Vol 13 No 1, January 2004
1009-1963/2004/13(01)/0030-06

Chinese Physics

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The closed-orbit and the photoabsorption spectra of lithium atom in varying magnetic fields*

Wang De-Hua(王德华)[a)b)] and Ding Shi-Liang(丁世良)[a)†]

[a)] *School of Physics and Microelectronics, Shandong University, Jinan* 250100, *China*

[b)] *Department of Mathematics and Physics, Shandong Institute of Architecture and Engineering, Jinan* 250014, *China*

(Received 21 March 2003; revised manuscript received 2 June 2003)

Using a simple analytic formula from closed orbit theory, we have calculated the photoabsorption spectra of Li atom in different magnetic fields. Closed orbits in the corresponding classical system have also been obtained for B=5.96T. We demonstrate schematically that the closed orbits disappear gradually with the decrease of the magnitude of the magnetic field. This gives us a good method to control the closed orbits in the corresponding system by changing the magnetic field, and thus changing the peaks in the photoabaorption spectra. By comparing the photoabsorption spectra of Li atom with those of hydrogen case, we find the core-scattered effects play an important role in multi-electron Rydberg atoms.

Keywords: closed-orbit theory, photoabsorption spectra, core-scattered effects
PACC: 3260, 0300, 0365

1. Introduction

Rydberg atoms in strong external fields have been shown to be real physical examples of nonintegrable systems to study the quantum manifestations of classical chaos both experimentally and theoretically. Closed-orbit theory [1,2] introduced new ways of looking at the photoabsorption spectrum of Hamiltonian having chaotic classical dynamics.[3] For light atoms, such as hydrogen and negative hydrogenic ions, in strong external fields, the closed-orbit theory has proven to be a quantitative and elegant method of calculating and interpreting the recurrence spectra.[4−7] However, a complete theoretical treatment of multi-electron atom in external fields remains a challenge. Recent works have found that the effects of a nonhydrogenic ionic core should be taken into account.[8−12] Following quantum-defect theory, the electron–core interactions are characterized by a set of energy independent quantum defects. Such results predict that when the ionic effects of multi-electronic atom are included, new recurrence peaks, called core-scattered recurrences,[13] emerge in large numbers.

To date, many researchers have studied the recurrence spectra of Li atom.[14,15] But they only calculated the spectra of Li atom in a uniform electric or magnetic field. Few calculations have been carried out for Li atom in external fields of varying magnitude. In this paper, we present theoretical computations of the photoabsorption spectra of Li atom in magnetic fields of five different magnitude using the closed orbit theory and analyse how the cross section varies with the magnetic fields. Finally, we compare the photoabsorption spectra of Li atom with those of the hydrogen case, and find that the spectra of Li atom oscillates in a much more complicated manner than those of hydrogen case. This suggests that the core-scattered effects play an important role in the multi-electron Rydberg atom.

2.Theory and quantitative formula

2.1. Closed-orbit theory

The closed-orbit theory was originally developed for the hydrogen atom in a magnetic field by Du and Delos [1,2] and has been extended to incorporate quan-

*Project supported by the National Natural Science Foundation of China (Grant No 20173031), the Science Foundation of Shandong Province, China, and the Doctoral Foundation from the Ministry of Education of China.

†Corresponding author. E-mail: shlaudin@sdu.edu.cn

tum defects by Gao and Delos.[16,17] For completeness we will only give a brief summary of this theory as well as the basic equations. The near-threshold absorption spectrum of an atom in an external field consists of a series of sinusoidal oscillations on a slowly varying background. Closed-orbit theory connects each oscillation to a classical electron orbit that is closed at the nucleus. Two different regions in space are distinguished: the region near the core ($r < r_b$, r_b=$50a_0$), where a quantum description is required, and the region far away from the core ($r > r_b$), where a semiclassical description is feasible.

In closed-orbit theory, the absorption of a photon by an atom in an external field excites an electron that leaves the core region in an almost zero-energy outgoing Coulomb wave at an initial launching angle θ_i to the field direction. For $r > r_b$, this wave propagates semiclassically; the electron follows a classical trajectories and its dynamics is governed by Hamiltonian equation of motion. Eventually, the trajectories will curl back in the combined external potential. The electron may then return to the core, its trajectory making an angle $\theta_f$with the field direction. Here again a quantum description is needed and a scattering wavefunction can be constructed. An electron orbit that closes exactly at the core results in an oscillation in the absorption spectrum as a consequence of interference between the returning waves scattering at the core and the original outgoing wave.

