The dynamical properties of a Rydberg hydrogen atom between two parallel metal surfaces*

Liu Wei(刘 伟)[a)†], Li Hong-Yun(李洪云)[b)],
Yang Shan-Ying(杨善迎)[b)], and Lin Sheng-Lu(林圣路)[c)]

[a)] *News Center, University of Jinan, Jinan* 250022, *China*
[b)] *Department of Information Engineering, Laiwu Vocational and Technical College, Laiwu* 271100, *China*
[c)] *College of Physics and Electronics, Shandong Normal University, Jinan* 250014, *China*

(Received 13 July 2010; revised manuscript received 22 August 2010)

This paper presents the dynamical properties of a Rydberg hydrogen atom between two metal surfaces using phase space analysis methods. The dynamical behaviour of the excited hydrogen atom depends sensitively on the atom–surface distance d. There exists a critical atom–surface distance $d_c = 1586$ a.u. When the atom–surface distance d is larger than the critical distance d_c, the image charge potential is less important than the Coulomb potential, the system is near-integrable and the electron motion is regular. As the distance d decreases, the system will tend to be non-integrable and unstable, and the electron might be captured by the metal surfaces.

Keywords: Poincaré surfaces of section, chaos, the phase space analysis methods
PACS: 34.35.+a, 03.65.Sq, 05.45.Mt **DOI:** 10.1088/1674-1056/20/3/033401

1. Introduction

The development of laser theory and technique has been a great influence on traditional atomic and molecular physics. With the help of the short intense laser pulse experiment, it is possible to prepare and probe highly excited Rydberg states, and therefore promote relative research and exploration.[1,2] As a typical theoretical and experimental model, the Rydberg atom near a metal surface can simulate many dynamical effects of an atom in strong fields, and its dynamical properties have attracted much attention for many years.[3−7] For example, Simonovic has studied classical chaos by analysing the Poincaré surface of section.[5] Ganesan and Taylor have calculated its quantum spectra.[6] The problem of a Rydberg atom at a large distance from the metal surface has been considered in the so-called instantaneous van der Waals interaction approximation. Salas and Simonovic have presented quantum mechanical, classical and semiclassical dynamics of a Rydberg hydrogen atom in the instantaneous van der Waals potential.[7] Compared to the studies performed on the Rydberg atom near a metal surface, the dynamical properties of the Rydberg hydrogen atom between two parallel metal surfaces has received little attention. Wang has studied the photoabsorption and recurrence spectra of the Rydberg hydrogen atom in the presence of two metal surfaces using the closed-orbit theory.[8,9] In this paper, we analyse the dynamical properties of the Rydberg hydrogen atom between two parallel metal surfaces using phase space analysis methods. We present that once the electronic energy E is fixed, the distance between the atom and the surface dominates the dynamical properties of the system. The electron motions are initially regular, but when subjected to a decrease in the atom–surface distance, will gradually transform to a chaotic state, which corresponds to the case of adsorption of electrons on the metal surface. Compared with the dynamical properties of the Rydberg atom near a metal surface, it is shown that the influence of image charge potential induced in the case of two metal surfaces is larger than that induced in a metal surface case.

2. Theory and method

We assume that the hydrogen nucleus lies on the origin of the coordinate system with the electron at a distance r from the nucleus. Two parallel metal surfaces are perpendicular to the z-axis and are placed at the planes $z = \pm d$ (see Fig. 1). Using the image charge

*Project supported by the National Natural Science Foundation of China (Grant No. 10774093) and the Natural Science Foundation of Shandong Province (Grant No. ZR2009FZ006).
†Corresponding author. E-mail: ave_liuw@ujn.edu.cn
© 2011 Chinese Physical Society and IOP Publishing Ltd

method,[10] we can write the Hamiltonian of the hydrogen atom in cylindrical coordinate (ρ, z) (we use atomic units hereafter except after extra explanation) as

$$H = \frac{1}{2}\left(p_\rho^2 + \frac{l_z^2}{\rho^2} + p_z^2\right) + U_{\rho z}(\rho, z), \tag{1}$$

$$\begin{aligned} U_{\rho z}(\rho, z) = & -\frac{1}{\sqrt{\rho^2 + z^2}} + \frac{1}{\sqrt{\rho^2 + (2d + z)^2}} \\ & - \frac{1}{4(d + z)} + \frac{1}{\sqrt{\rho^2 + (2d - z)^2}} \\ & - \frac{1}{4(d - z)}. \end{aligned} \tag{2}$$

