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## Near-threshold $K$ -shell photoionization of argon

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The  $K$ -shell photoionization cross section of argon near the threshold has been obtained with the multiconfiguration Hartree-Fock method for continuum wave functions. The electron correlation and the core-relaxation effects that are very important in this process have been taken into account in the calculation very accurately in the *ab initio* manner through the configuration-interaction procedure. The present results are compared with the experimental measurements and are found to be in excellent agreement. The two-electron resonances that have been observed immediately above the ionization threshold have been identified and assignments have been made to these based on accurate calculations.

### I. INTRODUCTION

It is well known that the interaction of atoms with an electromagnetic field is a convenient and effective method for studying their electronic structure. If the field is weak, it perturbs the atom and one can obtain information on atomic wave functions from the photoionization cross section.

Photoionization of deep inner atomic shells is a very interesting problem from a theoretical point of view. This process is accompanied by electron-shell rearrangement<sup>1</sup> of the residual ion under the influence of the inner-shell vacancy. This rearrangement leads to the variation of the wave functions of all the atomic electrons of the core, which alters the potential field in which the photoelectron moves. The inner-shell vacancy may decay subsequently by a radiative or Auger process. If the decay time is small compared to the time required for the photoelectron to leave the atom, it moves not in the potential field of the initial vacancy  $i$  but in the rearranged ion-core potential field. The inclusion of the rearrangement effects is important for the correct description of the photoionization of inner atomic shells.

At near-threshold energies not only the effects of core relaxation but also the electron-electron correlations are very important and these effects must be included in a realistic calculation of photoionization cross sections.

Deslattes *et al.*<sup>2</sup> made a detailed experimental study of the near-threshold behavior of  $K$ -shell absorption in argon which shows resonance structures due to two-electron excitation.

In general, the correct accounting of the allowance for the dynamics of the atomic core rearrangement and the effects of electron-electron correlation is a very complicated problem. Several attempts have been made to account for core relaxation in argon near-threshold  $K$ -shell photoionization. These effects provide useful information for a better understanding of the effects of core relaxation. Manson and Inokuti<sup>3</sup> calculated the  $K$ -shell photoionization cross section using wave functions generated in a local exchange central field potential (Herman and Skillman<sup>4</sup>) and found large deviations from smooth hy-

drogenic behavior for atoms with  $Z \leq 30$ . Their calculated argon  $1s$  cross section shows a peak at 40 eV above threshold, then decreases to a shoulder at about 135 eV above threshold instead of a sharp onset followed by a monotonic decrease. Amusia and his co-workers developed comparatively simple methods for the description of this process. Amusia *et al.*<sup>5</sup> considered the effect of the static rearrangement of an atom on the photoionization cross section of deep shells. They determined wave functions of the photoelectron in a completely rearranged self-consistent field of an atomic core. They have shown that static rearrangements significantly weaken the field at distances of the order of atomic radius. This leads to a decrease of the cross section at threshold. Amusia *et al.*<sup>6</sup> also considered the effect of a postcollision interaction due to the decay of the vacancy  $i$ . This increases the charge of the residual ion. In this case, the ejected electron immediately after its creation moves in the field of the doubly charged rearranged ion that is produced due to Auger decay. According to their simplified model the photoionization cross section is determined by a single-particle dipole matrix element calculated for a ground state of the neutral atom and a state of the electron that moves in the field of a rearranged doubly charged ion. They applied this method for the photoionization cross section of argon atom near the ionization threshold of the  $K$  shell. They have shown that their results agree well with Schnopper's<sup>7</sup> measurement.

