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Variation of photoelectron angular distributions along the Ar and Ca isonuclear sequences

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The dipole angular distribution asymmetry parameter, β, for photoelectrons resulting from $2p$ photoionization of Ar, Ar^{6+}, and Ar^{8+} and Ca, Ca^{2+}, and Ca^{8+} of the Ar ($Z = 18$) and Ca ($Z = 20$) isonuclear sequences, respectively, have been studied using the relativistic random-phase approximation over a broad range of photon energy. In the *absence of relaxation*, it is known that inner-shell cross sections are essentially unchanged, as a function of photon energy, upon the removal of outer-shell electrons. The present results show that this is not true for the photoelectron angular distribution asymmetry parameters, particularly near the ionization thresholds.

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I. INTRODUCTION

Reliable inner-shell photoionization cross sections are required for accurate models of stellar interiors and interstellar media [1]. Isonuclear studies are of great importance to assess theoretical data generated for applications in fusion plasmas, in tokamaks, and in astrophysics [2–4]. Despite the difficulty in producing ionic targets in sufficient density, several measurements of multiply charged ions are available [5,6]. Recently, photoionization measurements of isonuclear sequences for Xe [7], Cs [8], Ba [9], Fe [10], and Ce [11] have been reported. A number of theoretical calculations of the photoionization cross section of inner shells of isonuclear sequences for O [12], Fe [13], and Hg [14], based on the Hartree-Slater and Dirac-Slater methods, have been reported. Photoionization studies of members of Mg and Ar [15] using the relativistic random-phase approximation (RRPA) [16] have also been reported. These theoretical investigations led to the conclusion that the photoionization cross section of an inner subshell remains unchanged as a function of photon energy along an isonuclear sequence when outer electrons are removed. In a recent investigation [17], however, it was found that when core relaxation is taken into account, the photoionization cross section does show sensitivity to the removal of outer-shell electrons, contrary to earlier studies.

Photoionization remains one of the most effective tools for probing electron correlations in atoms and ions. Due to the availability of various experimental techniques, studies of inner-shell photoionization have gained much interest in recent years [18,19]. Now, the cross section is determined only by square of the matrix elements, but the photoelectron angular distribution asymmetry parameter is also sensitive to the phases of the continuum functions. It is therefore interesting to investigate how the asymmetry parameter behaves along the isonuclear sequence. To the best of our knowledge, no results have been reported yet for the dipole angular distribution asymmetry parameter, β, along an isonuclear sequence. To address this issue, in this paper we report a study of the dipole asymmetry parameter for photoelectrons ejected from the $2p$ subshell of Ar ($Z = 18$) and Ca ($Z = 20$) isonuclear sequences using the RRPA formalism. Ar and Ca sequences were chosen since these are of great astrophysical interest [20,21]. The RRPA was chosen since it includes the major electron correlation effects as well as the relativistic effects. The RRPA, rather than RRPA-R (RRPA *with* relaxation [17,22]) was chosen since the focus of the present work is to examine the difference, if any, in the behavior of the photoelectron angular distribution as opposed to that of a photoionization cross section, rather than a study of relaxation effects.

II. THEORY

The RRPA code of Johnson *et al.* [16] was used to obtain the matrix elements and the phases of the dipole eigenchannels which result in the dipole angular distribution asymmetry parameter β. In the present work, all dipole channels except the channels arising from the $1s$ shell are included for the Ar and Ca isonuclear sequences. The exclusion of channels from the $1s$ shell amounts to performing the computations in the truncated RRPA, and this could result in a loss of gauge invariance between the dipole-length and the dipole-velocity forms of the matrix elements. However, the $1s$ threshold from which the omitted channels would originate is energetically far from the photon energy range of interest in the present work, and here we find that the length and the velocity forms give nearly equal results. Accordingly, in the results explained below, only the length form is shown. As is usually done, the absolute values of the Dirac-Hartree-Fock (DHF) eigenvalues are used as the ionization threshold energies in the RRPA calculations.

In the RRPA, the photoionization cross section for subshell (n,κ) is given by [16]

$$\sigma_{n,\kappa} = \frac{4\pi^2\alpha\omega}{3}(|D_{nj\to j-1}|^2 + |D_{nj\to j}|^2 + |D_{nj\to j+1}|^2). \tag{1}$$

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The dipole matrix element $D_{nj\rightarrow j'}$ between an initial ground-state, bound orbital $n_b\kappa_b$ and a continuum orbital $\epsilon\kappa$ is given by [23]

$$D_{nj\rightarrow j'} = i^{1-l} e^{i\delta_\kappa} \langle \kappa \| Q_1^{(1)} \| \kappa_b \rangle, \tag{2}$$

where δ_κ and l are the phase shift and the orbital angular momentum of the continuum state, respectively. In addition to photoionization cross sections, the angular distribution asymmetry parameter β is also important. The parameter β results from interference between various electric dipole amplitudes [23] and depends on both the cosine of the phase-shift *difference* between various continuum states and the absolute values of the matrix elements.

