Higher multipole and retardation effects in the spin and polarization correlations of polarized photoelectrons ejected from the $2p_J$ - subshell by polarized photons - a nonrelativistic approach

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Abstract

We study spin and polarization correlations in atomic photoionization from np_J subshells, including the first retardation corrections to the dipole approximation. This extends previous work on distributions of unpolarized photoelectrons ejected by polarized photons [A. Bechler and R. H. Pratt, Phys. Rev. **A39**, 1774 (1989), **A42**, 6400 (1990)]. A non-relativistic Pauli-Schrödinger approach in a self-consistent central potential is used, neglecting spin-orbit coupling. There are nontrivial correlations, even in this non-relativistic approximation, even without taking into account spin-orbit coupling, provided the electron is ejected from a subshell with a definite value J of the total angular momentum. (However, if summation over J is performed, one would have to include the spin-orbit coupling in order to obtain any remaining spin and polarisation correlations in the non relativistic approach.). Explicit formulas are given in terms of dipole and quadrupole radial matrix elements and phase shift differences. Results are compared with exact numerical calculations. Corrections to the dipole approximation are generally small at low energies and low Z, but increase with energy and atomic number. Including the first retardation corrections significantly improves agreement.

1. Introduction

Recently there has been increasing interest in the angular distributions and polarization correlations, including non-dipolar effects, in atomic photoionization. In two recent papers Kim et al. (1992, 1995) considered the polarization correlations for high Z ns and npJ-subshell photoionization, using independent particle approximation (IPA) in a relativistic self-consistent atomic field of the Dirac-Slater type, including all significant multipole contributions. This extended earlier studies of the correlations by Pratt, Levee, Pexton and Aron (1964) and Pratt, Ron and Tseng (1973). The angular distributions and polarization correlations in photoionization and radiative recombination were also investigated by Scofield (1989). The full relativistic formulation of the IPA theory of atomic photoeffect, including the spin and polarization correlations, can be found, among others, in the papers of Pratt et al. (1973), Huang (1980, 1982), or in the paper of Lee (1974), which used the helicity formalism. Detailed knowledge of spin and polarization correlations is essential for the complete description of atomic and molecular photoionization.

It has long been known that photoelectrons are, in general, spin polarized. Fano (1969, 1969a) pointed out that the small difference in energy positions of Cooper minima, i.e. the zeros of radial matrix elements, in $ns \rightarrow \varepsilon p_{1/2}$ and $ns \rightarrow \varepsilon p_{3/2}$ channels due to the spin - orbit interaction, leads to a large spin polarization of the photoelectron in the visible and ultraviolet range. By now, it is well known that spin polarized electrons may be ejected from unpolarized atoms by photons of any polarization state, including unpolarized photons (Kessler 1985).

Spin polarization of photoelectrons was considered within a non-relativistic framework by Cherepkov (1979, 1983) in the random-phase approximation with exchange. In the case of an unpolarized atom and polarized light the ejected photoelectrons are usually spin- polarized. Polarization can arise from the spin-orbit interaction in the initial and final state. However, even if one does not take the spin-orbit coupling into account there are still nontrivial spin and polarization correlations, provided one selects an initial electron with a given value of the orbital angular momentum $\mathbf{L}^2$ and given value of the total angular momentum $\mathbf{J}^2$ (together with J_z these are good quantum numbers for the nonrelativistic electron). However, these polarizations cancel after summation over two possible values of the total angular momentum J, i.e. for J = L ± 1/2, so that there are no spin correlations in an nL-subshell cross section. (In the relativistic case, while L in fact is not a good quantum number, it may be understood as a label for the parity of the state.)

The non-dipolar effects in photoionization have also been investigated for a long time. For instance, the full non-relativistic multipole results for the angular distribution of 1s photoelectrons in the point-Coulomb case were obtained by Fischer (1931). [For a review of early results on non-dipolar effects see Tseng et al. (1978)]. Later first retardation corrections to the angular distributions of photoelectrons were considered by Amusia et al. (1975), Amusia and Cherepkov (1975), Wang et al. (1982), Bechler and Pratt (1989, 1990), Pratt and Kim (1993), Cooper (1990, 1993) and Ron et al. (1994). For instance, Amusia et al. (1975) showed that, for unpolarized light, the maximum of the angular distribution of ejected photoelectrons can be shifted, perpendicular to the incident photon direction for s-states in dipole approximation, can be shifted either backward or forward, depending on the photon energy. This effect has been also investigated later by Wang et al. (1982). Calculations of Bechler and Pratt (1989, 1990) for

1s, 2s and 2p subshells, and by Cooper (1990, 1993) for n = 1 - 4 subshells of rare gases showed that the retardation effects can be of the order of 10% for photoelectron energies ~100 eV and of the order 20 - 30% for ~2 keV in the case of initial s-subshells. For 1 - 2 keV photoelectrons ejected from p-subshells the retardation effects in the angular distributions are also quite pronounced (10 - 20%), although at lower energies they are smaller than in the s-subshells.

First experimental measurements of photoelectron angular distributions using high-energy x-rays were performed in the 1920s (Bothe 1924, Auger and Perrin 1927); they showed pronounced forward peaking of the distributions. Most subsequent experimental work was performed at photon energies a few tens to a few hundreds of keV above threshold. For a review of these experiments and comparison with theoretical predictions in this energy region see Tseng et al. (1978). First measurements of non-dipolar effects in the soft x-ray region were performed by Krause (1969) and Wuilleumier and Krause (1974); they showed a distinct increase of the photoelectron intensity in the forward direction. Recently measurements of non-dipolar effects in the angular distributions of unpolarized photoelectrons from K- and L-shells of noble gases for electron energies from a few tens of eV to 3 keV were performed by Krässig et al. (1995, 1996) and Jung et al. (1996). The angular distributions show forward or backward asymmetry, and the experimentally determined parameters describing angular distributions compare well with the results of recent calculations of Cooper (1993) and Bechler and Pratt (1989, 1990).