Here, $U_{\rho z}(\rho, z)$ is the potential energy. The last four terms in Eq. (2), called image charge potential, are induced by the metal surfaces, the higher-order image charge potentials are neglected. Because of the cylindrical symmetry, the z-component of angular momentum is conserved, therefore the φ-motion can be ignored, the system thus has two degrees of freedom. Here we only consider the case of $m = 0$ (i.e. $l_z = 0$) for convenience. Then the Hamiltonian is reduced to

$$\begin{aligned} H = & \frac{p_\rho^2 + p_z^2}{2} - \frac{1}{\sqrt{\rho^2 + z^2}} \\ & + \frac{1}{\sqrt{\rho^2 + (2d + z)^2}} - \frac{1}{4(d + z)} \\ & + \frac{1}{\sqrt{\rho^2 + (2d - z)^2}} - \frac{1}{4(d - z)}. \end{aligned} \tag{3}$$

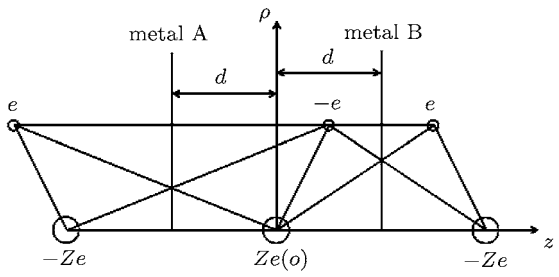


Fig. 1. Pictorial representation of a hydrogen atom and its image with two metal surfaces.

To eliminate the Coulomb singularity at the origin in the Hamiltonian, we adopt the semi-parabolic coordinates $u^2 = r + z$, $v^2 = r - z$ and the relative conjugate momentums $P_u = \mathrm{d}u/\mathrm{d}\tau$, $P_v = \mathrm{d}v/\mathrm{d}\tau$. The new time variable is defined as $\mathrm{d}\tau = \frac{1}{u^2+v^2}\mathrm{d}t$.[11] This results in a regularized Hamiltonian

$$\begin{aligned} h = & \frac{1}{2}(p_u^2 + p_v^2) - E(u^2 + v^2) \\ & + \frac{2(u^2 + v^2)}{\sqrt{(u^2 + v^2)^2 + 8(u^2 - v^2)d + 16d^2}} \\ & - \frac{u^2 + v^2}{2(2d + u^2 - v^2)} \\ & + \frac{2(u^2 + v^2)}{\sqrt{(u^2 + v^2)^2 - 8(u^2 - v^2)d + 16d^2}} \\ & - \frac{u^2 + v^2}{2(2d - u^2 + v^2)} = 2. \end{aligned} \tag{4}$$

After this transformation, the Coulomb singularity has been removed.

The classical trajectories in phase space often have very involved global features, which are in apparent contradiction with the locally smooth flow. Poincaré proposed to solve this problem by intercepting the flow at discrete times. The Poincaré surface of section is one good tool to analyse the classical properties of dynamic systems.[12] By numerical integration of the equations of motion associated with Eq. (4), we can build Poincaré surface of section and examine chaotic or regular behavious of the classical dynamics. For a Hamiltonian system with four-dimensional phase space and two degrees of freedom, the classical motion is restricted to a three-dimensional energy torus, the Poincaré surface of section is a two-dimensional cut of this torus.[13] Because the dimension of the section is one less than that of the flow, the map is easier to be analysed and there are an infinite number of ways to specify the surface of section in general. In this paper we have set the phase space by the surface of section with $p_u > 0$ and $u = 0$, thus obtain Poincaré surface of section in v, p_v plane. The boundary lines of the section can be obtained by

$$\begin{aligned} & p_v^2 - 4 - 2Ev^2 + \frac{4v^2}{4d - v^2} - \frac{v^2}{2d - v^2} \\ & + \frac{4v^2}{4d + v^2} - \frac{v^2}{2d + v^2} = 0. \end{aligned} \tag{5}$$

From Eq. (5), we find that if the electronic energy E is fixed, the boundary line of the section only depends on the atom–surface distance d.