The relativistic expression for β [16,23] reduces to the following for the $p_{1/2}$ and $p_{3/2}$ subshells:

$$\begin{aligned}\beta_{p_{1/2}} = {} & \big[\big|D_{p_{1/2}\rightarrow d_{3/2}}\big|^2 + 2\sqrt{2}\big|D_{p_{1/2}\rightarrow d_{3/2}}\big|\big|D_{p_{1/2}\rightarrow s_{1/2}}\big| \\ & \times \cos(\delta_{s_{1/2}} - \delta_{d_{3/2}})\big]\big(\big|D_{p_{1/2}\rightarrow s_{1/2}}\big|^2 + \big|D_{p_{1/2}\rightarrow d_{3/2}}\big|^2\big)^{-1},\end{aligned} \tag{3}$$

$$\begin{aligned}\beta_{p_{3/2}} = {} & \big[4\big|D_{p_{3/2}\rightarrow d_{5/2}}\big|^2 - 4\big|D_{p_{3/2}\rightarrow d_{3/2}}\big|^2 \\ & - 2\sqrt{5}\big|D_{p_{3/2}\rightarrow d_{3/2}}\big|\big|D_{p_{3/2}\rightarrow s_{1/2}}\big|\cos\big(\delta_{s_{1/2}} - \delta_{d_{3/2}}\big) \\ & - 6\sqrt{5}\big|D_{p_{3/2}\rightarrow d_{5/2}}\big|\big|D_{p_{3/2}\rightarrow s_{1/2}}\big|\cos\big(\delta_{s_{1/2}} - \delta_{d_{5/2}}\big) \\ & + 6\big|D_{p_{3/2}\rightarrow d_{3/2}}\big|\big|D_{p_{3/2}\rightarrow d_{5/2}}\big|\cos\big(\delta_{d_{3/2}} - \delta_{d_{5/2}}\big)\big] \\ & \times\big[5\big(\big|D_{p_{3/2}\rightarrow d_{3/2}}\big|^2 + \big|D_{p_{3/2}\rightarrow d_{5/2}}\big|^2 + \big|D_{p_{3/2}\rightarrow s_{1/2}}\big|^2\big)\big]^{-1},\end{aligned} \tag{4}$$

where $\delta_{s_{1/2}}$, $\delta_{d_{3/2}}$, and $\delta_{d_{5/2}}$ are the phase shifts of the continuum s and d states. Thus, in the abbreviated notation employed above, the arguments of the cosine function, such as that in the second term of Eq. (3), are $\delta_{s_{1/2}} - \delta_{d_{3/2}} = (\delta_{p_{1/2}\rightarrow s_{1/2}}) - (\delta_{p_{1/2}\rightarrow d_{3/2}})$. Other angles in Eq. (4) have been written similarly in an abbreviated notation. Note that these phase shifts are with respect to free waves; that is, they are the sum of the Coulomb and non-Coulomb phase shifts [24].

For spin-orbit splitting of a given nl shell into two different levels, it is conventional to use the weighted average given by

$$\beta_{nl} = \frac{\sum_\kappa \sigma_{n\kappa}\beta_{n\kappa}}{\sum_\kappa \sigma_{n\kappa}}. \tag{5}$$

