Spin polarization of photoelectrons from 3*d* electrons of Xe, Cs, and Ba

M. Ya. Amusia,[1,2] N. A. Cherepkov,[3] L. V. Chernysheva,[2] Z. Felfli,[4] and A. Z. Msezane[4]
[1]*Racah Institute of Physics, The Hebrew University, Jerusalem 91904, Israel*
[2]*A. F. Ioffe Physical-Technical Institute, St. Petersburg 194021, Russia*
[3]*State University of Aerospace Instrumentation, St. Petersburg 190000, Russia*
[4]*Department of Physics and Center for Theoretical Studies of Physical Systems, Clark Atlanta University, Atlanta, Georgia 30314, USA*
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The spin polarization parameters of photoelectrons from Xe, Cs, and Ba $3d_{5/2}$ and $3d_{3/2}$ levels are calculated using a modified version of the so-called spin-polarized random phase approximation with exchange. The effects of relaxation of excited electrons due to the creation of a 3*d* vacancy are also accounted for. We demonstrate that these parameters that characterize the photoionization process, as a function of the incoming photon frequency ω, acquire additional features when the interaction between electrons that belong to the $3d_{5/2}$ and $3d_{3/2}$ components of the spin-orbit doublet is taken into account. We conclude that through spin-orbit interaction polarization can be achieved and correlations probed.

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I. INTRODUCTION

Spin-polarization parameters that determine the orientation of the photoelectron spin relative to the photon flux or to their polarization direction are important characteristics of the photoionization process. It was demonstrated [1] that spin polarization of photoelectrons, although caused by the relatively weak spin-orbit interaction, is not a small relativistic effect. It was also found that the spin-orbit interaction acts as a leverage that reveals the degree of photoelectron spin polarization which can reach 100% at some emission angles [2]. The interest in the investigation of spin polarization of photoelectrons is in the context of the realization of the so-called complete experiment in atomic physics [3–5], since the five dynamic parameters [the partial photoionization cross section $\sigma_{nl}(\omega)$ of the *nl* subshell, the photoelectron's angular anisotropy parameter $\beta_{nl}(\omega)$, and the three characteristic photoelectron spin-polarization parameters $A^j_{nl}(\omega)$, $\alpha^j_{nl}(\omega)$, and $\xi^j_{nl}(\omega)$ where *j* is the total momentum of the ionized shell] are sufficient to determine completely five theoretical values, three photoionization amplitudes $D^j_{nli\to\epsilon(l\pm1)}(\omega)$, and two phase shift differences [5]. Later it was found that these parameters are not mutually independent, but are connected by one equation [6]. Therefore it is not possible to determine them from an experiment of that kind. Still, it is possible to determine that way three nonrelativistic values, two amplitudes, and one phase shift difference.

A recent experiment showed that the nonrelativistic approximation is quite sufficient even for an atom as heavy as Xe [6], and demonstrated the ability of this approach to describe satisfactorily the photoionization process. Different calculations demonstrated the important role played by multielectron correlations in photoionization and established that they can be taken into account accurately within the framework of the random phase approximation with exchange (RPAE) and some of its generalized versions, e.g., the GRPAE [7]. Recently, another example of the leveraging role of the spin-orbit interaction was found [8,9]; namely, it was demonstrated experimentally that there exists a strong interaction between the components of the spin-orbit doublet of the 3*d* electrons in Xe through the recent observation of an extra maximum in the Xe $3d_{5/2}$ partial cross section in the vicinity of the $3d_{3/2}$ ionization threshold [8]. This additional maximum was explained as due to the action of $3d_{3/2}$ upon $3d_{5/2}$ electrons. It was further demonstrated that the same effect, but considerably more pronounced, can be found in the 3*d* doublets of Cs and Ba [9]. Also, it has been shown that the intradoublet correlations are very important not only in dipole [10] but also in nondipole [11] angular anisotropy parameters, particularly in Cs and Ba.

The effect discussed here is a manifestation of the interaction between two channels of the photoionization, $3d_{5/2}\to\varepsilon f,p$ and $3d_{3/2}\to\varepsilon f,p$, which becomes observable due to the separation between the $3d_{5/2}$ and $3d_{3/2}$ ionization thresholds. It is still unclear whether the large magnitude of this interchannel interaction is a result of the relatively large energy splitting between these thresholds. In fact, the role of the intradoublet interaction in the 3*d* subshell photoionization of Xe, Cs and Ba was not investigated until very recently.

In this paper a case is investigated where the leveraging effect of spin-orbit interaction manifests itself simultaneously from two different perspectives: viz., as a cause of polarization and a means of revealing correlation effects. Therefore, our aim here is to study the spin polarization of the photoelectrons from the $3d_{3/2}$ and $3d_{5/2}$ levels in Xe, Cs, and Ba and show it is influenced by the intradoublet correlations. We expect that further specific features will appear in the spin-polarization parameters as was already observed in the partial cross sections.