In the present paper we investigate multipole and retardation effects in the spin and polarization correlations for 2p$_J$ photoelectrons in the nonrelativistic framework, using independent particle approximation. The electron wave function, both in the initial and final state, is treated nonrelativistically, and the photon plane wave is expanded in powers of the photon momentum **k** up to and including terms linear in **k**. This accounts for the standard nonrelativistic dipole approximation and the so-called first retardation (quadrupole) correction. We have shown previously (Bechler and Pratt 1989) that the first retardation correction to the matrix element is in general of order $Z\alpha$, or v/c in the point-Coulomb case, with relativistic corrections of the order $(Z\alpha)^2$ and $(v/c)^2$. It is therefore justified to consider the first retardation corrections to angular distributions and polarization correlations of photoelectrons using an otherwise nonrelativistic approach with nonrelativistic wave functions for the initial and final electron. This can be contrasted with integrated cross sections, in which corrections in the distributions proportional to $Z\alpha$ (v/c) integrate to zero. The result is that in total cross sections relativistic and surviving retardation corrections are of the same order of magnitude.

In the language of a multipole expansion of the incident photon field, including the dipole and first retardation contributions is equivalent to taking into account the electric dipole, electric quadrupole and magnetic dipole terms in their long wavelength limit, i.e. keeping the leading non-vanishing contributions of those multipoles in the limit that **k** (the photon momentum) goes to zero. The retardation correction then corresponds to the [$k \to 0$] limit of the electric quadrupole and magnetic dipole contributions, with the magnetic dipole contribution vanishing in independent particle approximation (Bechler and Pratt 1989, 1990, Cooper 1990)

The general form of the photoeffect cross-section with polarized light and polarized final photoelectrons is (Pratt et al. 1973)

$$\frac{d\sigma}{d\Omega}(\xi,\zeta)=\left(\frac{d\sigma}{d\Omega}\right)_{unpol}\frac{1}{2}\sum_{i,\,j=0}^{3}C_{ij}\xi_i\zeta_j\,, \tag{1.1}$$

where the photon polarization is characterized by Stokes parameters ξ_1,ξ_2,ξ_3 and ζ_1,ζ_2,ζ_3 specify the spin direction of the ejected electron in its rest frame. The parameters ξ_0 and ζ_0 are, by definition, equal to unity and also $C_{00}=1$. The spin and polarization correlation coefficients C_{ij} depend on the direction of the ejected photoelectron. It is the main purpose of the present paper to find their explicit form, including dipole and first retardation contributions. We also express the correlation coefficients C_{ij} in terms of the dynamical parameters introduced by Huang (1980, 1982), which are the coefficients of an expansion of the polarized cross-section for the photoeffect in terms of the matrix elements of the rotation group, $d^{\lambda}_{mn}(\theta)$. We will use the results for the correlation coefficients and dynamical parameters to discuss the polarization of the ejected electron, making a detailed examination of the case of transverse polarization in the production plane, and of case of the longitudinal polarization of the photoelectron ejected by a circularly polarized photon.

The paper is organized as follows. Section 2 contains general considerations concerning the spin and polarization correlations in the case of an initial electron in a npJ subshell, together with a discussion of the significance of higher multipoles at small and large energies. This section contains also some remarks concerning the applicability of the independent particle approximation at higher energies, in view of recent paper of Dias *et al.* (1997). Section 3 contains the formalism, based on our previous paper (Bechler and Pratt 1990), with the modifications necessary for the full description of the spin and polarization correlations. In Section 4 we give explicit expressions for the coefficients $C_{ij}(\theta)$ for npJ initial electron states in the dipole and first retardation approximations, in terms of radial matrix elements and phase shift differences. Explicit formulas for photoelectron spin are given both in terms of the correlation coefficients (Kim, Goldberg and Pratt 1995) and the dynamical parameters (Huang 1980, 1982). Section 5 presents and discusses results for the 2p dynamical parameters as functions of energy, for five values of the atomic number (Z = 6, 10, 18, 26 and 36), for photoelectron energies from threshold to 20 keV. Section 6 is devoted to a discussion of the spin of the photoelectron, based on these results, with a particular focus on the case of circularly polarized photons. Section 7 contains final remarks. Technical details of the calculation and explicit formulas for the rotation group matrix elements are given in Appendix A. Relations between the correlation coefficients and dynamical parameters, and explicit expressions for the latter in terms of radial matrix elements and phase shifts, are given in Appendix B.

2. General considerations

In this section we discuss some general issues related to the problem of spin and polarization correlations in photoionization. These are: the importance of spin - orbit coupling for the correlations and the justification of neglecting the spin - orbit interaction when a definite J - state is chosen as an initial state, the importance of higher multipoles at low energies, and the applicability of independent particle approximation.

As already mentioned in the Introduction, in a non relativistic approach weighted sums of the probabilities for $J=L-1/2$ and $L+1/2$ subshells show no correlations of spin and polarization unless the differences between radial matrix elements due to spin - orbit coupling are taken into account (Cherepkov 1979). In the present approach we take an initial electron state with given total angular momentum quantum number J, without performing a summation over J for a given value of L. This leads to nontrivial spin - polarization correlations even when spin - orbit coupling is neglected.