Recently Tulkki and Aberg<sup>8</sup> calculated the  $K$ -shell photoionization cross section of argon using the Dirac-Fock method. They took into account the complete relaxation effect by calculating separately the wave functions for the ground state and the final  $1s^{-1}$  hole state and by including all the resulting overlap matrix elements between the initial and the final state one-electron wave functions in the transition amplitude. They considered the effect of a postcollisional interaction by a relativistic generalization of the resonant scattering theory of threshold phenomena in inner-shell ionization.<sup>9,10</sup> Their results that include relaxation effects are seen to be in close agreement with experiment except for resonances. The most recent calculations are those of Cooper<sup>11</sup> who exam-

ined in detail the effects of core relaxation and electron correlation on the near-threshold  $K$ -shell absorption cross section. He calculated cross sections using wave functions obtained from both the center of gravity and the term-dependent  $^1P$  calculations. His results lie within 5% of the experimental values in the region immediately above the ionization threshold. At higher energies his calculations lie below the experimental results.<sup>2</sup> His further analysis indicated that although electron-electron correlations produce only small changes in the single-electron cross section, they can account for the two-electron resonances that have been observed immediately above the ionization threshold. Until now, no theoretical work has yet been reported on the  $K$ -shell photoionization of argon that can interpret the experimental results, in particular, the resonance structures in the cross section obtained by Deslattes *et al.*<sup>2</sup> As the electron-electron correlation and the core-relaxation effects are very important in the  $K$ -shell photoionization of argon, it is of interest to perform accurate calculations to understand the important interactions and to obtain accurate results for comparison with the experiment.

The numerical multiconfiguration Hartree-Fock approach<sup>12,13</sup> for continuum wave functions has already been proved to produce accurate results for the photoionization cross section of atoms.<sup>14-18</sup> The most recent successful application of this method was in the calculation of the  $K$ -shell photoionization cross section of the beryllium atom<sup>19</sup> for photon energies ranging from the  $(1s)^{-1}2s^2$  threshold at 123.6 to 144 eV. The results were found to be in very good agreement with the experiment. In the present paper we report a study of the  $K$ -shell photoionization cross section of argon using MCHF technique. As mentioned earlier, to understand the complicated dynamics of the  $K$ -shell photoionization, one has to consider both core relaxation and electron-electron correlation very accurately. The present MCHF method,<sup>19</sup> which can take into account the electron correlation and the core relaxation effects very efficiently through the configuration interaction procedure, will be very useful to understand the complex dynamics of the escape of the photoelectron from the  $K$ -shell of the argon atom.

## II. THEORY

### A. The MCHF wave function for the continuum state

The MCHF wave function for the final continuum state is expressed in a series of the form

$$\Psi(\gamma LS; N+1) = \sum_{j=1}^{m_c} a_j \Phi(\gamma_j L_c S_c; N) \phi_{kl} + \sum_{i=1}^m c_i \Phi(\gamma_i LS; N+1), \quad (1)$$

where  $\Phi(\gamma_j L_c S_c; N)$  is an  $N$ -electron bound configuration eigenstate of  $L_c$  and  $S_c$  of the ionic core, having configuration  $\gamma_j$  and mixing coefficients  $a_j$ , coupled to the continuum orbital function for the  $(N+1)$ th electron to give an eigenstate of  $L$  and  $S$ .  $\Phi(\gamma_i LS; N+1)$  are  $(N+1)$ -electron bound configurations that are eigen-

states with the same  $L$  and  $S$  and are included to allow for electron correlation effects.  $\phi_{kl}$  represents the one-electron continuum orbital with orbital angular momentum  $l$ .

The mixing coefficients  $a_j$  and the set of bound radial functions  $P_j(r)$ ,  $j=1, 2, \dots, N_c$  which describes the ionic-core wave function, are obtained from a separate MCHF calculation. In the calculation of the final-state continuum wave function all the radial functions describing the core are assumed to be fixed along with the mixing coefficients  $a_j$ . The coefficients  $c_i$  and a set of radial functions  $P_i(r)$   $i=1, 2, \dots, N_f$  describing the bound and the continuum orbitals, are determined variationally. All the radial functions  $P_i(r)$  satisfy the following coupled integro-differential equation:

$$\left[ \frac{d^2}{dr^2} + \frac{2Z}{r} - \frac{l(l+1)}{r^2} \right] P_i(r) = \frac{2}{r} [Y_i(r)P_i(r) + X_i(r) + I_i(r)] + \sum_{i'} \varepsilon_{ii'} P_{i'}(r), \quad (2)$$

where the off-diagonal energy parameters  $\varepsilon_{ii'}$  are related to Lagrange multipliers that ensure orthogonality assumptions.  $(2/r)Y_i(r)$  and  $(2/r)X_i(r)$  are, respectively, the screening and the exchange potentials.  $(2/r)I_i(r)$  represents terms arising from interaction between the configuration states.

The bound radial functions satisfy the boundary conditions

$$P_i(r) \underset{r \rightarrow 0}{\sim} r^{l+1}, \quad P_i(r) \underset{r \rightarrow \infty}{\sim} 0. \quad (3)$$

In this case the diagonal energy parameters  $\varepsilon_{ii}$  are eigenvalues of the integro-differential equations and hence need to be determined. The photoelectron is assumed to move asymptotically in a pure Coulombic field. The continuum wave function satisfies the following boundary conditions:

$$P_i(r) \underset{r \rightarrow 0}{\sim} r^{l+1}, \quad (4)$$

$$P_i(r) \underset{r \rightarrow \infty}{\sim} \left[ \frac{2}{\pi k} \right]^{1/2} \sin \left[ kr - \frac{l\pi}{2} + \frac{q}{k} \ln(2kr) + \sigma_l + \delta_l \right],$$

where  $k^2$  is the kinetic energy of the photoelectron and  $\varepsilon_{ii} = -k^2$ .  $q = Z - N$  is the net charge of the ion.  $\sigma_l = \arg \Gamma(l+1 - iq/k)$  is the Coulomb phase shift and  $\delta_l$  is the residual phase shift.

The coupled integro-differential equations are solved numerically by an iterative method. Both the bound and the continuum wave functions are computed using the same numerical multiconfiguration (MC) self-consistent-field (SCF) procedure. The bound radial functions are essentially localized and vary smoothly as  $r \rightarrow \infty$ . The continuum radial function is normalized by fitting the computed values at two adjacent points to the regular and irregular Coulomb functions as soon as the region is reached where the direct and the exchange potentials are vanishingly small, which may be at considerably smaller values of  $r$  than the asymptotic form represented by the

boundary condition of Eq. (4).

The coefficients  $c_i$ , which need to be determined, are solutions of the system of equations derived from the condition that  $\langle \Psi | H - E | \Psi \rangle$  is stationary with respect to the variations in the coefficients, where  $H$  is the Hamiltonian for the  $(N+1)$ -electron system and  $E = E_c + k^2/2$  (in a.u.).

The coefficients  $c_i$  are calculated by solving the system of equations

$$\sum_{i'=1}^m \langle \Phi_i | H - E | \Phi_{i'} \rangle c_{i'} + \sum_{j=1}^{m_c} \langle \Phi_i | H - E | \Phi_j \rangle a_j = 0, \quad i = 1, \dots, m \quad (5)$$

where

$$\Phi_j \equiv \Phi(\gamma_j L_c S_c; N) \phi_{kl}, \quad j = 1, \dots, m_c$$

and

$$\Phi_i \equiv \Phi(\gamma_i L S; N + 1), \quad i = 1, \dots, m.$$

### B. MCHF theory of photoionization

Having specified the initial- and the final-state wave functions we can now calculate the photoionization cross section. The total photoionization cross section is given in the dipole approximation by

$$\sigma(\omega) = 4\pi^2 \alpha a_0^2 \sum_{f,m} |\langle \Psi_f | T | \Psi_i \rangle|^2, \quad (6)$$