II. EQUATIONS FOR SPIN POLARIZATION

The formula for the photoelectron flux $I_{nlj}(\omega,\vec{x},\vec{s})$, which originates from photoionization of an atom with initial total

angular momentum equal to zero and final state ion momentum j, and for the corresponding polarization parameters $A^j_{nl}(\omega), \alpha^j_{nl}(\omega)$, and $\xi^j_{nl}(\omega)$ were derived in [2,5]. For circularly polarized light one has [5]

$$I_{nlj}(\omega,\vec{x},\vec{s}) = \frac{\sigma_{nlj}(\omega)}{8\pi}\left\{1-\frac{1}{2}\beta_{nl}(\omega)\left[\frac{3}{2}(\vec{x}\cdot\vec{s}_\gamma)^2-\frac{1}{2}\right]\right\} + A^j_{nl}(\omega) \times(\vec{s}\cdot\vec{s}_\gamma) - \alpha^j_{nl}(\omega)\left[\frac{3}{2}(\vec{x}\cdot\vec{s}_\gamma)(\vec{x}\cdot\vec{s})-\frac{1}{2}(\vec{s}\cdot\vec{s}_\gamma)\right] + \xi^j_{nl}(\omega)[\vec{s}\cdot(\vec{x}\times\vec{k}_\gamma)(\vec{x}\cdot\vec{k}_\gamma)], \quad (1)$$

where $\sigma_{nlj}(\omega)$ is the nl subshell photoionization cross section with the residual ion having momentum j; $\vec{s}_\gamma$ and $\vec{s}$ are unit vectors in the photon and photoelectron spin directions; $\vec{x}$ is the direction of motion of the photoelectron; and $\vec{k}_\gamma$ is the unit vector in the direction of motion of the photon. The photoelectron total momentum j can take two values, $j=l\pm 1/2$. A similar expression for linearly polarized light can be found in [5]. The parameters $\beta_{nl}(\omega), A^j_{nl}(\omega), \alpha^j_{nl}(\omega)$, and $\xi^j_{nl}(\omega)$ are given by the following relations [5]:

$$\beta_{nl}(\omega) = \frac{1}{2l+1}[(l+2)d^2_{l+1}+(l-1)d^2_{l-1} + \sqrt{l(l+1)}d_{l+1}d_{l-1}\cos(\delta_{l+1}-\delta_{l-1})][d^2_{l+1}+d^2_{l-1}],$$

where $\beta_{nl}(\omega)$ is the angular anisotropy parameter, while

$$A^j_{nl}(\omega) = \frac{(-1)^{j-l-1/2}}{(2j+1)}\frac{ld^2_{l+1}-(l+1)d^2_{l-1}}{d^2_{l-1}+d^2_{l+1}},$$

$$\alpha^j_{nl}(\omega) = \frac{2(-1)^{j-l-1/2}l(l+1)}{(2j+1)(2l+1)}\frac{1}{d^2_{l-1}+d^2_{l+1}}[l(l+2)d^2_{l+1}-(l-1)(l+1)d^2_{l-1}-3\sqrt{l(l+1)}d_{l+1}d_{l-1}\cos(\delta_{l+1}-\delta_{l-1})],$$

$$\xi^j_{nl}(\omega) = \frac{3(-1)^{j-l-1/2}\sqrt{l(l+1)}}{(2j+1)}\frac{d_{l+1}d_{l-1}\sin(\delta_{l+1}-\delta_{l-1})}{d^2_{l-1}+d^2_{l+1}}. \quad (2)$$

Here

$$d_{l\pm1} \equiv d_{nl,\epsilon l\pm1} = (-1)^{l_>}\sqrt{l_>}\int_0^\infty \phi_{nl}(r)r\phi_{\epsilon l\pm1}(r)dr, \quad (3)$$

with $l_>=l+1$ and $l_>=l$ for $l\to l+1$ and $l\to l-1$ transitions, respectively, while $\phi_{nl}(r)$ and $\phi_{\epsilon l'}(r)$ are the radial parts of the Hartree-Fock one-electron wave functions; $\delta_{l\pm1}$ are the photoelectron $l\pm1$ wave scattering phases.

In the RPAE or GRPAE the parameters $A^j_{nl}(\omega), \alpha^j_{nl}(\omega)$, and $\xi^j_{nl}(\omega)$ can be obtained using the following substitutions [5]:

$$d^2_{l\pm1} \to |D_{l\pm1}|^2,$$

$$d_{l+1}d_{l-1}\cos(\delta_{l+1}-\delta_{l-1}) \to \mathrm{Re}[D_{l+1}D^*_{l-1}e^{i(\delta_{l+1}+\Delta_{l+1}-\delta_{l-1}-\Delta_{l-1})}],$$

$$d_{l+1}d_{l-1}\sin(\delta_{l+1}-\delta_{l-1}) \to \mathrm{Im}[D_{l+1}D^*_{l-1}e^{i(\delta_{l+1}+\Delta_{l+1}-\delta_{l-1}-\Delta_{l-1})}], \quad (4)$$

where $D_{l\pm1}(\omega) \equiv |D_{l\pm1}(\omega)|\exp(i\Delta_{l\pm1})$ are the dipole photoionization amplitudes, expressed by RPAE (GRPAE) equations (see the next section) via $d_{l\pm1}$ and the interelectron interaction V.