2.2. Oscillator-strength density

According to the closed-orbit theory, the photoabsorption cross section is related to the oscillator-strength density $Df(E)$ by

$$\sigma(E) = \frac{2\pi^2 e^2}{m_e c} Df(E). \tag{1}$$

The oscillator strength for dipole transitions of an initial state ψ_i to final states at an energy E is

$$Df(E) = -\frac{2}{\pi}(E - E_i)\mathrm{Im}\langle D\psi_i|\hat{G}^+|D\psi_i\rangle, \tag{2}$$

where $\hat{G}^+$ is the outgoing Green function, and D is the dipole operator, for z-polarized light,

$$D = z = r\cos\theta. \tag{3}$$

We will consider the transition from Li 3s state to m=0, $E \approx 0$. According to the closed-orbit theory, the observed oscillator can be written as a combination of a smooth background term and a sum of sinusoidal oscillations [1]

$$Df(E) \approx Df_0(E) + \sum_k A_k \sin[T_k \cdot E + s_k - \phi_k]. \tag{4}$$

The first term is precisely the oscillator strength that would be reached without any external field. Each term in the summation corresponds to a closed orbit of the electron in the combined external fields.

2.2.1. The smooth-background part of the oscillator-strength density

It is easy to calculate the smooth-background term of the absorption spectra [13]

$$\begin{aligned} Df_0(E) &= -\frac{2}{\pi}(E - E_i)\mathrm{Im}\langle D\psi_i|\hat{G}^+_{\mathrm{dir}}|D\psi_i\rangle \\ &= 2(E - E_i)|B_{10}|^2, \end{aligned} \tag{5}$$

where $B_{lm} = \int \mathrm{d}r' D\psi_i(r') R_l^{0,\mathrm{reg}}(r') \mathrm{Y}^*_{l,m}(\theta', \varphi')$, for the photoabsorption from s state using z-polarized light, B_{10} is a constant. $R_l^{0,\mathrm{reg}}(r)$ is the wavefunction that is regular at the origin. For nonhydrogenic atoms, the asymptotic form for large r (valid for $5a_0 \le r \le 50a_0$) of the wavefunctions is [16]

$$\begin{aligned} R_l^{0,\mathrm{reg}}(r) = &\left[\frac{2}{\pi\sqrt{8r}}\right]^{\sqrt{1/2}} \\ &\times \cos\left[\sqrt{8r} - \left(l + \frac{1}{2}\right)\pi - \frac{\pi}{4} + \delta_l\right]/\sqrt{8r}, \end{aligned} \tag{6}$$

where δ_l is the phase shift of the Coulomb wave caused by the lithium core.

2.2.2. The oscillating part of the oscillator-strength density

The oscillating part is connected to some classical quantities of the closed orbit in the system, with the amplitude A_k and phase φ_k being

$$A_k = \sqrt{18\pi \sin\theta_{i,k} \sin\theta_{f,k}/|m_{12,k}|}\cos\theta_{i,k}\cos\theta_{f,k}, \tag{7}$$

$$\varphi_k = -2\delta_1 + \frac{\pi}{2}\alpha_k - \frac{\pi}{4}. \tag{8}$$

In the above equations, E and E_i are the energies of the final and initial states; $\theta_{i,k}$ and $\theta_{f,k}$ are the initial and final angles of the kth closed orbit; s_k and α_k are the classical action and the Maslov index of the closed orbit, respectively. T_k is the travel time along the closed orbit while $m_{12,k}$ is defined as [18]

$$m_{12,k} = \frac{r}{2}\det\left|\frac{\partial(r,\theta)}{\partial(t,\theta_i)}\right|.$$

