radius r_c

for the 4p excited state changes from positive to negative is 278.0203 a.u., which lies

between 200 a.u. and 300 a.u.. When the radius is less than r_c, the energy is positive,

which suggests that the pressure caused by the spherical microcavity is very large, the

electron has small possibility to escape from the microcavity, so the Shannon entropy

is relatively large. However, when the radius is larger than r_c, the confinement effect

caused by the spherical microcavity gets weakened. As a result, the electron has some

possibility to escape from the microcavity, so the Shannon entropy is decreased.

In Fig.7, we fix the radius of the spherical microcavity, and compare the

Shannon entropy for different excited states. Fig.7(a) shows the variation of the

Shannon entropy when the radius of the spherical microcavity is very small,

$r_d = 0.5$ a.u.. Under this condition, the Shannon entropies corresponding to the excited

state from 2s to 5p state are negative. The order of the Shannon entropy is:

$S_r^{5s} < S_r^{4s} < S_r^{3s} < S_r^{2s} < S_r^{5p} < S_r^{4p} < S_r^{3p} < S_r^{2p}$, which is quite different from the order

of the excited state energies as we show in Fig.5(a). As we increase the radius of the

spherical microcavity, the Shannon entropies changes from negative to positive and

the arrangement of the Shannon entropies corresponding to different excited states

changes accordingly. As the radius is very large, there is degeneracy among some

different excited states. For example, in Fig.7(f), $r_d = 200.0$ a.u., the Shannon entropy

$S_r^{4s} \approx S_r^{4p}, S_r^{5s} \approx S_r^{5p}$, which is similar to the energy degeneracy as we show in

Fig.5(f). In Table 3, we give the calculated values of theShannon entropy for the

confined hydrogen atom with the radius of the GaAs dielectric spherical microcavity.

Finally, we show the variation of the ground state energy and the Shannon entropy with the relative dielectric constant ε and the radius of the spherical microcavity r_d. The radius of the microcavity is given in each plot. Fig.8(a) shows the variation of the ground state energy when the radius of the microcavity is very small, $r_d = 0.5$ a.u. and $r_d = 1.0$ a.u. The results show that the ground state energy is positive and increases with the increase of the relative dielectric constant. In Fig.8(b), the radius of the microcavity becomes $r_d = 10$ a.u. and $r_d = 30$ a.u. It is shown when the relative dielectric constant ε is very small, the ground state energy is negative. With the increase of ε, the energy changes from negative to positive. As we further increase the radius of the spherical microcavity, the confinement effect on the ground state energy induced by the microcavity gets weakened. For example, in Fig.8(c), the difference between the ground state energy confined in the microcavity with the radius $r_d = 50$ a.u. and $r_d = 100$ a.u. is very small. In Fig.8(d), the radius of the spherical microcavity is very large, $r_d = 300$ a.u. and $r_d = 500$ a.u., it is found that the ground state energy becomes negative and the confinement effect on the ground state energy caused by the microcavity is nearly disappeared. The values of the ground state energy as a function of the relative dielectric constant ε and the radius of the microcavity r_d are given in Table 4.

In Fig.9, we show the variation of the ground state Shannon entropy change with the relative dielectric constant ε and the radius of the spherical microcavity r_d. It can be seen that the Shannon entropy change increases with the increase of the relative

dielectric constant. For small spherical microcavity radius as we show in Fig.9(a), $r_d = 0.5$ a.u. and $r_d = 1.0$ a.u., the Shannon entropy change increases very slowly with the relative dielectric constant, and the entropy change is always negative, which suggests that the effect of the spherical microcavity on the confined electron is very strong. The electron has no possibilities to escape from the spherical microcavity even though the relative dielectric constant is very large, and the electron density of the ground state is localized. The Shannon entropy change in the microcavity with the radius $r_d = 1.0$ a.u. is noticeably larger than the case with the radius $r_d = 0.5$ a.u.. In Fig.9(b), the radius of the microcavity is increased to $r_d = 10$ a.u. and $r_d = 30$ a.u., the Shannon entropy change becomes positive, which suggests that the confinement of the electron density gets delocalized. The electron has some possibilities to escape from the spherical microcavity due to the quantum tunneling effect. As we further increase the size of the spherical microcavity (Fig.9(c)), the difference between the Shannon entropy change is very small in the spherical microcavity with small relative dielectric constant. When the radius of the spherical microcavity is very large, such as in Fig.9(d), $r_d = 300$ a.u. and $r_d = 500$ a.u., the Shannon entropy changes are almost the same when the relative dielectric constant $\varepsilon \leq 40$. The difference between the Shannon entropy changes caused by the microcavity only appears at larger relative dielectric constant. In Table 5, we give the calculated values of the ground state Shannon entropy change as a function of the relative dielectric constant and the radius of the spherical microcavity.