III. RESULTS AND DISCUSSION

The calculated photoionization cross sections for the $2p$ subshell of the Ar isonuclear sequence are shown in Fig. 1; vertical solid lines denote the DF thresholds. It is observed that the photoionization cross sections for Ar, Ar^{6+}, and Ar^{8+} are essentially equal. Thus, removal of electrons from the $3p$ subshell of Ar^{6+}, and from the $3p$ and $3s$ subshells of Ar^{8+}, have virtually no effect on the $2p$ cross section other than a simple shift of threshold toward higher energy [15]. This occurs because the spherically averaged outer-shell charge density exerts no force at any point in the interior region; it only changes the potential by a constant amount, leaving the interior wave functions and the magnitude of the corresponding matrix elements unchanged. Accordingly, the energy dependence of the cross section which depends on the magnitude of the matrix elements does not change, as a function of photon energy, although the ionization thresholds change. The weighted average [Eq. (5)] of the dipole angular distribution asymmetry parameter for the $2p$ subshell of the Ar isonuclear sequence is given in Fig. 2. In the present case, the β values for the photoelectrons from the spin-orbit split subshells were essentially the same. The energy dependence of β is, however, qualitatively different from that of the photoionization cross section. At the highest energies in Fig. 2, the β values for the $2p$ subshell of Ar, Ar^{6+}, and Ar^{8+} are equal to each other, much like the case for cross sections. However, at lower energies near the thresholds, β values are different. The magnitudes of the dipole matrix elements that appear in Eqs. (3) and (4) are very nearly equal for the case of Ar, Ar^{6+}, and Ar^{8+}, as functions of the photon energy, as evidenced by the equality of the cross

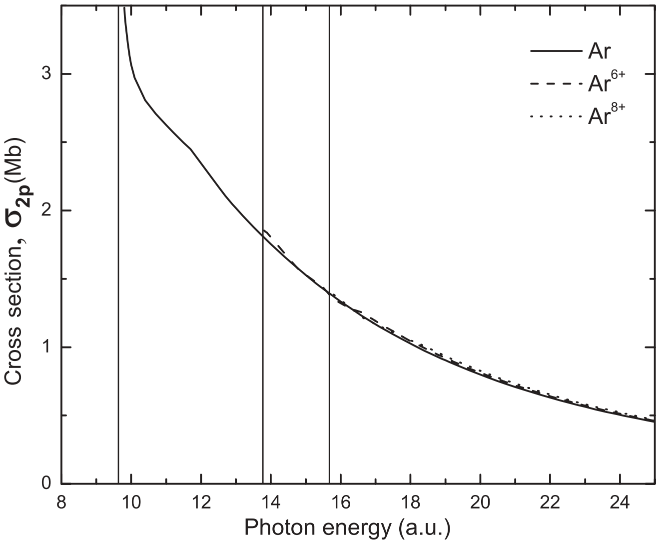

FIG. 1. Photoionization cross sections for the $2p$ subshell of Ar, Ar^{6+}, and Ar^{8+}. Vertical lines indicate the DHF $2p_{1/2}$ thresholds.

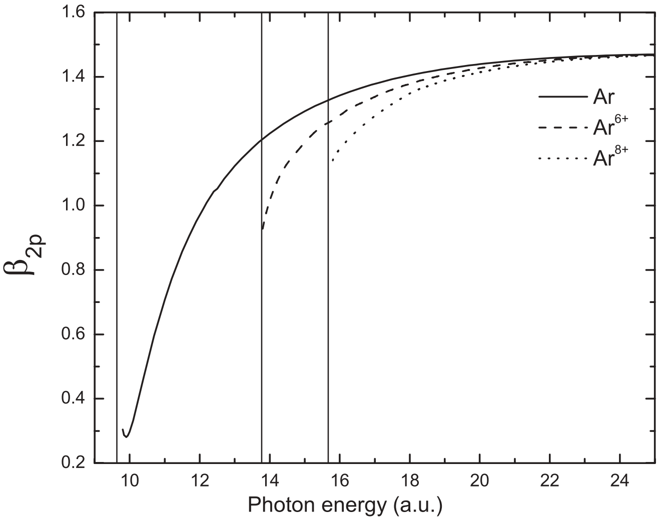

FIG. 2. $2p$ dipole angular distribution asymmetry parameter for the Ar isonuclear sequence. Vertical lines indicate the DHF $2p_{1/2}$ thresholds.