Since spin - orbit coupling does influence transition amplitudes it is necessary to check under what circumstances its influence on the correlations is small. For this purpose one can compare the magnitude of the residual correlation effects due to spin - orbit coupling for a particular np_J - subshell, with the spin - polarization correlations which are due to picking the J - state as an initial state. We examined sums of the probabilities for $np_{1/2}$ and $np_{3/2}$ initial states multiplied by their statistical weights (2 and 4 respectively). Using as an example recent results for the spin and polarization correlations in the photoionization of various subshells of Uranium (Kim, Goldberg and Pratt 1995, Goldberg 1995) one can show that for the 2p subshell the summed correlation coefficients C_{ij} are small up to outgoing electron energies of the order of few keV. We may expect therefore that for 2p subshells the spin - orbit coupling does not yield significant correlation effects at low energies. On the other hand, the full multipole results (not summed) for the correlation coefficients in the case of photoelectrons ejected from $2p_{1/2}$ and $2p_{3/2}$ subshells are not separately small (Kim, Goldberg and Pratt 1995) which shows that dominant contribution to the correlations is due to picking a particular $2p_J$ - state and not due to the spin - orbit coupling.

In two previous papers (Kim, Goldberg and Pratt 1992, 1995) the photon - electron polarization correlations were studied using full multipole numerical results for the polarization coefficients C_{ij}. For low energies of the ejected electron the dipole results reproduce well the angular dependence of exact full multipole polarization coefficients, with higher multipoles starting to play role at higher energies, and in those cases at lower energies, for which the C_{ij} vanished in the non relativistic dipole approximation. The numerical calculations show that multipoles beyond dipole and quadrupole start to play a significant role for energies exceeding ~ 2 keV . For energies below 2 keV either dipole or dipole + quadrupole terms give a quite accurate description of the angular dependence of the correlation coefficients. In the long - wavelength limit this corresponds to non relativistic dipole plus the first retardation correction. It is interesting to note that this formalism is sufficient for the regime in which atomic potential screening matters. Regarding screening effects it has been shown (Pratt and LaJohn 1995, LaJohn and Pratt 1998, 1998a) that, except for bound state normalization, they play a significant role only for low multipoles, since with increasing energy, when higher multipoles are needed, the point - Coulomb calculations become quite accurate.

Regarding applicability of the independent particle approximation, it has been argued in the recent paper by Dias et al. (1997) that in the photoionization of np subshells the interchannel coupling with the nearby ns channel persists for high energies of the outgoing electron, so that the independent particle approximation is insufficient at all energies. This conclusion was illustrated in 2p photoionization of Neon, where RPA calculations with interchannel coupling taken into account show deviations from the IPA results of the order of 30% at photon energies $\propto$ 1 - 1.4 keV, in agreement with experiment. An important question, not discussed in the paper of Dias et al., is the Z - dependence of the IPA breaking effects. Examining recent perturbative calculations of Drukarev (1998) we may argue that at high energies the relative magnitude of the final state interaction (FSI) correction is $\propto Z^{-1}$, independent of energy, which indicates a decreasing FSI effect for increasing atomic number. This is supported by previous experimental measurements of nondipolar angular distribution parameters for the 2p photoionization of Krypton (Jung et al. 1996), which compare well with the IPA calculations of Bechler and Pratt (1990) and Cooper (1993). Our conclusion is that, while the FSI effects require further investigation, and in particular their Z - dependence has to be understood, the independent particle calculations presented here give for high energies the dominant contribution, except perhaps in the lightest elements.

3. Formalism

To make the consideration of the spin and polarization correlations in the nonrelativistic limit complete we use as our starting point the fully relativistic expression for the photoeffect matrix element :

$$M_{fi} = \langle f|(\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon})e^{i\mathbf{k}\cdot\mathbf{r}}|i\rangle = \int d^3x \psi_f^\dagger (\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}) e^{i\mathbf{k}\cdot\mathbf{r}} \psi_i \ , \tag{3.1}$$

where $f(i)$ denotes the final (initial) state of the electron with the relativistic wave functions $\psi_f(\psi_i)$, $\boldsymbol{\varepsilon}$ is the photon polarization vector and $\mathbf{k}$ its momentum, and $\boldsymbol{\alpha}$ are the Dirac matrices. To obtain from this the nonrelativistic form of the matrix element we use the relation between the upper component of the Dirac wave function, φ, and the lower component χ, in the nonrelativistic limit:

$$\chi = \frac{1}{2}(\boldsymbol{\sigma}\cdot\mathbf{P})\varphi , \tag{3.2}$$

where $\mathbf{P}$ is the momentum operator, $\boldsymbol{\sigma}$ are the Pauli matrices, and we use the units $m = c = \eta = 1$. Substituting (3.2) into (3.1) we obtain the nonrelativistic expression for the matrix element including the Pauli-Schrödinger term (Bethe, Salpeter 1957) describing interaction of the electron spin with the magnetic part of the photon field:

$$M_{fi} = \langle f|(\boldsymbol{\varepsilon}\cdot\mathbf{P})e^{i\mathbf{k}\cdot\mathbf{r}}|i\rangle - \frac{1}{2}(\boldsymbol{\varepsilon}\times\mathbf{k})\langle f|\boldsymbol{\sigma}e^{i\mathbf{k}\cdot\mathbf{r}}|i\rangle , \tag{3.3}$$

where f(i) denote now the final (initial) state of the nonrelativistic spinning electron.

The wave function of the electron in the initial state has the form

$$\psi_i(\mathbf{r}) = R_{nL}(r)\Omega_{JLM}(\hat{\mathbf{r}}), \tag{3.4}$$

where $R_{nL}(r)$ is the nonrelativistic radial function and $\Omega_{JLM}(\hat{\mathbf{r}})$ is the spherical spinor describing the angular dependence of the wave function. We find it convenient to label the spherical spinors of the bound states by J, L and M. As has been discussed in the previous section, the spin and polarization correlation effects for an initial non relativistic electron in the nL_J subshell are due mainly to picking an initial state with given total angular momentum J, and not due to spin-orbit coupling, which can be neglected in this approximation. As a consequence we use the same radial wave function $R_{nL}(r)$ for $J = L - 1/2$ and $J = L + 1/2$ initial states.