4.Conclusions

In general, we present the energy and Shannon entropy for a hydrogen atom confined in a dielectric spherical microcavity. It is found that the energy and Shannon entropy for a confined hydrogen atom depend sensitively on the radius and the relative dielectric constant of the spherical microcavity. Taking the GaAs dielectric spherical microcavity as an example, we study the variation of the energy and Shannon entropy with the size of the microcavity. We found for smaller size of the microcavity, the force and pressure of the microcavity acting on the electron is very large, which causes the kinetic energy of the electron to increase due to the uncertainty principle in the quantum mechanics. Eventually the spatially confinement overcomes the attractive potential between the electron and the hydrogen atom, as a result the total energy of the electron becomes positive. However, the Shannon entropy change is negative, which suggests that the electron density is localized. With the increase of the size of the microcavity, the energy changes from positive to negative. On the contrary, the Shannon entropy change changes from negative to positive, which suggests the confinement of the electron density gets delocalized. As the radius of the microcavity is very large, the energy and Shannon entropy approach to a constant value. Another excited result is that the degeneracy of the excited state energy is broken due to the confinement of the spherical microcavity. There are crossings among some excited energies. At some given radius, the order of the excited state energies is different from the case of the free hydrogen atom, the energy of the $E_{n,l}$ orbit can be larger than $E_{n+1,l}$ orbit. Our calculation results also suggest that the energy and Shannon entropy vary with the relative dielectric constant of the spherical

microcavity. This study has some practical applications in metrology and quantum information processing, and may provide some guidance for future experimental studies for trapping and manipulating of atom and molecule in the microcavity or under high pressure environment.

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Figure and Table captions:

Fig.1. Comparison of the ground state energy for the hydrogen atom confined in the GaAs dielectric spherical microcavity and in the vacuum spherical microcavity.

Fig.2 The distribution of the ground state electron density ρ_{1s} in the GaAs dielectric spherical microcavity with different radius. The radius of the microcavity is as follows:(a) r_d=0.5a.u., (b) r_d =2.0a.u.,(c) r_d =5.0a.u.,(d) r_d =10.0a.u., (e) r_d =50.0a.u., (f) r_d =100.0a.u..

Fig.3. (a) The black line is the ground state Shannon entropy S_r for the hydrogen atom confined in the GaAs dielectric spherical microcavity. The red line denotes the Shannon entropy change ΔS_r relative to the free hydrogen atom. (b) Comparison the ground state Shannon entropy S_r for the hydrogen atom confined in the GaAs dielectric spherical microcavity with the case in the vacuum spherical microcavity.

Fig.4. Variation of the excited state energies for the confined hydrogen atom with the radius of the GaAs dielectric spherical microcavity.

Fig.5. Comparison of the excited state energies at a given size of the GaAs dielectric spherical microcavity. The radius of the spherical microcavity is as follows: (a) $r_d = 0.5$ a.u., (b) $r_d = 10$ a.u., (c) $r_d = 30$ a.u., (d) $r_d = 50$ a.u., (e) $r_d = 200$ a.u., (f) $r_d = 300$ a.u..

Fig.6. Variation of the excited state Shannon entropy for the confined hydrogen atom as a function of the radius of the GaAs dielectric spherical microcavity.

Fig.7 Comparison of the excited state Shannon entropy at a given size of the GaAs dielectric spherical microcavity. The radius of the spherical microcavity is as follows: (a) $r_d = 0.5$ a.u., (b) $r_d = 10$ a.u., (c) $r_d = 30$ a.u., (d) $r_d = 50$ a.u., (e) $r_d = 200$ a.u.,

(f) $r_d = 300$ a.u..