As a result, one has

$$A^j_{nl}(\omega) = \frac{(-1)^{j-l-1/2}}{(2j+1)}\frac{l|D_{l+1}|^2-(l+1)|D_{l-1}|^2}{|D_{l-1}|^2+|D_{l+1}|^2}, \quad (5)$$

$$\alpha^j_{nl}(\omega) = \frac{2(-1)^{j-l-1/2}l(l+1)}{(2j+1)(2l+1)(|D_{l-1}|^2+|D_{l+1}|^2)}\{l(l+2)|D_{l+1}|^2-(l-1)(l+1)|D_{l-1}|^2-3\sqrt{l(l+1)}[(\mathrm{Re}D_{l+1}\mathrm{Re}D_{l-1} + \mathrm{Im}D_{l+1}\mathrm{Im}D_{l-1})\cos(\delta_{l+1}-\delta_{l-1})-(\mathrm{Re}D_{l-1}\mathrm{Im}D_{l+1} - \mathrm{Re}D_{l+1}\mathrm{Im}D_{l-1})\sin(\delta_{l+1}-\delta_{l-1})]\}, \quad (6)$$

$$\xi^j_{nl}(\omega) = \frac{3(-1)^{j-l-1/2}\sqrt{l(l+1)}}{(2j+1)}\frac{1}{|D_{l+1}|^2+|D_{l-1}|^2} \times[(\mathrm{Re}D_{l+1}\mathrm{Re}D_{l-1}+\mathrm{Im}D_{l+1}\mathrm{Im}D_{l-1})\sin(\delta_{l+1}-\delta_{l-1}) + (\mathrm{Re}D_{l-1}\mathrm{Im}D_{l+1}-\mathrm{Re}D_{l+1}\mathrm{Im}D_{l-1})\cos(\delta_{l+1}-\delta_{l-1})]. \quad (7)$$

In this paper we study the spin-polarization parameters for d electrons, i.e., $l=2$. It is seen from Eqs. (5), (6), and (7) that the sets $A^{5/2}_{nl}(\omega), \alpha^{5/2}_{nl}(\omega)$, and $\xi^{5/2}_{nl}(\omega)$ and $A^{3/2}_{nl}(\omega), \alpha^{3/2}_{nl}(\omega)$, and $\xi^{3/2}_{nl}(\omega)$ differ only by their signs.

III. INCLUSION OF INTRADOUBLET CORRELATIONS

To perform calculations in the one-electron Hartree-Fock (HF) approximation, the matrix elements and phases were calculated using the computer codes described in [12]. The RPAE effects within a single channel, which correspond to ionization of either $3d_{3/2}$ or $3d_{5/2}$ electrons, are not important and the corresponding amplitudes are close to the HF values. However, the intradoublet correlations must be taken into account. For the problem under consideration, it is convenient to apply the nonrelativistic approach (see [7] for details). The main point of this approach is that it considers the $3d_{3/2}$ and $3d_{5/2}$ electrons as semifilled atomic levels, so that the method of accounting for interelectron correlations for semifilled subshells can readily be applied. The exchange between these two types of electrons is neglected, namely, between the six electrons which form the $3d_{5/2}$ (called "up") shell, and the four which form the $3d_{3/2}$ (called "down") shell. However, in the real half-filled $3d$ subshell one would have five electrons. But the corresponding corrections $5/6$ and $5/4$, respectively, can be introduced easily into the calculation scheme.

To atoms with half-filled shells one can apply the so-called spin-polarized random phase approximation with exchange (SPRPAE). The SPRPAE equations are rather complex and can be found in [7] or [12]. However, for the

intermediate 3*d* subshell the SPRPAE is not sufficient; the effects of rearrangement (relaxation) must be taken into account. This is achieved by going from RPAE to its generalized version (GRPAE) or, in our case, from the SPRPAE to the SPGRPAE. The latter takes into account that as the slow photoelectron leaves the atom, the field of the vacancy is modified due to the alteration of the states of all the other atomic electrons, resulting from the creation of an inner-subshell vacancy.

The GRPAE is discussed at length in [7,12], where the GRPAE equations are presented in matrix form. But to understand the structure and main features of this equation, it is sufficient to present it in the operator, symbolic form, in which it coincides with the RPAE equation:

$$D(\omega) = d + D(\omega)\chi(\omega)U. \tag{8}$$

The generalization of Eq. (8) to a system with two types of electrons up and down, represented by the transition from the GRPAE to the SPGRPAE, is straightforward. The symbolic version of the corresponding equations is as follows:

$$(D_\uparrow(\omega) \quad D_\downarrow(\omega)) = (d_\uparrow \quad d_\downarrow) + (D_\uparrow(\omega)\chi_{\uparrow\uparrow}(\omega) \quad D_\downarrow(\omega)\chi_{\downarrow\downarrow}(\omega)) \times \begin{pmatrix} U_{\uparrow\uparrow} & V_{\uparrow\downarrow} \\ V_{\downarrow\uparrow} & U_{\downarrow\downarrow} \end{pmatrix}, \tag{9}$$

where the signs $\uparrow$ and $\downarrow$ denote, respectively, the up and down photoelectron vacancy spin projections, $U_{\uparrow\uparrow(\downarrow\downarrow)}$ are the combinations of the direct V^{dir} and exchange V^{exc} Coulomb interelectron interaction matrix elements, $U_{\uparrow\uparrow(\downarrow\downarrow)} = V^{dir}_{\uparrow\uparrow(\downarrow\downarrow)} - V^{exc}_{\uparrow\uparrow(\downarrow\downarrow)}$ and $V^{dir}_{\uparrow\uparrow(\downarrow\downarrow)}$ are the pure Coulomb matrix elements that connect spin up with spin up (or spin down with spin down) states; $\chi_{\uparrow\uparrow(\downarrow\downarrow)}(\omega)$ describes the propagation of a HF electron-hole pair created after an atom absorbs a real or virtual photon. Again symbolically, the expression for $\chi_{\uparrow\uparrow(\downarrow\downarrow)}(\omega)$ is given by the relation

$$\chi_{\uparrow\uparrow(\downarrow\downarrow)}(\omega) = \frac{1}{\omega - \hat{H}^{HF}_{e\uparrow(\downarrow)} + \hat{H}^{HF}_{h\uparrow(\downarrow)}} - \frac{1}{\omega + \hat{H}^{HF}_{e\uparrow(\downarrow)} - \hat{H}^{HF}_{h\uparrow(\downarrow)}}. \tag{10}$$