The partial wave expansion of the relativistic continuum wave function has the form (Pratt *et al*. 1973)

$$\Psi_{\mathbf{p}}(\mathbf{r}) = 4\pi \sum_{\kappa m} \left[\Omega^{\dagger}_{\kappa m}(\hat{\mathbf{p}})\chi\right] i^{\lambda} \exp(-i\delta_{\kappa}) \begin{bmatrix} R_{\kappa}\Omega_{\kappa m}(\hat{\mathbf{r}}) \\ iS_{\kappa}\Omega_{-\kappa m}(\hat{\mathbf{r}}) \end{bmatrix}, \tag{3.5}$$

where $\mathbf{p}$ is the asymptotic momentum of the ejected electron, $\hat{\mathbf{p}}$ is the unit vector in its direction, χ is the Pauli spinor describing the spin state of the photoelectron, δ_{κ} are the phase shifts and R_{κ} , S_{κ} are the radial functions of the upper and lower components respectively. The quantum number κ combines total angular momentum and parity: $\kappa = \mu(j + 1/2)$ [??] for $j = \lambda \pm 1/2$. The spherical spinor can be labelled either by JLM, as in (3.4) and (3.7), or by κm, as in (3.5). In the non relativistic limit with spin-orbit coupling neglected we have $\delta_{\kappa} = \delta_{-\kappa} = \delta_{\lambda}$, $R_{\kappa} = R_{-\kappa} = R_{\lambda}$; using summation formulae for spherical spinors (Bechler 1993) given in Appendix A we obtain a partial wave series for the final electron wave function in the form

$$\psi_f(\mathbf{r}) = \sum_{l=0}^{\infty} i^l (2l+1) e^{-i\delta_l} P_l(\hat{\mathbf{p}} \cdot \hat{\mathbf{r}}) R_l(r) \chi. \tag{3.6}$$

The spherical spinors describing the angular momentum state of an electron are given by:

$$\Omega_{jlm}(\hat{\mathbf{r}}) = \begin{bmatrix} \left(\dfrac{j+m}{2j}\right)^{1/2} Y_{l,m-1/2}(\hat{\mathbf{r}}) \\ \left(\dfrac{j-m}{2j}\right)^{1/2} Y_{l,m+1/2}(\hat{\mathbf{r}}) \end{bmatrix} \tag{3.7}$$

for $j = l + 1/2$ $(\kappa = -j - 1/2)$, and

$$\Omega_{jlm}(\hat{\mathbf{r}}) = \begin{bmatrix} -\left(\dfrac{j-m+1}{2j+2}\right)^{1/2} Y_{l,m-1/2}(\hat{\mathbf{r}}) \\ \left(\dfrac{j+m+1}{2j+2}\right)^{1/2} Y_{l,m+1/2}(\hat{\mathbf{r}}) \end{bmatrix} \tag{3.8}$$

for $j = l - 1/2$ $(\kappa = j + 1/2)$.

To extract from the matrix element (3.3) the nonrelativistic dipole approximation plus the first retardation correction, we expand the photon plane wave in powers of k and keep in (3.3) the expansion through terms linear in k. This gives

$$M_{fi} = \langle f|(\boldsymbol{\varepsilon}\cdot\mathbf{P})(1+i\mathbf{k}\cdot\mathbf{r})|i\rangle - \frac{i}{2}(\boldsymbol{\varepsilon}\times\mathbf{k})\langle f|\boldsymbol{\sigma}|i\rangle. \qquad (3.9)$$

Including terms $\propto \mathbf{k}\cdot\mathbf{r}$ results in a retardation correction proportional to $Z\alpha$ (Bechler and Pratt 1989). On the other hand, the relativistic correction to the matrix element is $\propto (Z\alpha)^2$, which for lighter elements and low energies of the final electron is small compared to the first retardation correction.

It is convenient to write the first term in (3.9) in the length form :

$$\langle f|(\boldsymbol{\varepsilon}\cdot\mathbf{P})(1+i\mathbf{k}\cdot r)|i\rangle = i\omega\langle f|(\boldsymbol{\varepsilon}\cdot\mathbf{r})|i\rangle - \frac{1}{2}\omega k\langle f|(\hat{\mathbf{k}}\cdot\mathbf{r})(\boldsymbol{\varepsilon}\cdot\mathbf{r})|i\rangle - \frac{i}{2}(\boldsymbol{\varepsilon}\times\mathbf{k})\langle f|\mathbf{L}|i\rangle, \qquad (3.10)$$

where $\mathbf{L}$ is the orbital angular momentum operator. Substituting (3.10) into (3.9) and introducing the spin operator, $\mathbf{s} = 1/2\boldsymbol{\sigma}$, we get

$$M_{fi} = i\omega\langle f|(\boldsymbol{\varepsilon}\cdot\mathbf{r})|i\rangle - \frac{1}{2}\omega k\langle f|(\hat{\mathbf{k}}\cdot\mathbf{r})(\boldsymbol{\varepsilon}\cdot\mathbf{r})|i\rangle - \frac{i}{2}(\boldsymbol{\varepsilon}\times\mathbf{k})\cdot\langle f|\mathbf{L}+2\mathbf{s}|i\rangle. \qquad (3.11)$$

The first term in (3.11) gives the non relativistic dipole approximation to the matrix element, i.e. the long wavelength limit of the dipole contribution with retardation. The second term gives the long wavelength limit of the electric quadrupole term, and the last term gives the contribution from the magnetic dipole term in the same limit. In independent particle approximation the magnetic dipole contribution in (3.11) vanishes, due to the orthogonality of bound and continuum radial functions with the same value of orbital angular momentum.