3. Results and discussion

The free hydrogen atom is a real integrable system. When subjected to strong external fields, its integrability may be diminished. As to the atom between two metal surfaces, the image charge potential induced by the two metal surfaces acts on the electron beside the interaction with the nucleus. The motion of

the electron is closely related to the excited state and the atom–surface distance d. Irradiated by a continuous laser, the hydrogen atom staying initially at the ground state or a low excited state would be excited to the Rydberg state $n = 25$. Now the motion of the electron only depends on the atom–surface distance. In Fig. 2, the three-dimensional view and the corresponding contours of the effective potential $U_{\rho z}$ are plotted at two different atom–surface distances. Obviously there exists a deep 'groove' in Fig. 2(a), which disappears in Fig. 2(b). This means that the same electron excited state can escape more easily along the $\pm z$ orientation at $d = 400$ a.u. than at $d = 2000$ a.u. The shorter the atom–surface distance is, the greater the impact of image charge potential is, and the easier the electron is adsorbed on the metal surface.

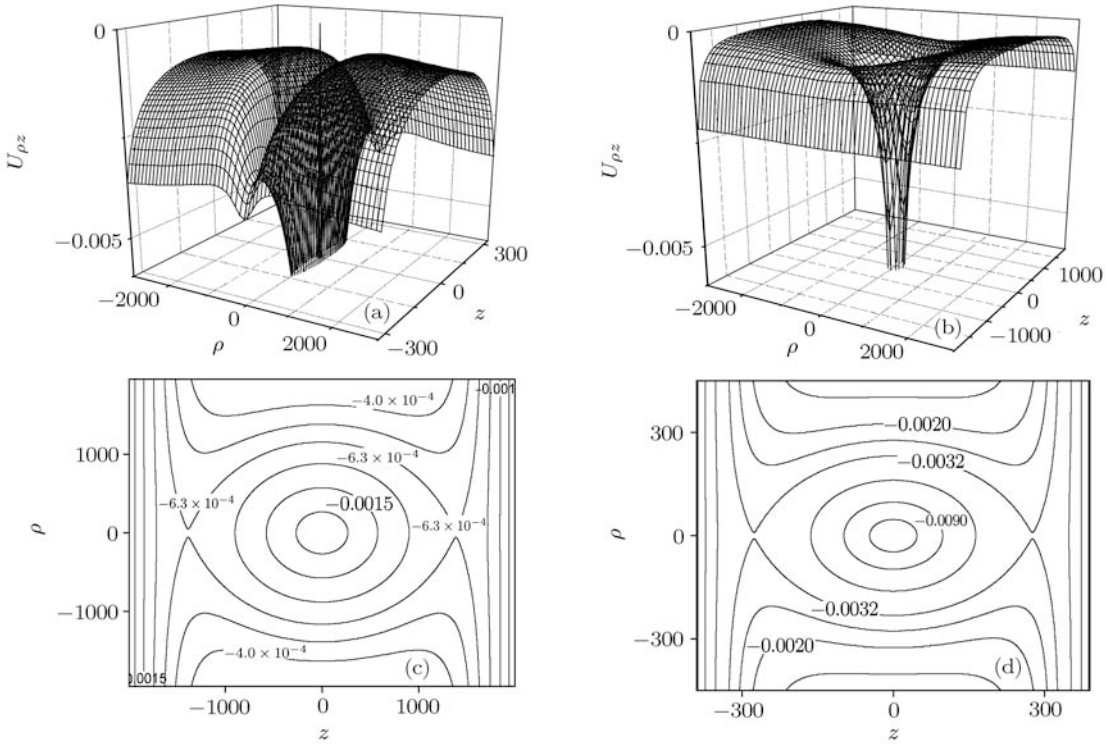


Fig. 2. The effective potential energy view of the electron between two metal surfaces in the cylindrical coordinate: (a) the three-dimensional view at $d = 400$ a.u.; (b) the three-dimensional view at $d = 2000$ a.u.; (c) the contours at $d = 400$ a.u.; (d) the contours at $d = 2000$ a.u.