Fig.8 Variation of the ground state energy with the relative dielectric constant and the radius of the spherical microcavity.

Fig.9 Variation of the ground state Shannon entropy with the relative dielectric constant and the radius of the spherical microcavity.

Table 1. The turning radius r_c for the first several s, p states.

Table 2. The excited state energy as a function of the radius of the GaAs dielectric spherical microcavity.

Table 3. The excited state Shannon entropy as a function of the radius of the GaAs dielectric spherical microcavity.

Table 4. The ground state energy as a function of the relative dielectric constant and the radius of the microcavity.

Table 5. The ground state Shannon entropy change as a function of the relative dielectric constant and the radius of the spherical microcavity.
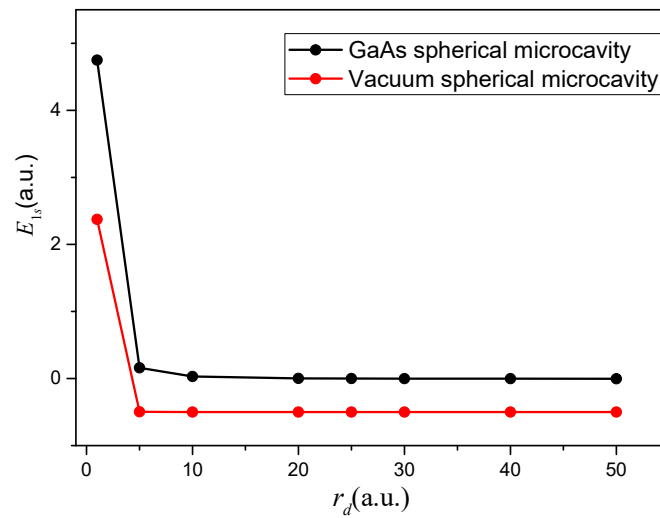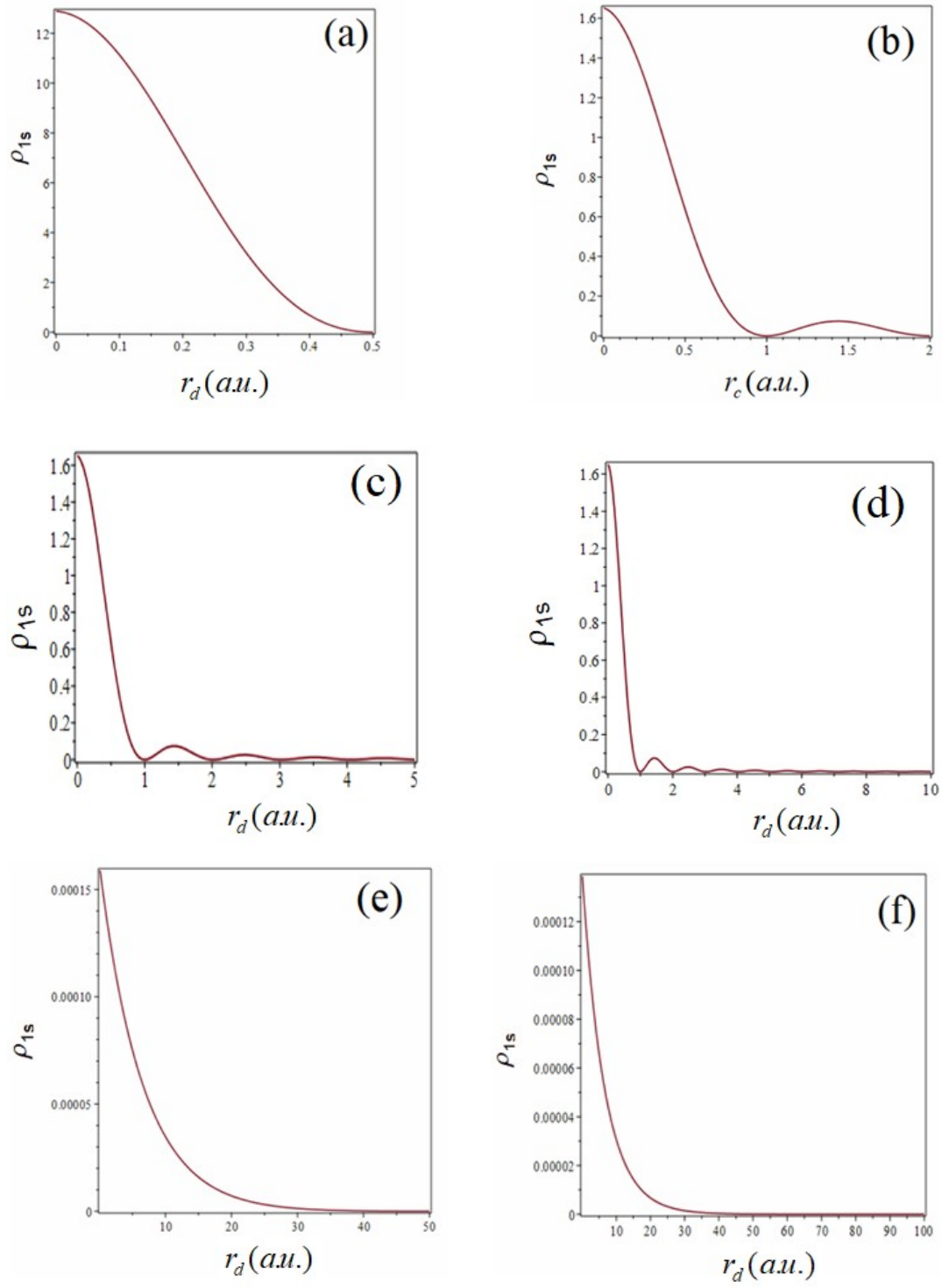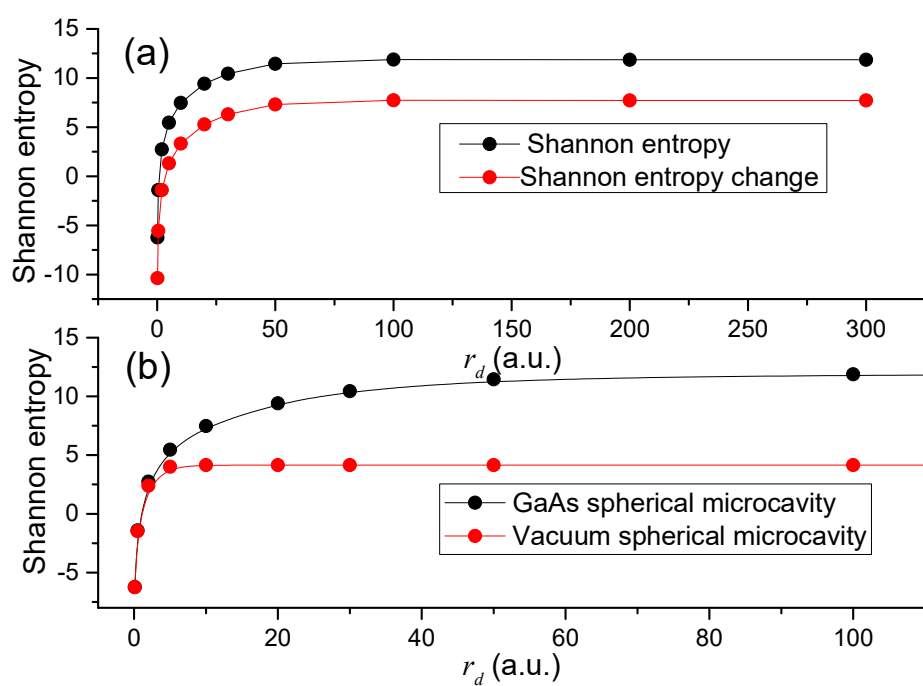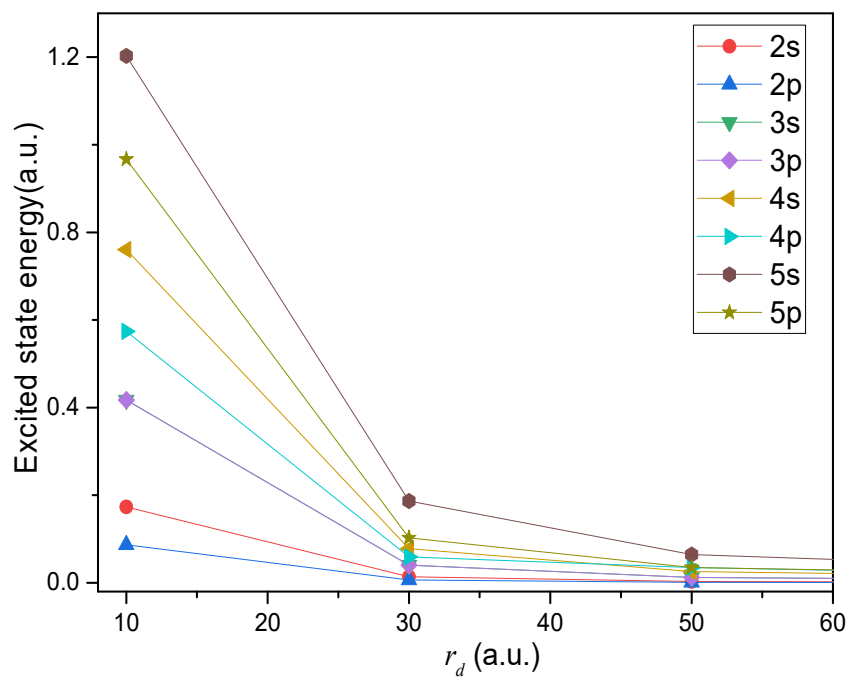