To calculate the dipole and quadrupole matrix elements from an initial p-state [first and second term in (3.11), respectively], we use (3.6) and explicit forms of the spherical spinors, (3.7) or (3.8) for $l=1$. The dipole selection rules pick up terms with $l=0$ and $l=2$ in ψ_f, and the quadrupole contribution is a sum of $l=1$ and $l=3$ terms. Using further the technique of angular integration described in the Appendix of Bechler and Pratt (1990), we obtain explicitly

$$\langle f|\boldsymbol{\varepsilon}\cdot\mathbf{r}|i\rangle = \frac{4\pi}{3}\left\{e^{i\delta_0}D_0\chi^\dagger\Omega_{J1M}(\boldsymbol{\varepsilon}) + e^{i\delta_2}D_2\chi^\dagger\left[\Omega_{J1M}(\boldsymbol{\varepsilon}) - 3(\boldsymbol{\varepsilon}\cdot\hat{\mathbf{p}})\Omega_{J1M}(\hat{\mathbf{p}})\right]\right\}, \qquad (3.12a)$$

$$\langle f|(\mathbf{k}\cdot\mathbf{r})(\boldsymbol{\varepsilon}\cdot\mathbf{r})|i\rangle = -\frac{4\pi}{5}ie^{i\delta_1}Q_1\chi^\dagger\left[(\boldsymbol{\varepsilon}\cdot\hat{\mathbf{p}})\Omega_{J1M}(\hat{\mathbf{k}}) + (\hat{\mathbf{k}}\cdot\hat{\mathbf{p}})\Omega_{J1M}(\boldsymbol{\varepsilon})\right] +$$

$$+\frac{4\pi}{5}ie^{i\delta_3}Q_3\chi^\dagger\left[-(\boldsymbol{\varepsilon}\cdot\hat{\mathbf{p}})\Omega_{J1M}(\hat{\mathbf{k}}) - (\hat{\mathbf{k}}\cdot\hat{\mathbf{p}})\Omega_{J1M}(\boldsymbol{\varepsilon}) + 5(\boldsymbol{\varepsilon}\cdot\hat{\mathbf{p}})(\hat{\mathbf{k}}\cdot\hat{\mathbf{p}})\Omega_{J1M}(\hat{\mathbf{p}})\right], \qquad (3.12b)$$

where J, M are the total angular momentum quantum numbers of the initial electron state, and D_0, D_2, Q_1, Q_3 are the dipole and quadrupole radial matrix elements for the dipole transitions to continuum $\lambda = 0$ and $\lambda = 2$ states, and quadrupole transitions to continuum $\lambda = 1$ and $\lambda = 3$ states:

$$D_l = \int_0^\infty drr^2 R_l(r) r R_{np}(r), \qquad Q_l = \int_0^\infty drr^2 R_l(r) r^2 R_{np}(r). \tag{3.13}$$

The formulas (3.12) for the dipole and quadrupole matrix elements have so far been written in a form independent of a particular choice of coordinate system. In general, however, it is convenient to make a definite choice of coordinate system. The specific form of the correlation coefficients depends on this choice, and it is therefore desirable to choose a coordinate system in which their form is as simple as possible. Such a coordinate system is shown in Fig. 1a; the z-axis is chosen in the direction of the photon momentum and the photoelectron momentum is in the xz-plane. With this choice of coordinate system, the angular dependence of the correlation coefficients enters only through the angle between the electron and photon momenta.

Another convenient coordinate system, which has been used in the recent measurement of the non-dipolar effects in the angular distributions of photoelectrons (Krässig et al. 1995, 1996, Jung et al. 1996) is shown in Fig. 1b. The z-axis is chosen along the direction of the photon polarization vector and the x-axis along the direction of the photon momentum. With passive interpretation of the rotations (i.e. axes are rotated, not vectors), the matrix of transformation from the coordinate system Fig. 2b, to that of Fig. 2a is

$$\hat{R} = \begin{bmatrix} 0 & \sin\phi & \cos\phi \\ 0 & -\cos\phi & \sin\phi \\ 1 & 0 & 0 \end{bmatrix}. \tag{3.14}$$

The polarization of the incident photon may be characterized by Stokes parameters, which in the coordinate system Fig. 2a are expressed in terms of the components of the photon polarization vector as

$$\xi_1 = |\varepsilon_x|^2 - |\varepsilon_y|^2, \ \ \xi_2 = \varepsilon_x\varepsilon_y^* + \varepsilon_x^*\varepsilon_y, \ \ \xi_3 = i\left(\varepsilon_x\varepsilon_y^* - \varepsilon_x^*\varepsilon_y\right), \tag{3.15}$$

and in the other coordinate system Fig. 2b (primes refer to the vector components in this coordinate system)

$$\xi_1' = |\varepsilon_y'|^2 - |\varepsilon_z'|^2, \ \ \xi_2' = \varepsilon_z'\varepsilon_y'^* + \varepsilon_z'^*\varepsilon_y', \ \ \xi_3' = i\left(\varepsilon_y'\varepsilon_z'^* - \varepsilon_y'^*\varepsilon_z'\right). \tag{3.16}$$

Expressing the components of the polarization vector in both coordinate frames with the use of (3.14), we can find the relation between the two sets of Stokes parameters as

$$\begin{aligned} \xi_1 &= -\xi_1'\cos 2\phi + \xi_2'\sin 2\phi, \\ \xi_2 &= -\xi_1'\sin 2\phi - \xi_2'\cos 2\phi, \end{aligned} \tag{3.17}$$

$$\xi_3 = \xi_3'.$$

We give also relations between the two sets of angles, θ,ϕ and θ',ϕ', shown in Fig. 2a and 2b:

$$\begin{aligned} &\cos\theta = \cos\phi'\sin\theta', \\ &\cos\theta' = \cos\phi\sin\theta. \end{aligned} \tag{3.18}$$