Once the electron is excited to a fixed Rydberg state, there exists a critical atom–surface distance d_c, where the Coulomb interaction is comparable with the atom–surface interaction. According to Eq. (2) and solving $\partial U/\partial\rho = 0$, $\partial U/\partial z = 0$, we find the critical atom–surface distance $d_c = 1586$ a.u. and the critical point position $\rho = 0$, $z = \pm 1096$ a.u. When the atom–surface distance $d > d_c$, the electron is trapped in bound orbits for all time. When $d < d_c$, the electron may escape and be adsorbed on the metal surface. Some adsorbed orbits at $d = 1000$ a.u. are plotted in Fig. 3 (z is the horizontal axis and ρ is the vertical axis).

The classical properties of the system can be illustrated with the Poincaré surface of section. The evolution of the Poincaré surface of section of the Rydberg hydrogen atom between two parallel metal surfaces at different atom–surface distance is showed in Fig. 4. The atom–surface distance are: (a) $d = 1900$ a.u.; (b) $d = d_c = 1586$ a.u.; (c) $d = 1300$ a.u.; (d) $d = 1000$ a.u.; (e) $d = 700$ a.u.; (f) $d = 400$ a.u. Here we move the two metal surfaces synchronously and ensure the equality of the distance between the atom and each surface. The broken line in Fig. 4 obtained by Eq. (5) denotes the boundary of the section. When $d \geq d_c$, the boundary of the section is closed (the broken line in Figs. 4(a) and 4(b)), while the boundary of the section is opened when $d < d_c$ (the broken line in Figs. 4(c)–4(f)). When the two metal surfaces are far away from the nucleus, the image charge potential is less important than the Coulomb potential, and the Rydberg electron can not be captured by the

metal surface, so the boundary of section is elliptic and closed, the electron can only move inside this ellipse. With the decrease of the atom–surface distance, the role of the image charge potential is enhanced. When $d < d_c$, the electron has a chance to be captured by the metal surface, and the boundary of section becomes open. As the atom–surface distance reduces further, more and more electrons can be adsorbed on the metal surface and the boundary of section becomes more open.