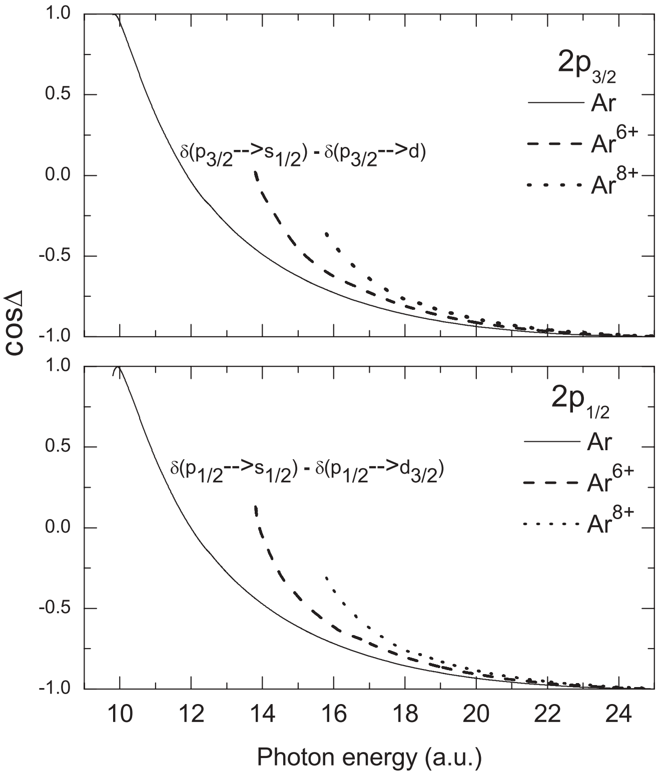

FIG. 3. Cosine of the phase-shift differences for the photoionization channels from the $2p_{3/2}$ subshell (upper panel) and the $2p_{1/2}$ subshell (lower panel) for three ions of the Ar isonuclear sequence. The phase-shift differences $\delta(p_{3/2} \to s_{1/2}) - \delta(p_{3/2} \to d_{3/2})$ and $\delta(p_{3/2} \to s_{1/2}) - \delta(p_{3/2} \to d_{5/2})$ are almost identical so the difference is designated as $\delta(p_{3/2} \to s_{1/2}) - \delta(p_{3/2} \to d)$. Cosines of the phase-shift difference $\delta(p_{3/2} \to d_{3/2}) - \delta(p_{3/2} \to d_{5/2})$ for Ar, Ar^{6+}, and Ar^{8+} are essentially unity and are not shown.

sections (Fig. 1). Thus, the fact that the β values for these three cases are different in the low-energy near-threshold region must be due to the only other quantities that β depends on: the phase factors that appear in Eqs. (3) and (4). The dominant part of the energy dependence of the phase shifts near threshold are the components of the Coulomb phase shifts, which depend not on photon energy but only on the photoelectron kinetic energy and the asymptotic charge of the residual ion [24]. To highlight this analysis, shown in Fig. 3 is the cosine of the phase shift differences that appear in Eqs. (3) and (4). The near-threshold differences in the magnitude and energy dependence of these cosine factors are explicitly manifest in this figure, thereby explaining the differences in the angular distribution asymmetry parameters along the Ar isonuclear sequence (Fig. 2). At higher energies, the contribution of the Coulomb phase shifts becomes insignificant [24], and the β values therefore agree with each other for the three cases Ar, Ar^{6+}, and Ar^{8+}.

Photoionization cross sections for the $2p$ subshell of three members (Ca, Ca^{2+}, and Ca^{8+}) of the Ca isonuclear sequence are presented in Fig. 4. In this case too the cross sections of the three species merely differ in threshold energy, but the low-energy angular distribution asymmetry parameters, shown in Fig. 5 for the three cases, are different, again owing to the dependence of the Coulomb phase shift on the photoelectron energy and asymptotic charge, as discussed for the case of the Ar isonuclear sequence. The cosines of the phase shift differences in this case are presented in Fig. 6 and these results underscore the differences near the threshold and the confluence at higher energies. Note that the curves in Figs. 5 and 6 for the cases of Ca and Ca^{2+} are not very different from each other; this is due to the fact that their thresholds are not very much separated.

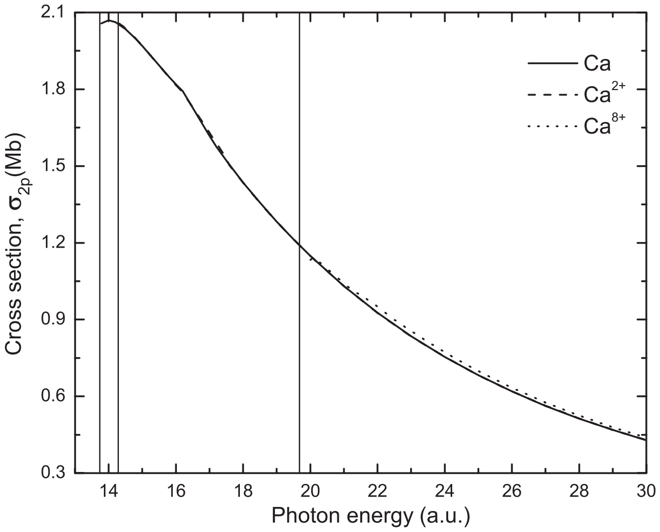

FIG. 4. Photoionization cross sections for the $2p$ subshell of Ca, Ca^{2+}, and Ca^{8+}. Vertical lines indicate the DHF $2p_{1/2}$ thresholds.