Fig.1

Fig.2

Fig.3

Fig.4
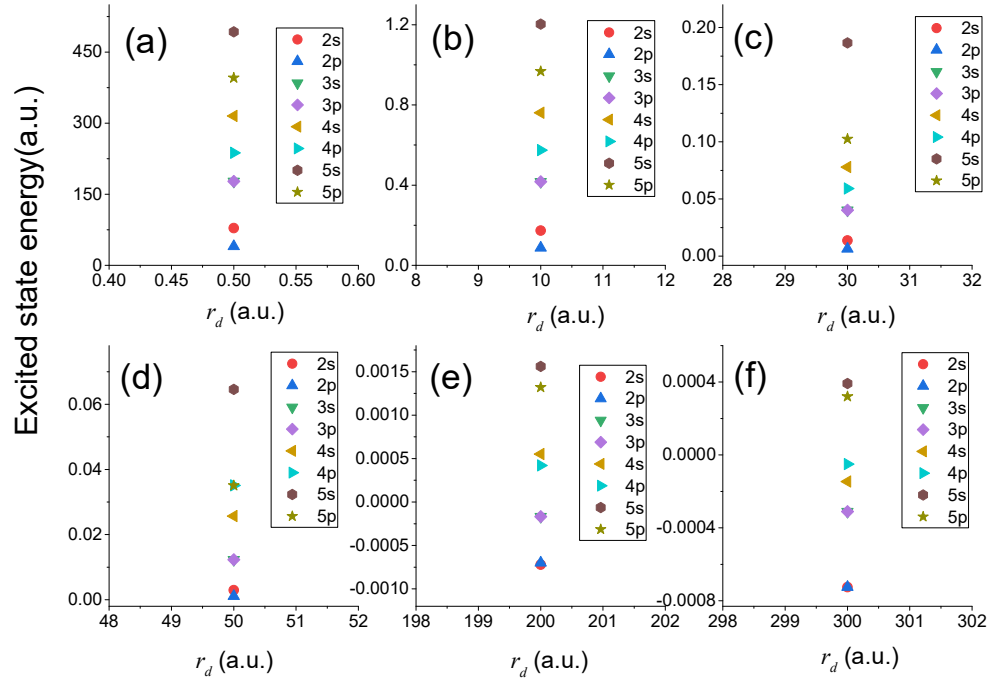
Fig.5
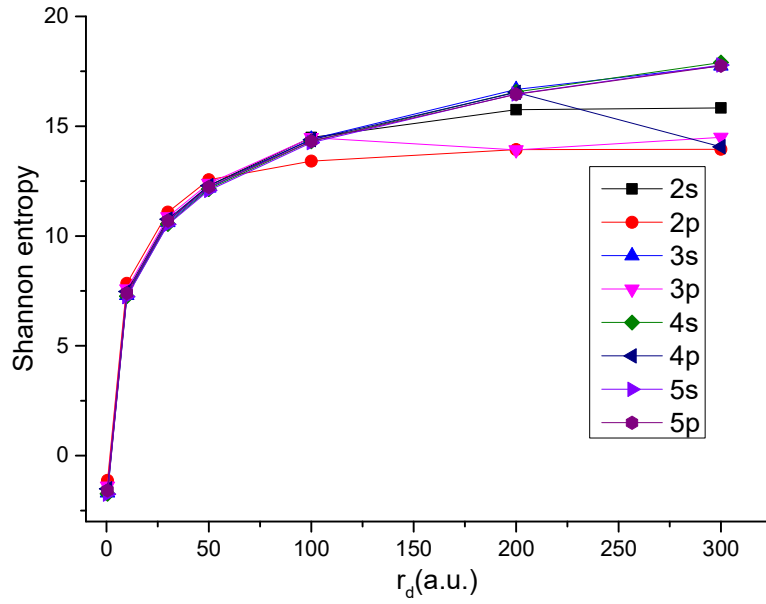