where  $\omega$  is the energy of the incident photon in atomic units;  $\alpha$  is the fine structure constant, and  $a_0$  is the Bohr radius of the hydrogen atom.  $\Psi_i$  and  $\Psi_f$  are the initial- and the final-state wave functions, respectively, and the sums run over final configurations and all magnetic quantum numbers.  $T$  is the dipole transition operator which is given by

$$\{ 1s^2 3s^2 3p^6, 1s^2 3s 3p^6 4s, 1s^2 3s^2 3p^5 4p, 1s^2 3s 3p^5 3d 4p, 1s^2 3s 3p^5 3d 4f, 1s^2 3s 3p^5 4s 4p, 1s^2 3s 3p^5 4p 4d, 1s^2 3s 3p^5 4d 4f, 1s^2 3p^6 3d 4d, 1s^2 3p^6 3d^2, 1s^2 3p^6 4s^2, 1s^2 3p^6 4p^2, 1s^2 3p^6 4d^2, 1s^2 3p^6 4f^2, 1s^2 3s^2 3p^4 3d 4s, 1s^2 3s^2 3p^4 3d 4d, 1s^2 3s^2 3p^4 4p 4f, 1s^2 3s^2 3p^4 3d^2, 1s^2 3s^2 3p^4 4s^2, 1s^2 3s^2 3p^4 4p^2, 1s^2 3s^2 3p^4 4d^2, 1s^2 3s^2 3p^4 4f^2 \}^1 S.$$

The radial wave functions for the different orbitals were obtained by the MCHF procedure, varying all the orbitals simultaneously except  $1s$ ,  $2s$ ,  $2p$ ,  $3s$ , and  $3p$  which were obtained from the Hartree-Fock (HF) calculation of the argon atom and were kept fixed.

The final-state continuum wave function expansion for the  $^1P$  state contains 18 configurations:

$$\{ 1s 3s^2 3p^6 k p_1, 1s 3s^2 3p^5 3d^2 (^3P, ^1D, ^1S), 1s 3s^2 3p^5 4s^2, 1s 3s^2 3p^5 4p^2 (^3P, ^1D, ^1S), 1s 3s^2 3p^5 4d^2 (^3P, ^1D, ^1S), 1s 3s^2 3p^5 4f^2 (^3P, ^1D, ^1S), 1s 3s^2 3p^5 (^3P, ^1P) 3d 4s, 1s 3s (^3S, ^1S) 3p^6 4s 4p_2 \}^1 P^0.$$

The  $1s$ ,  $2s$ ,  $2p$ ,  $3s$ , and  $3p$  orbitals were obtained from the Hartree-Fock calculation of  $\text{Ar}^+$  core state. The configuration mixing coefficients  $c_i$  and the other bound orbitals were optimized at each photon energy. In this

$$T = T_L = \sum_{j=1}^n Z_j$$

in the length form and

$$T = T_V = \sum_{j=1}^n \frac{\nabla_j^Z}{i\omega}$$

in the velocity form. If  $\Psi_i$  and  $\Psi_f$  are exact solutions of the same Hamiltonian, the length and the velocity forms of the cross sections will be identical. Following Scofield<sup>20</sup> the many electron matrix elements in Eq. (6) can be expressed as a superposition of products of one-electron overlap and the dipole matrix elements.

### III. COMPUTATIONAL PROCEDURE

We consider the process

$$\hbar\omega + \text{Ar}(1s^2 2s^2 2p^6 3s^2 3p^6 ^1S) \rightarrow \text{Ar}^+(1s 2s^2 2p^6 3s^2 3p^6 ^2S) + k p ^1P^0.$$

We mentioned earlier that electron correlations in the initial state and both electron correlation and the core relaxation in the final state are very important for the study of the  $K$ -shell photoionization of argon. The multiconfiguration Hartree-Fock method described in the earlier papers,<sup>12-19</sup> which can take into account both of these effects very accurately is used for the calculation. In order to study the presence of the autoionization resonances that characterize the spectrum found in the experiment, particular attention was placed to the inclusion of the double electron excitations in the MCHF calculation of the initial- and the final-state wave functions. First of all, a set of radial functions was determined for the initial state by the traditional MCHF method.<sup>21</sup>

The MCHF wave function expansion for the initial ground-state argon was over the set of 38 configuration states coupled to form a  $^1S$  term:

way the core relaxation and the electron correlation effects were considered in the calculation of the final-state wave function.