3. The classical motion

3.1. Hamiltonian

The Hamiltonian of the Li atom in a static magnetic field aligned along the z-axis is described (in atomic units and cylindrical coordinates) as

$$H = \frac{1}{2}\left(p_\rho^2 + \frac{l_z^2}{\rho^2}\right) + \frac{\gamma(t)}{2}l_z + \frac{1}{8}\gamma^2(t)\rho^2 + \frac{1}{2}p_z^2 + V(r), \tag{9}$$

where $\gamma(t) = B(t)/2.35 \times 10^5 (B(t)$ is the magnetic field strength), for m=0 state, $l_z = 0$. The magnetic field changes with time according to

$$B(t) = 5.96\sin(\pi t), \tag{10}$$

where t ranges from 0.1 to 0.5, and $V(r)$ is the potential. Since we are dealing with the Rydberg Li atom in which only one electron is excited to the ionization threshold while the ionic core remains in the ground state, thus the nuclear charge is screened by other electrons and the exact problem can be simplified to the movement of a highly excited electron in an attractive Coulomb potential modified by a short-range core potential combined with external fields. Thus the potential $V(r)$ can be in the following form:[14]

$$V(r) = V_{\text{Coulomb}}(r) + V_{\text{core}}(r) = -\frac{1}{r} - \frac{Z-1}{r}\mathrm{e}^{-\frac{r}{a}}, \tag{11}$$

where Z is the nuclear charge and a is a free length parameter determining the range of the core and quantum defects. For a Li atom, we choose Z=3 and a=1/2.13. In quantum mechanics, the ionic effects are described by the quantum defects. In our calculation, we choose $\delta_1 = 0.06\pi$.

3.2. Closed-orbit search

For the system we consider in this paper, because of the existence of a magnetic field, the Hamiltonian is not separable and the motion is nonintegrable. Therefore, we have to integrate the equation of motion in order to find the closed orbit. We use the fifth-order Cash–Karp Runge–Kutta method to integrate the equations of motion. In order to search the accurately closed orbit and calculate the relevant classical quantities, we take three steps in the computer codes, as follows: (1) Because of the symmetry of the problem, we search for those nearly closed orbits in the range of (0°, 90°) instead of (0°, 180°). In order to save computing time, we set the step size of the initial launching angle θ_i to be 0.1°. It is recorded as a nearly closed orbit when the trajectory returns to the vicinity of the nucleus for $|r - r_b| < 1.0a_0$. (2) We change the step size of θ_i to 0.01°, then we search for two nearly closed orbits found in step 1. (3) Since we have launched trajectories in the radial direction, the accurately closed orbits must return to the spherical surface perpendicularly, which means that $p_\theta = 0$. We search for all the closed orbits of this system with five different magnetic fields, B=5.96, 5.67, 4.82, 3.5 and 1.84T respectively. For each of the closed orbits, we calculate the classical action s_k, Maslov index α_k and the amplitude A_k.

4. Results and discussion

By integrating the Hamiltonian equations of motion, we obtain all the closed orbits of this system with varying magnetic field. From the calculation, we find that with the decrease of the magnitude of the magnetic field, the closed orbits disappear gradually. Figure 1 presents some important closed orbits of Li atom with the applied magnetic field B=5.96T. Using Eq.(4), we calculate the absorption spectra of Li atom in various magnetic fields. As seen in Figs.2(a)–(e), the spectra become more and more complicated as $B(t)$ increases. It is easy to understand the underlying physical reason of this: as the magnetic force becomes stronger, the electron can travel much nearer to the nucleus before it is turned back by the magnetic field.

Figure 2(f) is the photoabsorption of H atom in the magnetic field, B=5.96T. From Figs.2(e) and (f) we can see that the spectrum of Li atom oscillates in a much more complicated manner than that of H atom. This can be interpreted as follows: by comparing the closed orbits of Li atom and those of H atom in the same magnetic field,[1] we find that the number of the closed orbits of Li atom is much larger than that of the H atom and some different types of nonhydrogen closed orbits exist in the Li atom. This is caused by the scattering of the core potential. A trajectory of Li atom starting at almost the same initial direction as a hydrogenic closed orbit leaves the nucleus radially and evolves hydrogen-like outside the region of the ionic core. As the orbit returns to the nucleus it is scattered by the core potential. Outside the ionic core the electron again evolves hydrogen-like and may then be scattered a second time, a third time, etc. until finally it returns to the nucleus exactly where the orbit is closed. Thus the nonhydrogenic closed orbit appears to be composed of two or more hydrogenic orbits. For example, Fig.1(e) can be seen as a combination of two

hydrogenic orbits, Fig.1(f) can be seen as a combination of three hydrogenic orbits, whereas Fig.1(h) can be seen as composed of more than three hydrogenic orbits. Therefore it causes a huge and rapid increase of the number of multiple-scattered closed orbits. From the above, we can see that the core-scattered effects play a great role in the nonhydrogenic atom case.