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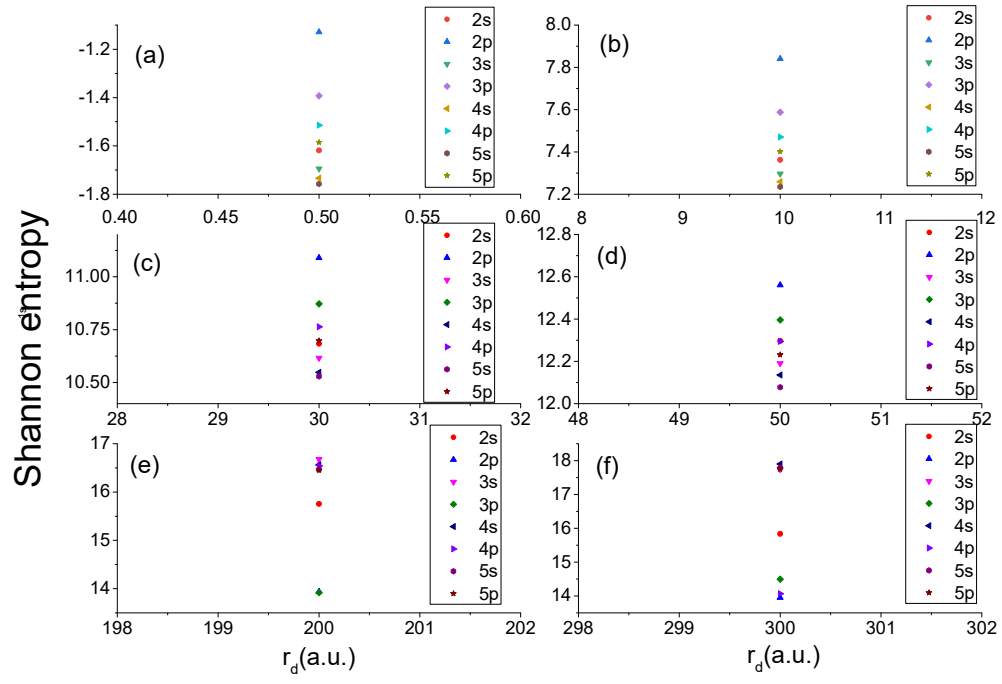
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