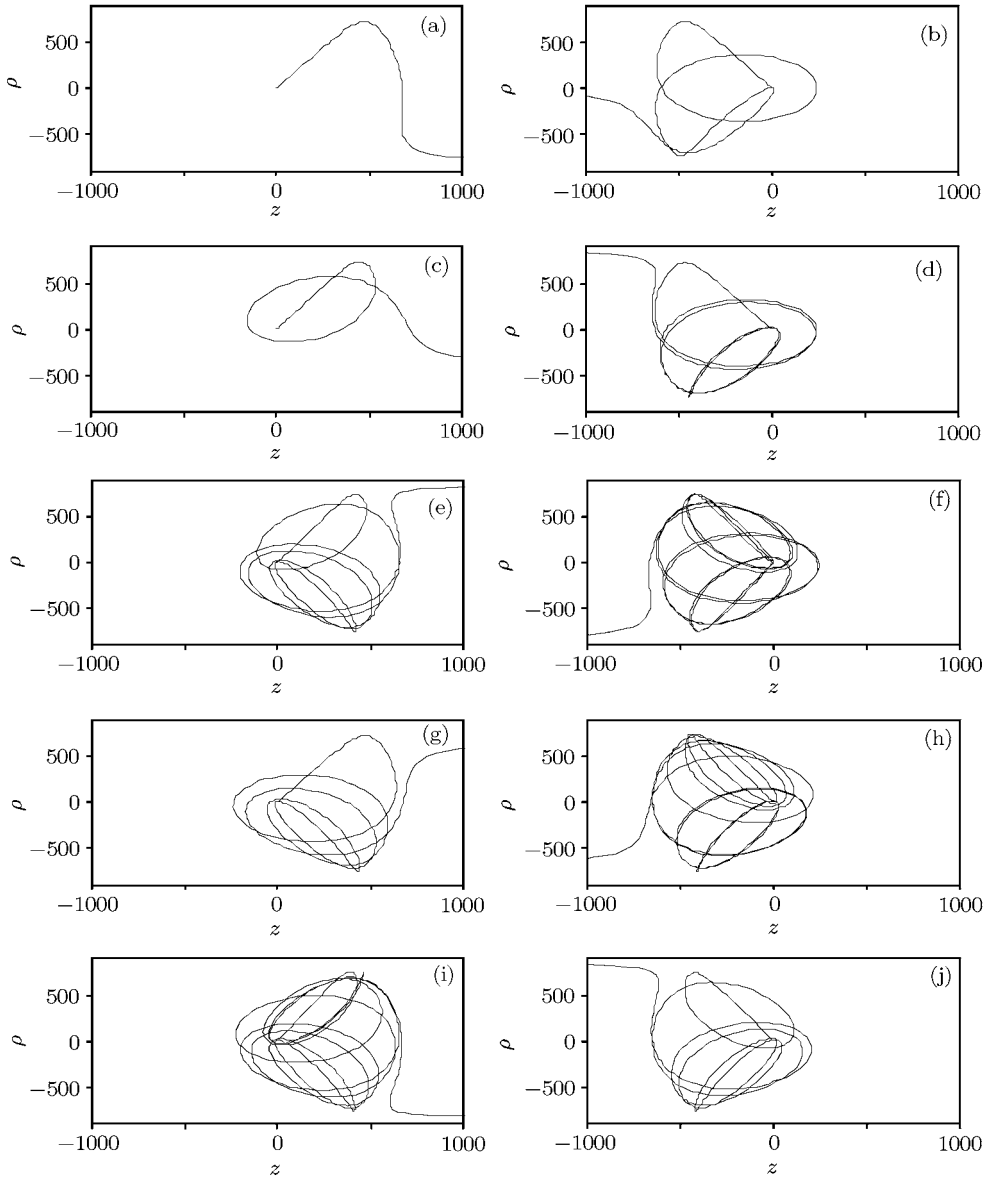


Fig. 3. Some adsorbed orbits at the atom–surface distance $d = 1000$ a.u. The initial outgoing angles are (a) 60.447°, (b) 119.353°, (c) 61.882°, (d) 119.411°, (e) 63.197°, (f) 116.328°, (g) 60.561°, (h) 116.781°, (i) 65.065°, (j) 116.804°. (a), (c) (e), (g), (i) are the orbits captured by the right metal surface; (b), (d), (f), (h), (j) are the orbits captured by the left metal surface.

For the ulterior atom–surface distance, the image charge potential caused by the metal surfaces is very weak, the system is near-integrable (Figs. 4(a) and 4(b)) and the electron's motion is regular. Several isolated fixed points in the surface of section are the centres of concentric closed loops, which define a basin or a mountain as that in a topographic map. The section divided into four separate regions by the separatrix corresponds to the orbits. The ellipses in the central region are vibrational types of orbits since the electron oscillates from the origin towards the right metal surface (Fig. 5(a)). The regions situated sym-

metrically left and right from the central region are rotational types of orbits (Fig. 5(b)). The outer ellipses situated between the separatrix and boundary line are also filled by vibrational-type orbits. However, in this case the electron oscillates from the origin towards the left metal surface, opposite to the orbits in the central region (Fig. 5(c)).