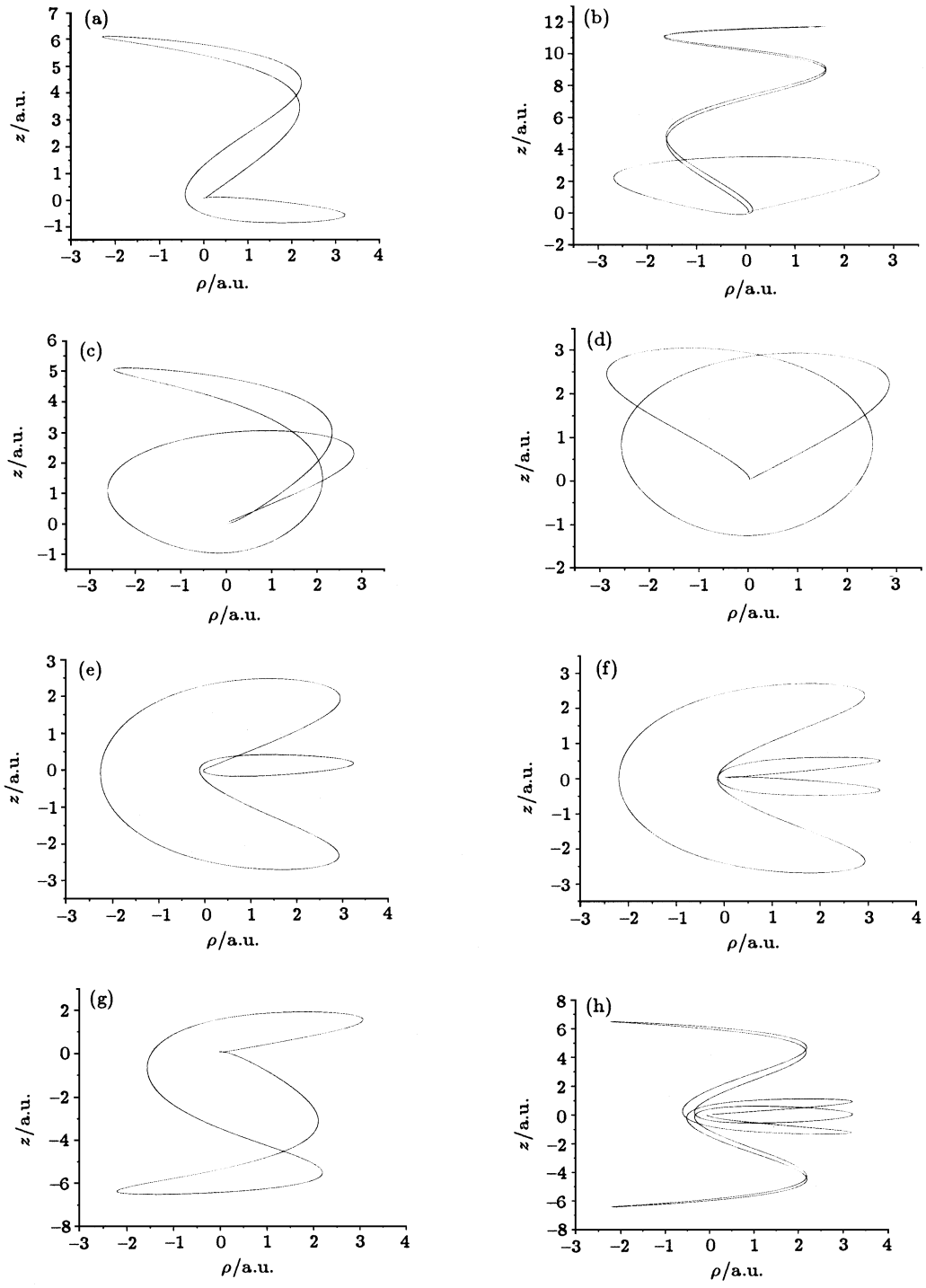


Fig.1. Some closed orbits of Li atom in the magnetic field with B=5.96T. The figures are plotted in the ρ–z plane.