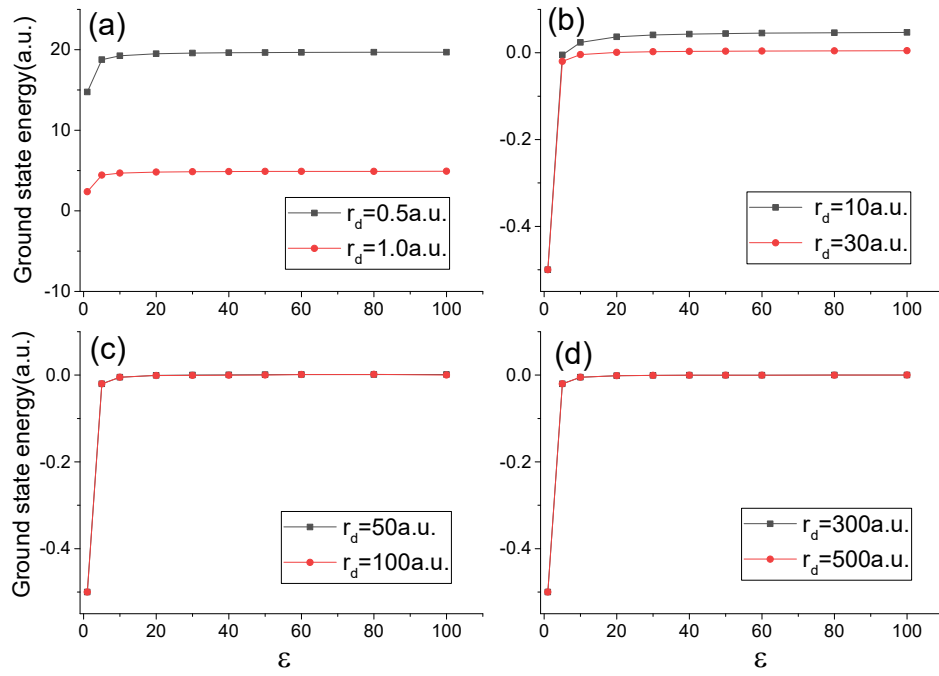
Fig.8
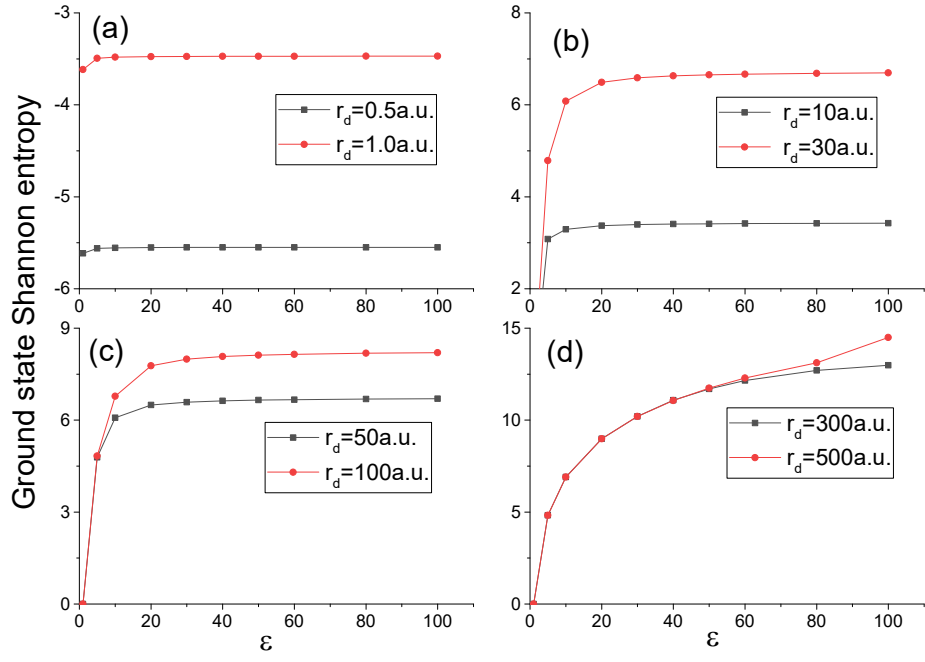
Fig.9