The spin measurement direction for the ejected electron in its rest frame is specified by the unit vector $\boldsymbol{\zeta}$, with (Pratt et. al. 1973)

$$\boldsymbol{\zeta} = \chi^{\dagger}\boldsymbol{\sigma}\chi, \tag{3.18}$$

where χ is the two-component Pauli spinor describing the spin degrees of freedom of the ejected electron, and $\boldsymbol{\sigma}\cdot\boldsymbol{\zeta}\chi = \chi$. In the electron rest frame, with the z-axis along the direction of the electron momentum, we have

$$\begin{aligned} \zeta_1 &= \frac{(\hat{\mathbf{y}}\times\hat{\mathbf{p}})\cdot\boldsymbol{\zeta}}{|\hat{\mathbf{y}}\times\hat{\mathbf{p}}|}, \\ \zeta_2 &= \hat{\mathbf{y}}\cdot\boldsymbol{\zeta}, \\ \zeta_3 &= \hat{\mathbf{p}}\cdot\boldsymbol{\zeta}, \end{aligned} \tag{3.19}$$

with $\hat{\mathbf{y}} = \left(\hat{\mathbf{k}}\times\hat{\mathbf{p}}\right)/\left|\hat{\mathbf{k}}\times\hat{\mathbf{p}}\right|$. Relations between the correlation coefficients C_{ij} and C'_{ij} in the coordinate frames, Fig. 2a and 2b respectively, are given in the next section.

4. Spin and polarization correlations

In this section we obtain explicit formulas for the p state correlation coefficients and dynamical parameters. We explicitly write out the expressions for the $p_{1/2}$ initial state. To obtain the corresponding quantities for the $p_{3/2}$ state one should use formulas (4.6), (4.30) and (4.31). Keeping in mind that the magnetic dipole term in the large wave length limit gives no contribution to the matrix element within the independent particle approximation, we get from (3.11)

$$M_{fi} = i\omega\langle f|\boldsymbol{\varepsilon}\cdot\mathbf{r}|i\rangle - \frac{1}{2}\omega k\langle f|\left(\hat{\mathbf{k}}\cdot\hat{\mathbf{r}}\right)(\boldsymbol{\varepsilon}\cdot\mathbf{r})|i\rangle. \tag{4.1}$$

The modulus squared of this matrix element, up to terms linear in k, is

$$\left|M_{fi}\right|^2 = \omega^2\left\{\langle f|\boldsymbol{\varepsilon}\cdot\mathbf{r}|i\rangle^2 + k\,\mathrm{Im}\left[\langle f|\boldsymbol{\varepsilon}\cdot\mathbf{r}|i\rangle\langle f|\left(\hat{\mathbf{k}}\cdot\hat{\mathbf{r}}\right)(\boldsymbol{\varepsilon}\cdot\mathbf{r})|i\rangle^*\right]\right\}. \tag{4.2}$$

Assuming that the spin of the initial electron is not taken into account, we have to average over the magnetic quantum number M of the initial state. As can be seen from (3.12) the expression (4.2) is bilinear both in the spherical spinors Ω_{JLM} and the Pauli spinors χ characterizing the spin state of the ejected electron. The summation over M can be performed with the use of summation formulas for spherical spinors (Bechler 1993), which we summarize in Appendix A. Substituting (3.12) into (4.2), performing the summation over magnetic substates, and using (3.16) together with the auxiliary formulas given in Appendix A, we obtain an expression bilinear in the Stokes parameters $\boldsymbol{\xi}$ of the photon and the spin parameters $\boldsymbol{\zeta}$ of the ejected photoelectron. The spin and polarization dependent differential cross section is of the form [c.f. also (1.1)]:

$$\frac{d\sigma}{d\Omega}(\boldsymbol{\xi},\boldsymbol{\zeta})=\left(\frac{d\sigma}{d\Omega}\right)_{unpol}\frac{1}{2}\sum_{i,\,j=0}^{3}C_{ij}\xi_i\zeta_j\,, \tag{4.3}$$

where $C_{00}=1$, and we give the C_{ij} below.

For the $p_{1/2}$ state we use (A.2) with $J=1/2, L=1$:

$$\sum_M \Omega_{\frac{1}{2},1,M}(\hat{\mathbf{a}})\Omega^{\dagger}_{\frac{1}{2},1,M}(\hat{\mathbf{b}})=\frac{1}{4\pi}\hat{\mathbf{a}}\cdot\hat{\mathbf{b}}+\frac{i}{4\pi}\left(\hat{\mathbf{a}}\times\hat{\mathbf{b}}\right)\cdot\boldsymbol{\sigma}. \tag{4.4}$$

The first term here gives contributions of the type C_{00} and $C_{10}\xi_1$, containing no spin variables, while the second term contributes to the part of the cross-section describing correlations between photon and electron polarizations, $C_{ij}\xi_i\zeta_j$ with $j\neq 0$. For the $p_{3/2}$ state we use (A.1) with $J=3/2,\ L=1$:

$$\sum_M \Omega_{\frac{3}{2},1,M}(\hat{\mathbf{a}})\Omega^{\dagger}_{\frac{3}{2},1,M}(\hat{\mathbf{b}})=\frac{1}{2\pi}\hat{\mathbf{a}}\cdot\hat{\mathbf{b}}-\frac{i}{4\pi}\left(\hat{\mathbf{a}}\times\hat{\mathbf{b}}\right)\cdot\boldsymbol{\sigma}. \tag{4.5}$$

Comparing (4.4) and (4.5) we see that after averaging over initial magnetic states

$$C_{i0}\left(p_{3/2}\right)=C_{i0}\left(p_{1/2}\right)\qquad C_{ij}\left(p_{3/2}\right)=-\frac{1}{2}C_{ij}\left(p_{1/2}\right)\ \ j\neq 0. \tag{4.6}$$

Formulas (4.6) are only valid under the assumption that we neglect the spin-orbit interaction, since only then are the $p_{1/2}$ and $p_{3/2}$ states described non-relativistically by the same radial functions. With spin-orbit coupling included the radial matrix elements for $p_{1/2}$ and $p_{3/2}$ initial states are different and equations (4.6) are not valid (Cherepkov 1979).

