Angular Distribution of Electrons Following Photoionization of $n'sns\ ^1S_0$ Rydberg States in the Alkaline-Earth Atoms*

DAI Changjian (C.J.Dai)
Department of Physics, Zhejiang University, Hangzhou 310027

(Received 17 January 1994)

A new characterization of the angular distribution of electron ejected from n'pns autoionizing states in the alkaline-earth atoms has been carried out from the most general expression of differential cross section of photoabsorption. The same approach may be extended to more complicated cases where the traditional treatment becomes invalid. The comparison between the two methods is presented.

PACS: 34. 50. Lf, 32. 80. Rm, 32. 80. Dz

The photoexcitation process in general may lead either to the excitation of a structureless continuum or a structured continuum consisting of autoionizing states. Recent study on the angular distribution measurements of ejected electron from autoionizing *3pns* states of magnesium[1] has shown that the angular distribution measurements involve more complex sets of channels and wavefunctions than those of the line-shape measurements of corresponding autoionizing Rydberg states.[2]

Study of the $n'pns$ autoionizing states is especially appealing, as the initial states of the transitions are spherically symmetric, and $J=1$ is the only allowed final excited-state angular momentum. Systematic studies on angular distributions of electrons ejected from alkaline-earth elements in analogous doubly excited autoionizing Rydberg states $n'pns$ ($n'=3$—6 for Mg,[1] Ca,[3] Sr,[4] and Ba,[5] respectively) have been performed. In all cases, angular-momentum-transfer theory[6] was employed to derive the expression of the asymmetry parameter necessary to describe the angular distribution. In this paper we present an alternative approach to the same problem and point out the differences between them.

For the most general cases, more than one asymmetry parameters have to be used to describe the angular distribution.[7] One must start from the most general formula for $d\sigma/d\Omega$ of an atom absorbing a linearly-polarized photon and then emitting an electron, i. e.

$$\frac{d\sigma}{d\Omega}=\sum_k a_k P_k(\cos\theta)\ , \tag{1}$$

where

$$a_k=-\frac{N^2}{4\pi}\sum_{\substack{J_cJ_{cs}\\ ll'JJ'}}(-1)^{J_{cs}}[J][J'][l][l'][k]^2 CD_{J_{cs}lJ}D^*_{J_{cs}l'J'}\ . \tag{2}$$

* Supported by the National Natural Science Foundation of China, and the State Commission of Education of China, and Science Foundation of Zhejiang University.

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In Eq. (1), $P_k(\cos\theta)$ is the kth Legendre polynomial, and θ is the polar angle between the laser polarization and the direction of the emitted electron. The coefficient a_k is a sum of contributions corresponding to different magnitudes of the angular momentum transferred to a target. In Eq. (2), N^2 is a normalization constant, J_c is the total residual ion core angular momentum, $J_{cs} = J_c + s$, where s is the spin of the outer electron, l is the orbital angular momentum of the outer electron, J is the total angular momentum of the system, i. e. $J = J_{cs}+l$. The symbol $[x]$ is defined as $(2x+1)^{1/2}$, where $x = J, J', l, l'$ or k. $D_{J_{cs}lJ}$ in Eq. (2) is an abbreviation of the reduced matrix elements, i. e.,

$$D_{J_{cs}lJ} = \langle (J_{cs}l)J - ||r^{(1)}||J_i\rangle \ , \tag{3}$$

where $r^{(1)}$ is a first-rank tensor, J_i is the total angular momentum of the initial state, and, $J_i = 0$ for $n'sns$ Rydberg states. The minus sign in the matrix element indicates that the wave function of final state is normalized according to incoming-wave boundary conditions, namely at large r the wave function has the form of a plane wave plus incoming spherical waves. The coefficient C in Eq. (2) is a product of $3j$ and $6j$ symbols, i. e.,

$$C = \begin{bmatrix} J_i & 1 & J \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} J' & 1 & J_i \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} l' & l & k \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} k & J' & J \\ 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} k & J' & J \\ J_{cs} & l & l' \end{Bmatrix} . \tag{4}$$

Since $J = 1$ is the only possible angular momentum for the $n'pns$ autoionizing states, the non-zero $6j$-symbol requires $k = 0, 2$ only. Therefore Eq. (1) reduces to a well-known expression:

$$\frac{d\sigma}{d\Omega} = a_0 + a_2 P_2(\cos\theta) = \frac{I_0}{4\pi}[1 + \beta P_2(\cos\theta)] \ , \tag{5}$$

which immediately yields

$$I_0 = 4\pi a_0 \tag{6}$$

and

$$\beta = \frac{a_2}{a_0} \ . \tag{7}$$

I_0 as a function of energy gives the total photoabsorption cross section, or line shape of the transition. The asymmetry parameter β varies as a function of energy which determines the differential photoabsorption cross section of the transition. Thus armed with the general expression of the coefficient a_k, we are able to calculate line shape of transition, or autoionization spectrum, and the angular distribution of ejected electrons from autoionizing states.