Here $\hat{H}^{HF}_{e\uparrow(\downarrow)}$ is the HF Hamiltonian of an electron in an excited state, and $\hat{H}^{HF}_{h\uparrow(\downarrow)}$ is that of a hole, i.e., an electron in an occupied level.

In solving Eq. (9) we concentrate on the investigation of the influence of the up and down electrons upon each other and demonstrate the effect of the down electrons upon the up ones. To adjust the up and down approach to the situation with the $5/2$ and $3/2$ electrons, the second term in Eq. (9) is multiplied by $6/5$ for up and by $4/5$ for down electrons. Thus we obtain $D_{l\pm1;5/2,3/2}(\omega)$ as complex quantities that are required to calculate the spin-polarization parameters $A^{5/2}_{nl}(\omega)$, $\alpha^{5/2}_{nl}(\omega)$, and $\xi^{5/2}_{nl}(\omega)$, and $A^{3/2}_{nl}(\omega)$, $\alpha^{3/2}_{nl}(\omega)$, and $\xi^{3/2}_{nl}(\omega)$.

To clarify what is really taken into account by our calculations when going from the HF one-electron approximation to the RPAE, to the GRPAE, to the SPRPAE, and, finally, to the SPGRPAE, we will present some details. More details can be found in [7,12]. We start with the HF approximation adjusted to half-filled shell atoms, namely, spin-polarized HF or SPHF method. This equation takes into account that, for a given spin projection of an electron state, there is no exchange:

$$\left[\hat{H}^{HF}_{h\uparrow(\downarrow)} + \int d\mathbf{r}'\rho_{\downarrow(\uparrow)}(\mathbf{r}')V(|\mathbf{r}-\mathbf{r}'|) - \varepsilon_{k\uparrow(\downarrow)}\right]\varphi_{k\uparrow}(\mathbf{r}) \equiv 0$$

or simply

$$[\hat{H}^{SPHF}_{h\uparrow(\downarrow)} - \varepsilon_{k\uparrow(\downarrow)}]\varphi_{k\uparrow}(\mathbf{r}) = 0, \tag{11}$$

where $\rho_{\downarrow(\uparrow)}(r)$ is the density for spin down (up) electrons and $\hat{H}^{HF}_{h\uparrow(\downarrow)}$ is the HF operator for up (down) electrons only that include the so-called self-consistent field formed by all atomic electrons. Equation (11) determines the one-electron wave functions of occupied levels. The same equation is applicable to vacant discrete states and continuous spectrum electrons.

It was demonstrated [7] that by eliminating the interaction of the outgoing electron with the electron *i* eliminated in the photoionization, an important piece of electron correlations is taken into account. By introducing such a correction we arrive at the so-called frozen core approximation. If Eq. (11) is modified by removing the interaction with the ionized electron *i*, it is said that the relaxation (R) of the atomic core due to hole *i* creation is taken into account. The corresponding spin-polarized HF states calculated taking into account the presence of the hole *i* are denoted as $\varphi^{RSP}_{k\uparrow}(\mathbf{r})$ and the corresponding one-electron Hamiltonian is denoted as $\hat{H}^{RSPHF}_{h\uparrow(\downarrow)}$.

If one uses $\varphi^{RSP}_{k\uparrow}(\mathbf{r})$ to calculate all matrix elements that enter Eq. (9) and takes the corresponding RSP one-electron energies from Eq. (11), then Eq. (9) represents the SPGRPAE approximation. Equation (9) is used in this paper to calculate the matrix elements $D_{\uparrow(\downarrow)}(\omega)$ that determine using Eqs. (5)–(7) the spin-polarization parameters of photoelectrons from the $3d_{5/2,3/2}$ levels of Xe, Cs, and Ba.

In order to clarify what sort of equations were actually solved, let us present one of them explicitly, say that for $D_\uparrow(\omega)$, in its matrix form:

$$\begin{aligned} D_{i\uparrow f\uparrow}(\omega) = {} & d_{i\uparrow f\uparrow} \\ & + \sum_{k\uparrow\leqslant F\uparrow, q\uparrow > F\uparrow} D_{k\uparrow q\uparrow}(\omega)\frac{2(\varepsilon_{q\uparrow} - \varepsilon_{k\uparrow})}{\omega^2 - (\varepsilon_{q\uparrow} - \varepsilon_{k\uparrow})^2}U_{k\uparrow i\uparrow q\uparrow f\uparrow} \\ & + \sum_{k\downarrow\leqslant F\downarrow, q\downarrow > F\downarrow} D_{k\downarrow q\downarrow}(\omega)\frac{2(\varepsilon_{q\downarrow} - \varepsilon_{k\downarrow})}{\omega^2 - (\varepsilon_{q\downarrow} - \varepsilon_{k\downarrow})^2}V_{k\downarrow i\uparrow q\downarrow f\uparrow}. \end{aligned} \tag{12}$$

Replacing everywhere in Eq. (12) $\uparrow$ by $\downarrow$ and vice versa, an equation for $D_{i\downarrow f\downarrow}(\omega)$ can be obtained.