We can see from Fig. 4 that the shape of the Poincaré surface of section changed obviously with the decrease of the atom–surface distance. The blank regions are capture scope, which means that the electron can not reach those regions, i.e. as soon as the electron reaches the regions, it can be captured by the metal surfaces. When the boundary of the section is opened and the electron may be captured, some anomalistic dots appear, which imply that chaotic motion appears. With the further decrease of the atom–surface distance, regular regions reduce inchmeal and chaotic regions increase. At $d = 400$ a.u., regular regions disappear and the phase space is globally chaotic (Fig. 4 (f)). In addition, we can see from the figures that the blank regions appear simultaneously in the inner and outer regions when $d < d_c$.

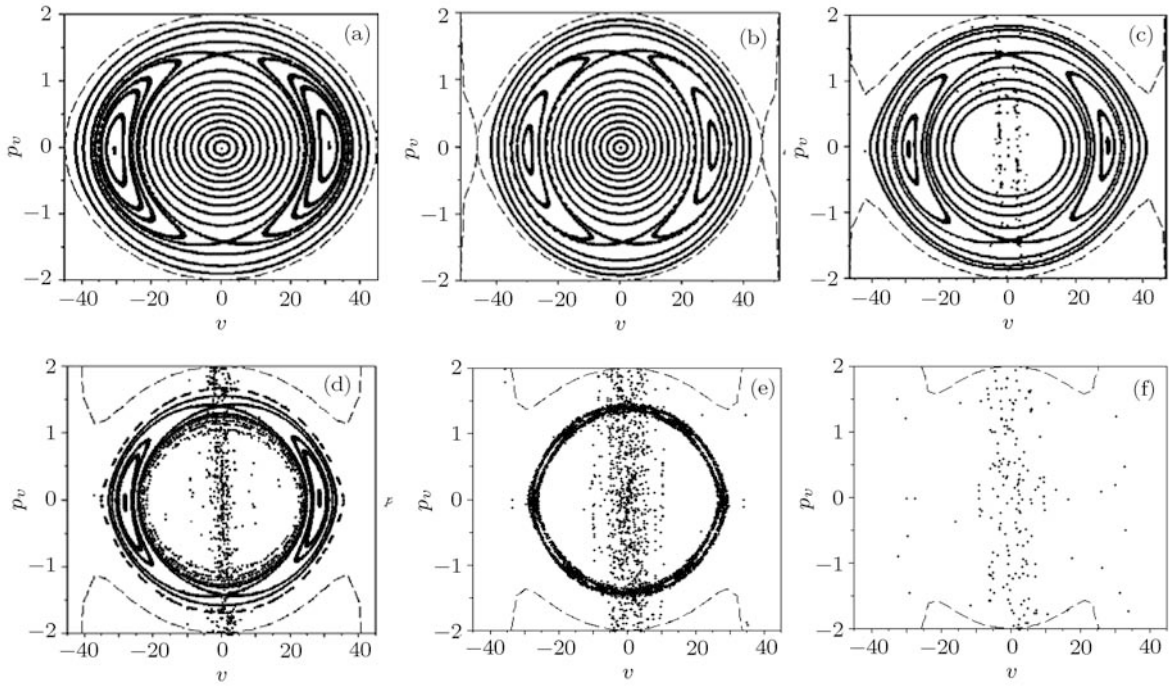


Fig. 4. The evolution of the Poincaré surface of section of the Rydberg hydrogen atom between two parallel metal surfaces: (a) $d = 1900$ a.u.; (b) $d = 1586$ a.u.; (c) $d = 1300$ a.u.; (d) $d = 1000$ a.u.; (e) $d = 700$ a.u.; (f) $d = 400$ a.u.