The above sets of configurations were selected after a

series of tests had been performed and represent the sets of configurations which contribute considerably to the dipole matrix elements. In the selection of the configurations it has been found that the configurations with  $1s$  excitation in both the initial neutral and the final ionic state contribute negligibly small not only in the dipole matrix elements but also in the mixing coefficients compared to that of the configurations with outer-shell excitations.

#### IV. RESULTS

##### A. Energy levels

The Hartree-Fock energy of the initial bound state derived from the use of the single configuration was found to be  $-526.817512$  a.u. In the MCHF calculation of the initial state it was found that the configurations with double electron excitation  $3p^4 3d^2$  mix very strongly. The binding energy obtained in the MCHF calculation was  $-527.031246$  a.u. The HF energy of the ionic core ( $1s^{-1}2s$ ) was  $-409.389067$  a.u. It should be mentioned that the correlation of the ionic core does not change the photoionization cross section considerably.

The HF energy levels of the different states of the different configuration are presented in Table I relative to the HF energy of the ground state of the ionic core. In the calculation of HF energy of the different states of the different configuration, all the orbitals were varied except the  $1s$ ,  $2s$ ,  $2p$ ,  $3s$ , and  $3p$  orbitals that were kept frozen to the HF  $1s$ ,  $2s$ ,  $2p$ ,  $3s$ , and  $3p$  orbitals of the ionic state. As already mentioned, in the MCHF calculation of the final state all the orbitals were varied except the  $1s$ ,  $2s$ ,  $2p$ ,  $3s$ , and  $3p$  orbitals that were kept fixed to the ionic state HF value.

TABLE I. Hartree-Fock energy levels relative to ionic core state ( $1s^{-1}$ ) of argon (HF energy =  $-409.389067$  a.u.).

Configuration state	Energy (eV)
$1s^{-1}3p^{-1}3d^2(^3P)^1P^o$	22.19
$1s^{-1}3p^{-1}3d^2(^1D)^1P^o$	21.49
$1s^{-1}3p^{-1}3d^2(^1S)^1P^o$	22.14
$1s^{-1}3p^{-1}4s^2^1P^o$	16.72
$1s^{-1}3p^{-1}4p^2(^3P)^1P^o$	20.19
$1s^{-1}3p^{-1}4p^2(^1D)^1P^o$	21.12
$1s^{-1}3p^{-1}4p^2(^1S)^1P^o$	21.91
$1s^{-1}3p^{-1}4d^2(^3P)^1P^o$	25.96
$1s^{-1}3p^{-1}4d^2(^1D)^1P^o$	26.33
$1s^{-1}3p^{-1}4d^2(^1S)^1P^o$	26.87
$1s^{-1}3p^{-1}4f^2(^3P)^1P^o$	27.50
$1s^{-1}3p^{-1}4f^2(^1D)^1P^o$	28.33
$1s^{-1}3p^{-1}4f^2(^1S)^1P^o$	28.76
$1s^{-1}3p^{-1}(^3P)3d4s^1P^o$	19.13
$1s^{-1}3p^{-1}(^1P)3d4s^1P^o$	19.08
$1s^{-1}3p^{-1}1P^o$	32.62
$1s^{-1}3p^{-1}3P^o$	31.75
$1s^{-1}3s^{-1}(^3S)4s4p^1P^o$	37.01
$1s^{-1}3s^{-1}(^1S)4s4p^1P^o$	39.93
$1s^{-1}3s^{-1}1S$	53.19
$1s^{-1}3s^{-1}3S$	51.47