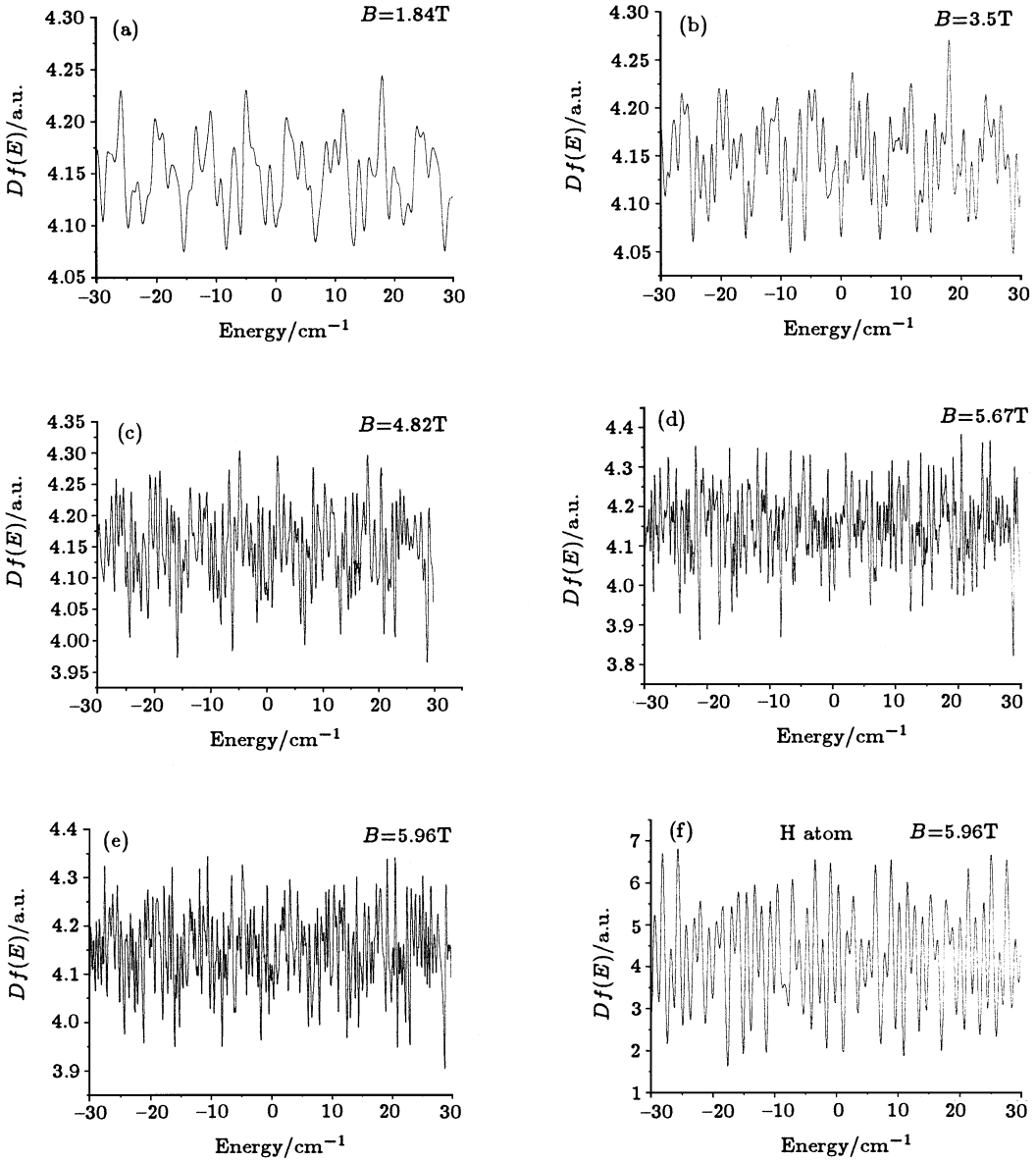


Fig.2. (a)–(e) are the photoabsorption spectra of Li atom in different magnetic fields. (f) is the photoabsorption spectra of H atom in a magnetic field.

5. Conclusion

We have calculated the photoabsorption spectra of Li atom in different magnetic field in terms of using the closed-orbit theory. We have shown that the closed orbits disappear gradually with the decrease of the magnitude of the magnetic field. We think this gives us a good method to control the closed orbits in the corresponding system by changing the magnetic field, and thus changing the peaks in the photoabaorption spectra. By comparing the spectra of Li atom with those of the hydrogen case, we find that the core–scattered effects play a great role in multi-electron Rydberg atom. Presently no experiments on the photoabsorption spectra of Li atom in varying magnetic fields have been carried out. Our calculations show that there are interesting phenomena that may arouse future measurements.

Acknowledgements

We also thank Professor S L Lin for his kind help and valuable discussion.

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