IV. RESULTS OF CALCULATIONS

The results of calculation for Xe, Cs, and Ba are presented in Figs. 1, 2, and 3, respectively. The calculations for the

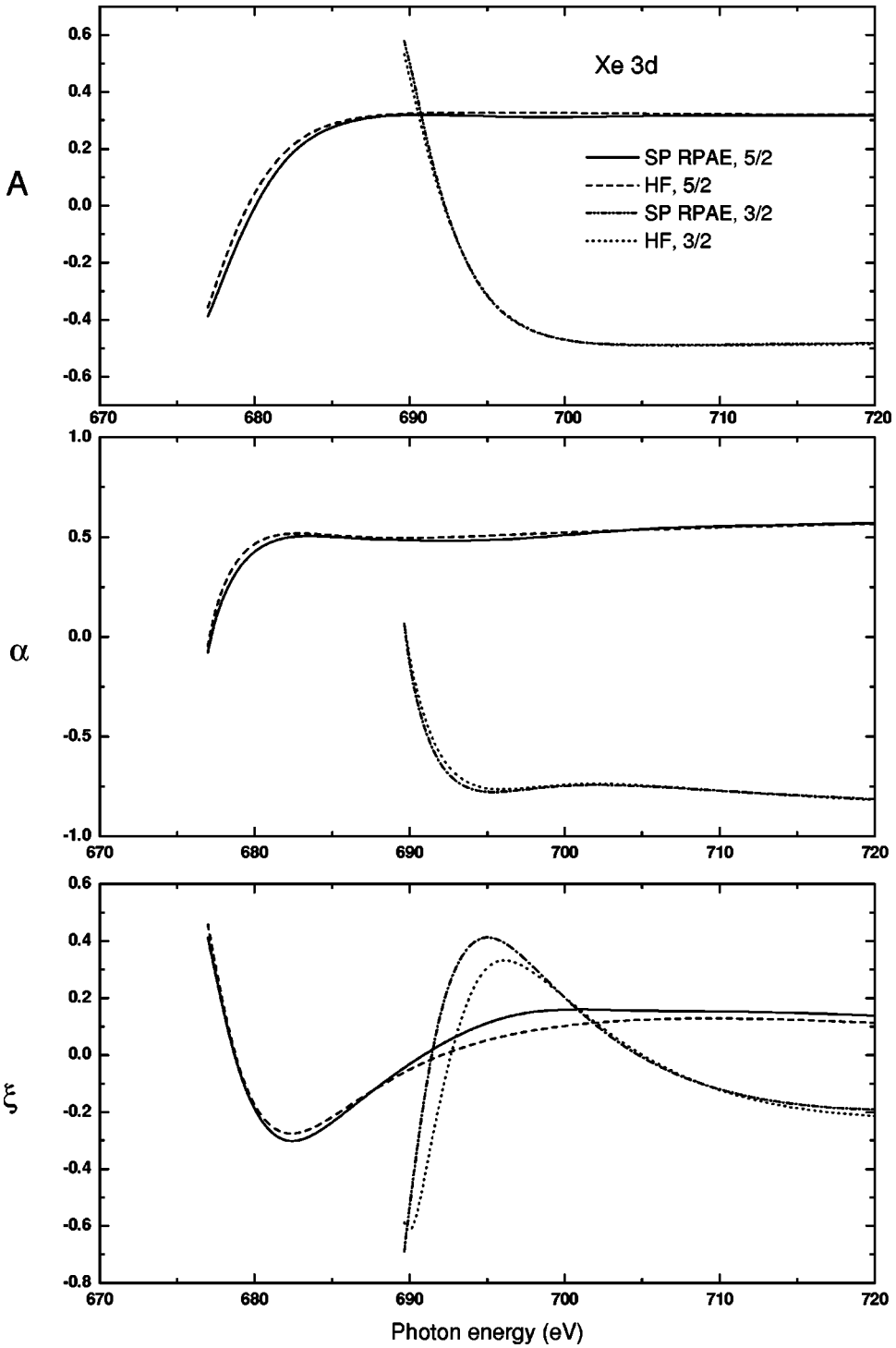

FIG. 1. Calculated values of the spin-polarization parameters A, α, and ξ for Xe $3d_{5/2}$ and $3d_{3/2}$ subshells in correlated many-electron (SPRPAE) and one-electron (HF) approximations.

spin-polarization parameters for Xe, Cs, and Ba were performed in both the dipole-length and dipole-velocity formulations. However, only the dipole-length values are presented in the figures to minimize cluttering them. The dipole-length and dipole-velocity values of the parameters agree in most cases within 5%. The values of the $3d_{5/2}$ and $3d_{3/2}$ thresholds are respectively 676.71 and 689.27 eV for Xe, 726.63 and 740.55 eV for Cs, and 780.56 and 795.76 eV for Ba. We see that for Cs and Ba, all the parameters in the considered energy region, about 5–25 eV above the $3d_{5/2}$ threshold, are rather complicated functions of ω. Their variation is particularly strong in the vicinity of thresholds. Inclusion of intradoublet interaction affects the parameters of the $5/2$ level, leaving almost unaltered that of the $3/2$ one, just as for the partial cross sections [9] as well as for the dipole [10] and nondipole [11] angular anisotropy parameters. While the effect of intradoublet interaction is small in Xe, its role in Cs and Ba is indeed very large.