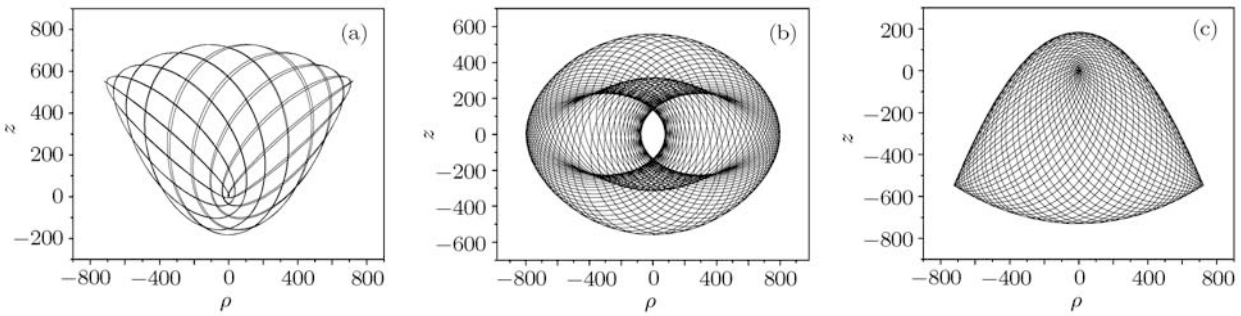


Fig. 5. Examples for vibrational and rotational types of orbits: (a) and (c) are vibrational type of orbits; (b) is rotational type of orbits.

In Fig. 6, we give the evolution of the Poincaré surface of section of the Rydberg hydrogen atom near a metal surface at different atom–surface distances. The metal surface lies on the left side of the nucleus and the atom–surface distances are the same as that in Fig. 4. Compared with Fig. 4, the general tendency of the evolution of the Poincaré map is the same. With the decrease of the atom–surface distance, the system also changes from the regular state to the chaotic state, but there are a few differences. First of all, because the role of the image charge potential is different, the degree of chaos is also different. For example, when $d = 1300$ a.u., chaotic phenomenon has appeared in Fig. 4(c), while it is inexistent in Fig. 6(c). When $d = 400$ a.u., the classical dynamics are globally chaotic in Fig. 4(f), while some small regular motion still exists in Fig. 6(f). Secondly, the critical atom–surface distance is different. Because of the mutual restriction of two metal surfaces, the electron between two metal surfaces can not be easily captured and the critical atom–surface distance of the hydrogen atom between two metal surfaces is less than that of the hydrogen atom near a metal surface. Through calculation, we find the critical atom–surface distance of the hydrogen atom near a metal surface to be 1865 a.u. We also can see from Figs. 4(b) and 6(b) that the boundary of the section is closed in Fig. 4(b) and is already open in Fig. 6(b). In addition, with the decrease of the atom–surface distance, the blank regions are different. When an electron lies near a metal surface, the blank regions only occur in the outer region. When an electron lies between two metal surfaces, they occur in the inner and outer regions at the same time. We know that the outer ellipses in the Poincaré surface of section correspond to the orbits from the central regions towards the left metal surface, while the inner ellipses correspond to the orbits from the central regions towards the right metal surface. When the hydrogen atom is near a metal surface, the electron moved towards the metal surface can be captured first and the outer ellipses disappear first (Figs. 6(c)–6(e)). When an electron is influenced by both side metal surfaces, the inner and outer ellipses reduce at the same time (Figs. 4(c)–4(e)).