Now we are in a position to obtain the specific expressions of the parameters I_0 and β. An $n'pns$ $J = 1$ autoionizing state may decay to $n's_{1/2}\epsilon p$ continuum which determines all the quantum numbers, i. e. $J_c = 1/2$, $J = J' = J_- = 1$, and $J_{cs} = 0,1$, respectively. Obviously, $l = l' = 1$ is the only possible electron ejected from $n'pns$ states. In other words, when $l = J = 1$ the ejected electron is an outgoing p wave. For this simple case, determination of a_k is straightforwards, and

$$a_0 = \frac{N^2}{4\pi} \sum_{J_{cs}=0}^{1} (-1)^{J_{cs}} C |D_{J_{cs}lJ}|^2 \tag{8}$$

with

$$C = \frac{1}{9}\begin{Bmatrix} 0 & 1 & 1 \\ J_{cs} & 1 & 1 \end{Bmatrix} \tag{9}$$

or write them together,

$$a_0 = \left(\frac{N^2}{4\pi}\right)\frac{1}{3}[|D_{011}|^2 + |D_{111}|^2] \,. \tag{10}$$

Similarily, we obtain

$$a_2 = \left(\frac{N^2}{4\pi}\right)\frac{1}{3}[2|D_{011}|^2 - |D_{111}|^2] \,, \tag{11}$$

which immediately yields the β parameter and the total cross section of photoabsorption for the $n's_{1/2}$ core respectively as

$$\beta_{n's_{1/2}} = \frac{a_2}{a_0} = \frac{2|D_{011}|^2 - |D_{111}|^2}{|D_{011}|^2 + |D_{111}|^2} \tag{12}$$

and

$$\sigma_{n's_{1/2}} = \frac{I_0}{4\pi} = a_0 = \left(\frac{N^2}{4\pi}\right)\frac{1}{3}[|D_{011}|^2 + |D_{111}|^2] \,. \tag{13}$$

Clearly, calculations of the reduced matrix elements D_{011} and D_{111} are crucial parts of determining both β and σ. The procedures to determine $D_{J_{cs}lJ}$ are well documented.[4] Usually one can apply multichannel quantum-defect theory[8] (MQDT) or the combination of MQDT with R-matrix calculation[1] to a given theoretical model in which the number of channels may be quite different from Mg to Ba.

It is worthwhile to make a comparison between the present result and that of traditional approach performed in alkaline-earth metals. It is well-known that the β parameter for the p-wave electrons may be expressed as[4]

$$\beta_{n's_{1/2}} = \frac{2|S_p(0)|^2 - 3|S_p(1)|^2}{|S_p(0)|^2 + 3|S_p(1)|^2} \tag{14}$$

with the scattering matrix elements

$$S_l(J_t) = A(-1)^{J_0 - J - 1}[J]\begin{Bmatrix} J_{cs} & 1 & J \\ 1 & J_0 & J_t \end{Bmatrix} D_{J_{cs}lJ} \,, \tag{15}$$

where A is a factor related to photon energy $\hbar\nu$ by

$$A(2\alpha\hbar\omega^3/3c^2)^{1/2} \,, \tag{16}$$

where $S_l(J_t)$ are characterized by quantum numbers of the transferred angular momentum J_t and the orbital angular momentum of outgoing electron. The α and c are the fine-structure constant and the velocity of light, respectively. For the special case under consideration, $J_t = J_{cs}$. Thus it is straightforward to carry out the specific expression for $S_l(J_t)$, i.e.

$$S_p(0) = A\, D_{011} \,, \tag{17}$$

$$S_p(1) = -\frac{A}{\sqrt{3}} D_{111} \,. \tag{18}$$

Substitution of Eqs. (17) and (18) into Eq. (14) enables us to verify that Eq. (14) is indeed equivalent to Eq. (12).

The advantage of the present approach is apparent. It is based on a general expression of differential cross section of photoabsorption so that it is suitable to both cases in which the initial state is polarized and unpolarized targets. The validity of Eqs. (1) and (2) on a polarized target, the Mg $3snd$ Rydberg state, was tested successfully.[7] Furthermore, the expressions of the β and σ in terms of the reduced matrix elements are derived without knowledge of angular-momentum-transfer theory and the scattering matrix element $S_l(J_t)$, which significantly simplifies the problem. Note that the results presented here are applicable to all alkaline-earth metals.

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