It is known that the spin-polarization parameters, like the angular anisotropy parameter β, do not change dramatically when many-electron correlations are taken into account. In particular, that happens when the phase shifts do not change

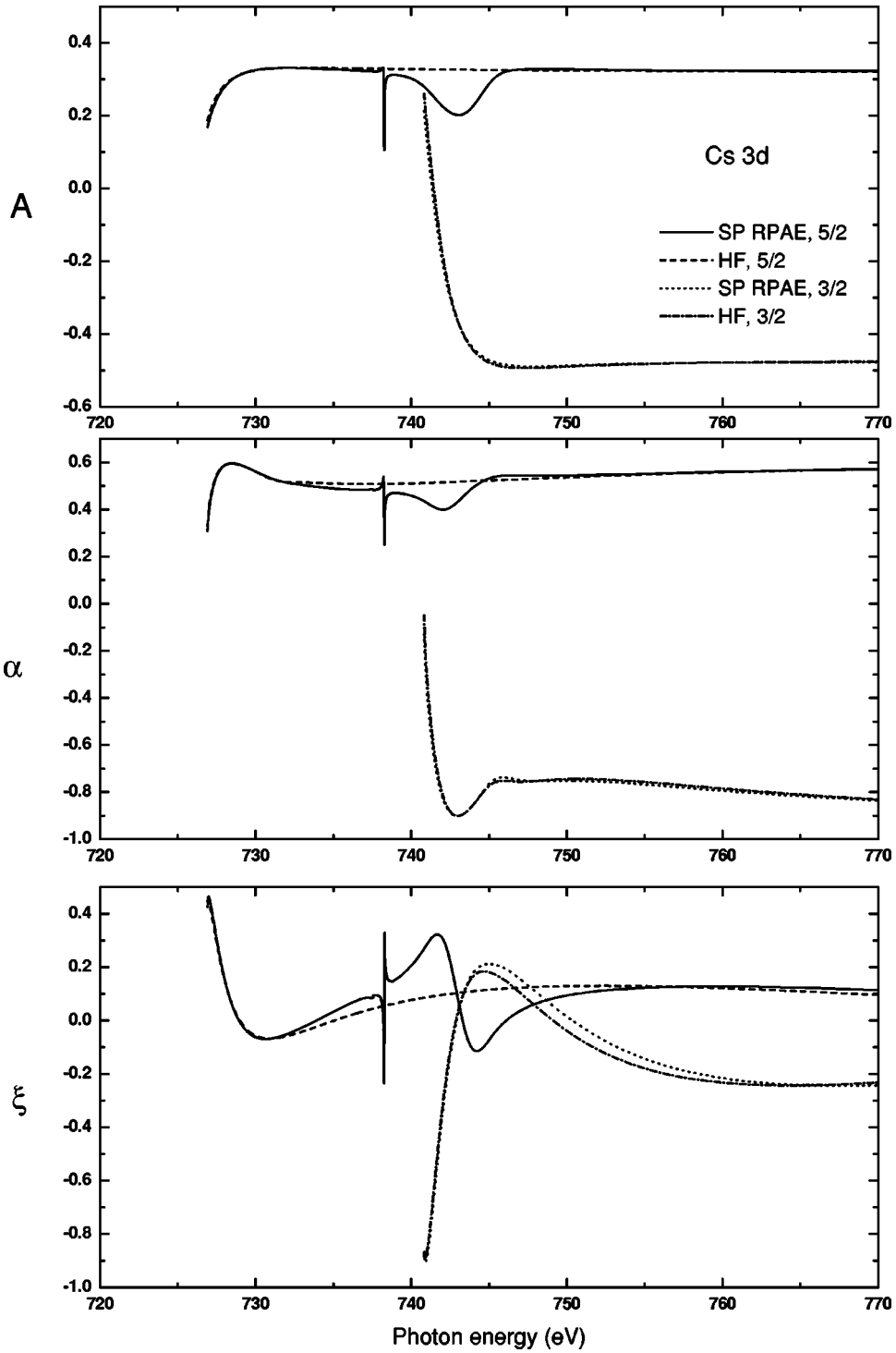

FIG. 2. Calculated values of the spin-polarization parameters A, α, and ξ for Cs $3d_{5/2}$ and $3d_{3/2}$ subshells in correlated many-electron (SPRPAE) and one-electron (HF) approximations.