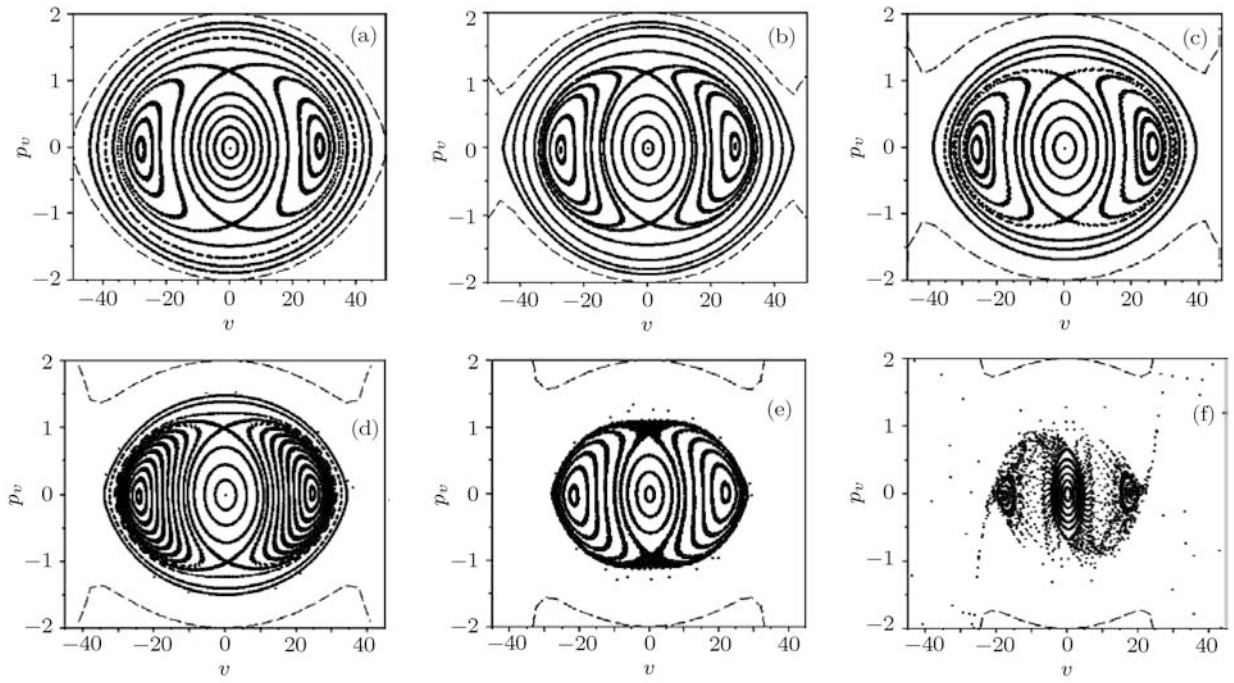


Fig. 6. The evolution of Poincaré surface of section of Rydberg hydrogen atom near a metal surface: (a) $d = 1900$ a.u.; (b) $d = 1586$ a.u.; (c) $d = 1300$ a.u.; (d)$d = 1000$ a.u.; (e) $d = 700$ a.u.; (f) $d = 400$ a.u.

4. Conclusions

The Rydberg hydrogen atom between two metal surfaces is an important example to reveal quantum chaos. By analysing the Poincaré surface of section of the phase space, we study its dynamical properties. We present that once the electronic energy E

is fixed, the atom–surface distance parameter d dominates the dynamical properties of the system. With the decrease of the atom–surface distance, the electron motions gradually transform from an initially regular state to a chaotic state. Compared with the dynamical properties of the Rydberg atom near a metal surface, we find that the influence of electrical mirror image potential induced by two metal surfaces is larger than that induced by a metal surface.

References

[1] Johnson T A, Urban E, Henage T, Isenhower L, Yavuz D D, Walker T G and Saffman M 2008 *Phys. Rev. Lett.* **100** 113003

[2] Hamilton E L, Greene C H and Sadeghpour H R 2002 *J. Phys.* B **35** L199

[3] Landragin A, Courtois J Y, Labeyrie G, Vansteenkiste N, Westbrook C I and Aspect A 1996 *Phys. Rev. Lett.* **77** 1464

[4] Huang K Y and Wang D H 2010 *Chin. Phys.* B **19** 063402

[5] Simonovic N S 1997 *J. Phys.* B **30** L613

[6] Ganesan K and Taylor K T 1996 *J. Phys.* B **29** 1293

[7] Salas J P and Simonovic N S 2000 *J. Phys.* B **33** 291

[8] Wang D H 2006 *Chin. Phys. Lett.* **23** 2745

[9] Wang D H 2007 *Chin. Phys.* **16** 0692

[10] Jackson J D 1975 *Classical Electrodynamics* (2nd) (New York: John Wiley)

[11] Dando P A, Monteiro T S, Delande D and Taylor K T 1996 *Phys. Rev.* A **54** 127

[12] Courtney M and Kleppner D 1996 *Phys. Rev.* A **53** 178

[13] Meyer H D 1986 *J. Chem. Phys.* **84** 3147