The unpolarized differential cross section is given by (Kim *et al* 1980)

$$\left(\frac{d\sigma}{d\Omega}\right)_{unpol}=\frac{\sigma}{4\pi}g(\theta), \tag{4.7}$$

where σ is the total cross section, and

$$g(\theta) = 1 - \frac{1}{2}\beta^{(d)} P_2(\cos\theta) + B_1^{(r)} P_1(\cos\theta) + B_3^{(r)} P_3(\cos\theta) \; . \tag{4.8}$$

The first two terms in this expression give the dipole approximation to the unpolarized differential cross section, with the asymmetry parameter β for the p subshell

$$\beta^{(d)} = 2\frac{D_2^2 - 2D_0 D_2 \cos\Delta_{20}}{D_0^2 + 2D_2^2} , \tag{4.9}$$

where D_0 , D_2 are the dipole radial matrix elements [c.f. (3.13)], and Δ_{20} is the phase shift difference, defined in general as

$$\Delta_{\lambda\lambda'} \equiv \delta_\lambda - \delta_{\lambda'} \, . \tag{4.10}$$

The first retardation correction to the unpolarized differential cross section is given by the last two terms in (4.8), with the coefficients B_1 and B_3 (Bechler and Pratt 1990)

$$B_1^{(r)} = \frac{3}{10} k \frac{\frac{10}{5} F_{23} - \frac{2}{5} F_{21} + 2F_{01}}{D_0^2 + 2D_2^2} , \tag{4.11a}$$

$$B_3^{(r)} = \frac{3}{10} k \frac{2F_{03} - \frac{8}{5} F_{23} + \frac{12}{5} F_{01}}{D_0^2 + 2D_2^2} , \tag{4.11b}$$

where the $F_{\lambda\lambda'}$ are defined as in Bechler and Pratt (1990):

$$F_{ll'} \equiv D_l Q_{l'} \cos\Delta_{ll'} , \tag{4.12}$$

with the quadrupole radial matrix element Q_λ given by (3.13).

The normalized correlation coefficients C_{ij} in (4.3) can be written in the form

$$C_{ij}(\theta) = \frac{c_{ij}(\theta)}{g(\theta)} , \tag{4.13}$$

where $c_{00}(\theta) \equiv g(\theta)$ so that $C_{00} = 1$, and dipole contributions to c_{ij} for the $p_{1/2}$ initial state are given by [details of the calculations leading to (4.14) and (4.15) below are given in Appendix C] [??}:

$$c_{10}^{(d)} = \frac{3}{2} \frac{\left(D_2^2 - 2D_0 D_2 \cos\Delta_{20}\right)\sin^2\theta}{D_0^2 + 2D_2^2} , \tag{4.14a}$$

$$c_{31}^{(d)} = -\frac{\left(D_0^2 - 2D_2^2 - 2D_0 D_2 \cos\Delta_{20}\right)\sin\theta}{D_0^2 + 2D_2^2}, \tag{4.14b}$$

$$c_{33}^{(d)} = \frac{\left(D_0^2 + D_2^2 + 2D_0 D_2 \cos\Delta_{20}\right)\cos\theta}{D_0^2 + 2D_2^2}, \tag{4.14c}$$

$$c_{21}^{(d)} = -\frac{3D_0 D_2 \sin\Delta_{20}\sin\theta}{D_0^2 + 2D_2^2}, \tag{4.14d}$$

$$c_{23}^{(d)} = 0, \tag{4.14e}$$

$$c_{02}^{(d)} = c_{12}^{(d)} = \frac{3D_0 D_2 \sin\Delta_{20}\sin\theta\cos\theta}{D_0^2 + 2D_2^2}. \tag{4.14f}$$

For the first retardation correction to c_{ij} in the case of the $p_{1/2}$ subshell we have

$$c_{10}^{(r)} = -\frac{5}{2} B_3 \sin^2\theta\cos\theta, \tag{4.15a}$$

$$c_{31}^{(r)} = k\frac{-\frac{9}{10}F_{01} + \frac{3}{2}F_{23} + \frac{3}{5}F_{03}}{D_0^2 + 2D_2^2}\sin\theta\cos\theta, \tag{4.15b}$$

$$c_{33}^{(r)} = \frac{3}{5}kP_2(\cos\theta)\frac{F_{01} + F_{03} + F_{21} + F_{23}}{D_0^2 + 2D_2^2}, \tag{4.15c}$$

$$c_{21}^{(r)} = \frac{3}{10}k\frac{G_{01} - 4G_{03} - 4G_{21} - G_{23}}{D_0^2 + 2D_2^2}\sin\theta\cos\theta, \tag{4.15d}$$

$$c_{23}^{(r)} = \frac{3}{10}k\frac{G_{01} + G_{03} - G_{21} + G_{23}}{D_0^2 + 2D_2^2}\sin^2\theta, \tag{4.15e}$$

$$c_{02}^{(r)} = c_{12}^{(r)} = k\frac{-\frac{3}{10}G_{01} - \frac{3}{10}G_{03} - \frac{3}{5}G_{21} + \frac{3}{5}G_{23}}{D_0^2 + 2D_2^2}\sin\theta + k\frac{\frac{3}{2}G_{03} + \frac{9}{5}G_{21} - \frac{3}{10}G_{23}}{D_0^2 + 2D_2^2}\sin\theta\cos^2\theta, \tag{4.15f}$$

where

$$G_{ll'} \equiv D_l Q_{l'} \sin\Delta_{l_> l_<}, \tag{4.16}$$

with $l_>(l_<)$ denoting the larger (smaller) of l and l'. There are seven non-vanishing correlation coefficients C_{ij} (six in dipole approximation, since then $C_{23} = 0$). This number of non-trivial spin and polarization correlations is not particular to our approximation but is a general feature of the photoeffect, following from time reversal invariance (Pratt et. al. 1973).