substantially, and both dipole allowed amplitudes change similarly, because β and all spin-polarization parameters depend on the ratios of the amplitudes. Consequently, a strong variation of the cross section is not always related to strong variations of the spin-polarization parameters. Therefore it is not too surprising that in Xe the spin-polarization parameters obtained in the SPRPAE remain very close to the results obtained in the HF approximation. However, the situation in Cs is rather different. For the $3d_{3/2}$ subshell the influence of correlations is still small as in Xe, while for the $3d_{5/2}$ subshell the effect is substantial. The parameter $A^{5/2}$, which depends only on the difference between the squared moduli of the dipole matrix elements, acquires a minimum in the region where the cross section has an additional maximum. Clearly, from Eq. (2) the minimum must be related to the relative minimum of the dipole matrix element corresponding to the $3d_{5/2} \rightarrow \epsilon f$ transition. The sharp oscillation of the parameter $\xi^{5/2}$ in the same region evidently reflects the variation of the phase shift difference between the p and f partial waves as seen from Eq. (2). Finally, the $\alpha^{5/2}$ parameter varies less dramatically because it contains both the squares of the dipole matrix elements and the interference terms with the

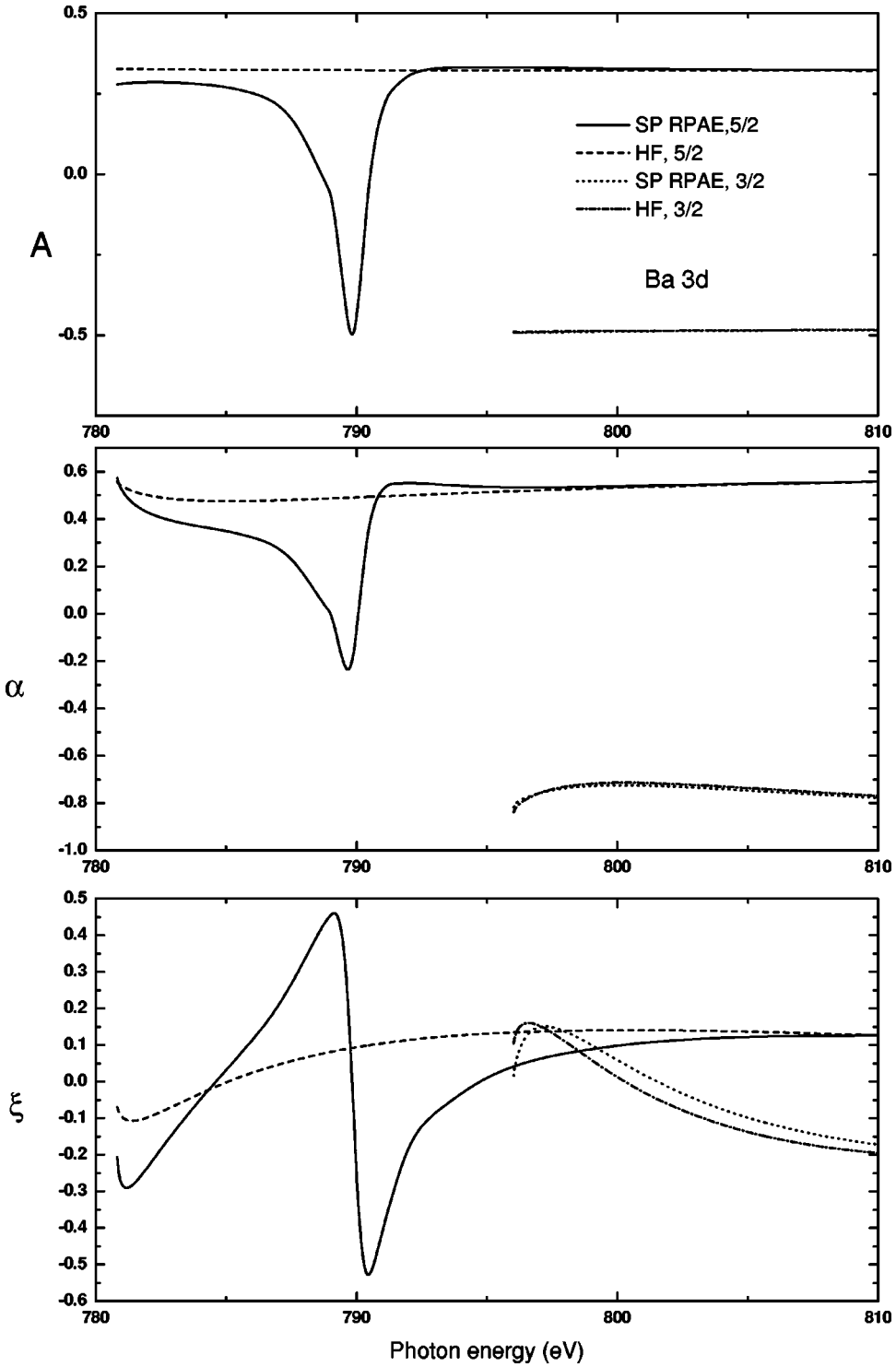

FIG. 3. Calculated values of the spin-polarization parameters A, α, and ξ for Ba $3d_{5/2}$ and $3d_{3/2}$ subshells in correlated many-electron (SPRPAE) and one-electron (HF) approximations.

cosine function of the phase shift difference, which partially cancel each other. From the comparison of these parameters in the corresponding figures one can conclude that the behavior of the $\alpha^{5/2}$ parameter resembles that of the parameter $A^{5/2}$. This means that the main contribution comes from the squares of the dipole matrix elements. There is, however a rapid variation in all parameters at about 737.12 eV, Fig. 2, connected with the autoionization resonance $3d_{3/2} \rightarrow 4f$. There are many more resonances which have not been taken into account in our calculation.