Table 1.

r_c(a.u.) / ε	1s	2s	3s	4s	5s	2p	3p	4p	5p
1.0	1.8352	6.1523	12.9374	22.1901	33.9102	5.0883	11.9097	21.1744	32.9001
13.13	24.0968	80.7798	169.8685	291.3560	445.2410	66.8095	156.3743	278.0203	431.978
30.0	55.0574	184.5692	388.1230	665.7029	1017.3062	152.6492	357.2909	635.2329	987.0032
50.0	91.7623	307.6153	646.8716	1109.5048	1695.5103	254.4154	595.4848	1058.7216	1645.0053
80.0	146.8197	492.1846	1034.9945	1775.2077	2712.8165	407.0647	952.7757	1693.9545	2632.0085
100.0	183.5246	615.2307	1293.7431	2219.0096	3391.0207	508.8308	1190.9697	2117.4431	3290.0107

Table 2.

r_c(a.u.)	2s	2p	3s	3p	4s	4p	5s	5p
0.5	78.4821	40.0990	177.117	119.0013	315.2481	237.3911	492.8671	395.270
10	0.17341	0.08672	0.41721	0.28042	0.76042	0.57420	1.20292	0.96691
30	0.01372	0.00641	0.04020	0.02711	0.12673	0.05921	0.18661	0.10243
50	0.00291	0.00101	0.01226	0.00826	0.02568	0.01963	0.06459	0.03506
100	-0.00043	-0.00058	0.00171	0.00111	0.00494	0.00384	0.00922	0.00761
200	-0.00072	-0.00072	-0.00017	-0.00020	0.00055	0.00042	0.00156	0.00132
300	-0.00072	-0.00072	-0.00003	-0.000030	-0.00002	-0.00005	0.00039	0.00033

Table 3.

r_c(a.u.)	2s	2p	3s	3p	4s	4p	5s	5p
0.5	-1.6188	-1.1285	-1.6946	-1.3925	-1.7336	-1.51467	-1.7575	-1.5856
10	7.3625	7.84059	7.29681	7.5882	7.2594	7.47033	7.2356	7.40123
30	10.6832	11.0898	10.6157	10.87199	10.5477	10.7629	10.5287	10.6972
50	12.297	12.5607	12.1906	12.3957	12.1353	12.2944	12.078	12.2312
100	14.4905	13.4092	14.4156	14.4782	14.3099	14.3836	14.2486	14.3214
200	15.7557	13.9379	16.6782	13.9205	16.563	16.5403	16.4657	16.4534
300	15.8341	13.9486	17.7441	14.4962	17.8995	14.0658	17.7860	17.7504

Table 4

ε / r_0(a.u.)	1.0	5.0	10	20	30	40	50	60	80	100
0.5	14.7480	18.7597	19.2506	19.4952	19.5766	19.6173	19.6417	19.6579	19.6782	19.6900
1.0	2.3740	4.4428	4.6899	4.8126	4.8534	4.8738	4.8860	4.8940	4.9043	4.9104
10	-0.4999	-0.0050	0.0237	0.0369	0.0411	0.0432	0.0444	0.0453	0.0463	0.0469
30	-0.5000	-0.0199	-0.0042	0.0011	0.00264	0.0034	0.00381	0.0041	0.0045	0.0047
50	-0.5000	-0.0200	-0.0049	-0.0008	0.0002	0.0007	0.0009	0.0011	0.0014	0.0015
100	-0.5000	-0.0200	-0.0050	-0.0012	-0.0005	-0.0002	-0.0001	0.0014	0.0016	0.0002
300	-0.5000	-0.0200	-0.0050	-0.0013	-0.0006	-0.0003	-0.0002	-0.0001	-0.0001	-0.00004
500	-0.5000	-0.0200	-0.0050	-0.0013	-0.0006	-0.0003	-0.0002	-0.0001	-0.0001	-0.00005

Table 5.

ε r_0 (a.u.)	1.0	5.0	10	20	30	40	50	60	80	100
0.5	-5.6151	-5.5609	-5.5547	-5.5516	-5.5506	-5.5501	-5.5498	-5.5496	-5.5498	-5.5491
1.0	-3.6157	-3.4943	-3.4815	-3.4752	-3.4732	-3.4722	-3.4716	-3.4711	-3.4706	-3.4704
10	-0.0001	3.0803	3.2921	3.3721	3.3957	3.4069	3.4135	3.4178	3.4231	3.4263
30	0.0	4.7888	6.0794	6.4915	6.5879	6.6298	6.6531	6.6680	6.6858	6.6960
50	0.0	4.8282	7.3032	7.7717	8.0542	8.0744	8.1204	8.1488	8.1818	8.2005
100	0.0	4.8283	6.9079	9.5312	9.5721	9.8511	9.9880	10.1337	10.1278	10.1998
300	0.0	4.8283	6.9078	8.9872	10.2038	11.0808	11.6968	12.1558	12.7058	12.9872
500	0.0	4.8283	6.9078	8.9872	10.2036	11.0668	11.7363	12.2871	13.1172	14.4943