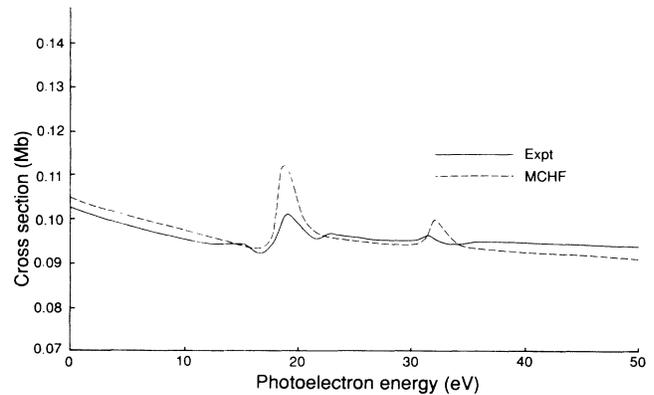


FIG. 1. Calculated and experimental cross section plotted as a function of photoelectron energy.

##### B. Cross section

The photoionization cross sections obtained from the MCHF calculation are presented in Fig. 1 as a function of photoelectron energy ranging from 0 to 50 eV. The cross section shown in the figure are the total cross sections that are obtained by adding the present calculated cross sections with the extrapolated  $L$ - and  $M$ -shell contributions obtained from Ref. 20. The experimental<sup>2</sup> total cross sections are plotted for comparison. We also calculated the photoionization cross sections in the HF calculation with initial- and the final-state orbitals computed separately. In this case the final-state bound orbitals were calculated with a vacancy in the  $1s$  orbital and the photoelectron wave function was calculated in this rearranged potential field of the core. The photoionization cross section was obtained in this approximation by including all the resulting overlap matrix elements between the initial and the final one-electron orbitals in the transition amplitude. The present HF results were found to be the same as those obtained by Tulkki and Aberg<sup>8</sup> and by Cooper.<sup>11</sup> The present length and velocity results in the HF approximation differ by approximately less than 5%. In the MCHF calculation the length and velocity results agree very well so that only the length results are shown in the figure. The present calculation shows two resonances in the cross section. These resonances are due to the presence of the doubly excited bound states  $1s^{-1}3p^5 3d^2(^3P)^1P^o$  at 19.0 eV and  $1s^{-1}3s(^3S)3p^6 4s4p^1P^o$  at 32.2 eV. The position of these resonances agrees very well with the experimental values 19.0 and 31.4 eV, respectively. From the figure it is seen that the theoretical results are slightly higher than the experiment at very near to the threshold from 0 to 12 eV and from 34.5 to 50 eV, the theoretical results are a little lower. However, there is overall excellent agreement with the experimental observation.<sup>2</sup> The experiment also indicated a few more resonances in the cross section, which were not found in the present calculation with the set of configurations used in the present case.

#### V. CONCLUSION

We have made a detailed study of the effects of core relaxation and electron correlation on the near-threshold behavior of the  $K$ -shell photoionization of argon using

the multiconfiguration Hartree-Fock method.<sup>12,13</sup> Our calculations show that electron correlation in the initial state and complete relaxation of the ionic core and electron correlation of the final state are essential to obtain reliable cross section of atomic argon near the 1s threshold. The core relaxation and the electron correlation which are found to be very important in this case have been taken into account very accurately in the *ab initio* manner through the configuration interaction procedure. The present results agree very well with the experimental results of Deslattes *et al.*<sup>2</sup> The positions of the two-electron resonances that have been found immediately above the ionization threshold are in excellent agreement with the experimental values. Moreover, excellent agreement between the present length and velocity cross sec-

tions shows the accuracy of the initial- and the final-state wave functions. Finally our success in this difficult calculation shows that the MCHF method extended for continuum wave function that can take into account the correlation and the relaxation effects very accurately in the *ab initio* manner produces reliable results.

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