The situation in Ba is significantly different from that in Cs. Now the near threshold resonance has moved into the discrete spectrum, and the cross section of the $3d_{3/2}$ subshell does not contain any maximum. The cross section of the $3d_{5/2}$ subshell is dominated by the autoionization resonance corresponding to the $3d_{3/2} \rightarrow 4f$ transition. The variations of the spin-polarization parameters are evidently defined by this resonance. In particular, the parameter $A^{5/2}$ has a deep minimum at the position that coincides with the minimum (close to zero) of the dipole matrix element corresponding to the

$3d_{5/2} \rightarrow \epsilon f$ transition. The parameter $\xi^{5/2}$ has a rapid variation in this region, as in Cs, defined by the sine of the phase shift difference. Finally the $\alpha^{5/2}$ parameter varies less rapidly and shows a minimum at the same energy as the $A^{5/2}$ parameter. The values of all the parameters at the cross section minimum (when $d_f \rightarrow 0$) follow directly from Eq. (2) and are given by

$$\alpha^{5/2} = -0.2, \quad A^{5/2} = -0.5, \quad \xi^{5/2} = 0.$$

These values agree exactly with the limiting values at the photon energy of about 791.52 eV.

V. DISCUSSION AND CONCLUSIONS

According to the calculations reported in [9], in Xe and Cs there are maxima in the $3d_{5/2} \rightarrow \varepsilon f$ and $3d_{3/2} \rightarrow \varepsilon f$ transitions just above the ionization thresholds of the corresponding subshells which are already predicted in the HF approximation. Due to the spin-orbit activated interchannel coupling between the $3d_{3/2}$ and $3d_{5/2}$ subshells, the near threshold resonance in the $3d_{3/2} \rightarrow \varepsilon f$ channel is transferred to the $3d_{5/2} \rightarrow \varepsilon f$ channel and reveals itself as an additional strong maximum in the $3d_{5/2}$ subshell cross section just above the threshold of the $3d_{3/2}$ subshell. This maximum also manifests itself in the angular anisotropy parameter β as a very tiny increase in Xe and as a substantial maximum in Cs [11].

It is natural to expect a similar influence of this coupling on the spin-polarization parameters. Our calculation demonstrated that this is the case. In Xe the influence of interchannel coupling on the spin-polarization parameters is again rather negligible, just as with the partial cross sections, while in Cs it leads to the appearance of a substantial minimum in the $A_{3d}^{5/2}$ and $\alpha_{3d}^{5/2}$ parameters. The parameter $\xi_{3d}^{5/2}$ becomes oscillatory in that energy region as seen from Fig. 2. Interestingly, the largest deviation of the correlated spin-polarization parameters from the corresponding HF values in Cs occurs not at the energy where the additional maximum of the cross section occurs (about 747 eV), but at some lower energy (742–743 eV) where the matrix element of the $3d_{5/2} \rightarrow \varepsilon f$ transition has a local minimum. The oscillation of the $\xi_{3d}^{5/2}$ parameter is a consequence of a strong variation of the phase shift difference in that energy region.

In Xe the near threshold maximum appears at about 20 eV above the ionization threshold, while in Cs it occurs only at 5 eV above threshold. In Ba the situation is changed dramatically; the maximum is shifted to the discrete spectrum and reveals itself as a strong autoionization resonance corresponding to the $3d_{3/2} \rightarrow 4f$ transition. This resonance is very strong in the partial cross section (rising up to 120 Mb; see [9]), and has a typical Fano profile [15]. As a result, there are strong variations of all spin-polarization parameters in that resonance as shown in Fig. 3. Deep minima appear in the $A_{3d}^{5/2}$ and $\alpha_{3d}^{5/2}$ parameters while the parameter $\xi_{3d}^{5/2}$ acquires a strong oscillation. This behavior of the parameters is typical for resonances and was demonstrated in [5] for the case of the Tl atom. In Cs the $3d_{3/2} \rightarrow 4f$ resonance is relatively weak though visible as demonstrated in Fig. 2.

Previously, the spin-polarization parameters for Xe were calculated [14] using the relativistic version of the RPAE, the RRPA [13]. There the spin-orbit splitting of the 3*d* subshell is naturally taken into account in the zeroth order Dirac-Fock approximation, and the interchannel coupling between the $3d_{3/2}$ and $3d_{5/2}$ subshells was also included. In addition, the relaxation of atomic orbitals after the creation of a deep 3*d* hole was taken into account. The results obtained in [14] agree reasonably well with the present ones.

We have demonstrated that the strong interchannel coupling between the transitions from the spin-orbit split sublevels $3d_{3/2}$ and $3d_{5/2}$ of Xe, Cs, and Ba produces remarkable variations in the spin-polarization parameters of the $3d_{5/2}$ subshells in the regions of the additional maxima. The experimental study of these variations can shed light on the role of many-electron correlations in deep atomic shells which, for a long time, were believed to be much less important [15].

The rapid variation of these parameters in the vicinity of threshold is particularly significant. This is due to the rather fast variations of the phase differences and their sine and cosine functions that enter the expressions (5)–(7) of the spin-polarization parameters. It is interesting to compare our results for Xe with those obtained using the relativistic version of the RPAE, the RRPA [13], developed in [14]. The calculations in [14] were performed with account of relaxation. The two calculations, viz., the present and Ref. [14], for all the parameters agree reasonably well. We conclude that through spin-orbit interaction polarization can be realized and correlations probed.

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