The present calculations do not include the effect of core relaxation [17]. Nevertheless, inclusion of the core relaxation does not affect the essential results of the present work since the angular distributions not being invariant along an isonuclear sequence does not depend on invariant cross sections; it is the Coulomb phase shifts, which are not just a function of photon energy, that causes the variation along the sequence. This variation will remain and probably be more pronounced with the addition of relaxation effects.

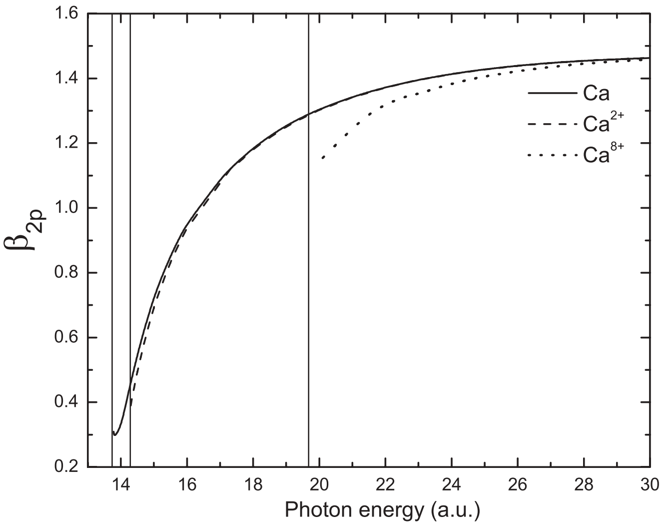

FIG. 5. $2p$ dipole angular distribution asymmetry parameter for the Ca isonuclear sequence. Vertical lines indicate the DHF $2p_{1/2}$ thresholds.

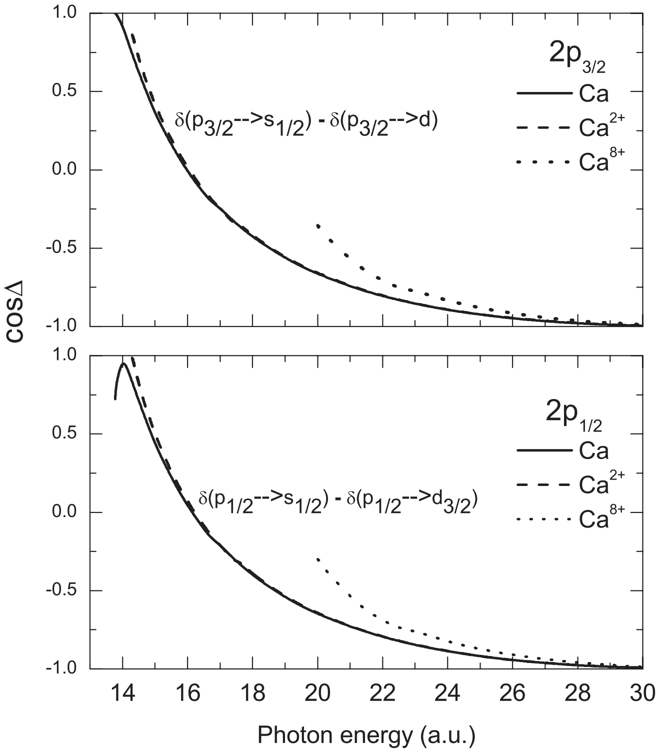

FIG. 6. As in Fig. 3, but for the Ca isonuclear sequence.

IV. CONCLUSIONS

In the study of inner-shell photoionization of members of an isonuclear sequence, it has been known hitherto that the cross sections remain essentially invariant across the members of the sequence, unless relaxation effects are included [17]. In the present work, we find that even when the effects of relaxation are not included, the angular distributions of the photoelectrons show a different dependence on photon energies near respective thresholds since the Coulomb phase shifts depend on the photoelectron's kinetic energy and the asymptotic charge "seen" by the photoelectron, rather than the photon energy. In fact, one can expect all other photoionization parameters, such as the spin-polarization parameters, to show similar differences in the low-energy photoionization domain because these properties also depend on phase-shift differences. It is hoped that the present results prompt some experiments on the measurement of the angular distribution asymmetry parameters for photoelectrons across members of an isonuclear sequence to test the predictions made.

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