To obtain the differential cross-section for an electron in the p-subshell, (i.e. characterized by the orbital angular momentum, not by total angular momentum) we have to sum the probabilities for $p_{1/2}$ and $p_{3/2}$ initial states multiplied by corresponding statistical weights and then divide by the total weight of the p-subshell.. All terms in the separate p_J-cross sections involving spin degrees of freedom cancel. There are no correlations between photon and electron polarizations. To obtain nontrivial spin and polarization correlations for the complete p - subshell one has to take into account the spin-orbit interaction (Cherepkov 1979).

The spin state of the photoelectron is described by a unit vector ζ (3.18)-(3.19) characterizing the direction along which the spin of the photoelectron is measured. The degree of polarization of the photoelectron along the direction ζ is given by (Kim, Goldberg and Pratt 1995)

$$P_\zeta = \frac{\frac{d\sigma}{d\Omega}(\xi,\zeta) - \frac{d\sigma}{d\Omega}(\xi,-\zeta)}{\frac{d\sigma}{d\Omega}(\xi,\zeta) + \frac{d\sigma}{d\Omega}(\xi,-\zeta)}. \tag{4.17}$$

The denominator in this formula is the differential cross section for the ejection of an unpolarized electron and can be obtained from (4.3) by performing a summation over ζ:

$$\frac{d\sigma}{d\Omega}(\xi,\zeta) + \frac{d\sigma}{d\Omega}(\xi,-\zeta) = \left(\frac{d\sigma}{d\Omega}\right)_{unpol}\left(1 + C_{10}\xi_1\right). \tag{4.18}$$

For the degree of polarization in the three directions $\hat{\mathbf{y}} \times \hat{\mathbf{p}}$, $\hat{\mathbf{y}}$, $\hat{\mathbf{p}}$, with $\hat{\mathbf{y}} = \left(\hat{\mathbf{k}} \times \hat{\mathbf{p}}\right) / \left|\hat{\mathbf{k}} \times \hat{\mathbf{p}}\right|$, we obtain (Kim, Goldberg and Pratt 1995)

$$P_1(\theta) = \frac{\xi_2 C_{21}(\theta) + \xi_3 C_{31}(\theta)}{1 + \xi_1 C_{10}(\theta)}, \tag{4.19a}$$

$$P_2(\theta) = \frac{C_{02}(\theta) + \xi_1 C_{12}(\theta)}{1 + \xi_1 C_{10}(\theta)}, \tag{4.19b}$$

$$P_3(\theta) = \frac{\xi_2 C_{23}(\theta) + \xi_3 C_{33}(\theta)}{1 + \xi_1 C_{10}(\theta)}. \tag{4.19c}$$

Expressions for P_1, P_2 and P_3 can be also written in an alternative form (Huang 1982), employing an expansion of the cross section in terms of the rotation group matrix elements $d^{\lambda}_{mm'}(\theta)$. Following Huang (1982) we write

$$P_1 F(\theta) = \xi_3 \sum_{l \geq 1} \xi_{3l} d_{01}^l + \xi_2 \sum_{l \geq 2} \left(\xi_{2l} d_{21}^l + \eta_{2l} d_{2-1}^l \right), \tag{4.20a}$$

$$P_2 F(\theta) = \sum_{l \geq 1} \eta_{0l} d_{01}^l - \xi_1 \sum_{l \geq 2} \left(\xi_{2l} d_{21}^l - \eta_{2l} d_{2-1}^l \right), \tag{4.20b}$$

$$P_3 F(\theta) = \xi_3 \sum_{l \geq 0} \zeta_{3l} d_{00}^l + \xi_2 \sum_{l \geq 2} \zeta_{2l} d_{20}^l \,, \tag{4.20c}$$

where

$$F(\theta) = 1 + \sum_{l \geq 1} \beta_{0l} d_{00}^l - \xi_1 \sum_{l \geq 2} \beta_{1l} d_{20}^l \,. \tag{4.21}$$

Table 1 shows non vanishing dipole and first retardation contributions to the dynamical parameters, $\xi_{3\lambda}$, $\xi_{2\lambda}$, $\eta_{2\lambda}$, $\eta_{0\lambda}$, $\zeta_{3\lambda}$, $\zeta_{2\lambda}$, $\beta_{0\lambda}, \beta_{1\lambda}$. The relations between correlation coefficients and dynamical parameters, and explicit expressions for the dynamical parameters including dipole and first retardation contributions, are given in Appendix B.

We may give the relations between the correlation coefficients C_{ij} and C'_{ij} in the coordinate frames Fig. 2a and 2b respectively. Writing the differential cross section (4.3) in the coordinate frame Fig. 2b we have

$$\frac{d\sigma}{d\Omega}(\xi', \zeta) = \frac{1}{2} \left(\frac{d\sigma}{d\Omega} \right)_{unpol} \sum_{i,j} C'_{ij}(\theta', \phi') \xi'_i \zeta_j \,, \tag{4.22}$$

where the angles θ' and ϕ' are shown in Fig. 2b. Substituting into (4.3) the Stokes parameters ξ_i expressed by ξ'_i [Eqs. (3.17)], we obtain

$$\begin{aligned} \frac{d\sigma}{d\Omega}(\xi', \zeta) = \frac{1}{2} \left(\frac{d\sigma}{d\Omega} \right)_{unpol} \Bigg[& \sum_j \left(C_{0j} + C_{3j} \xi'_3 \right) \zeta_j + \sum_j C_{1j} \left(-\xi'_1 \cos 2\phi + \xi'_2 \sin 2\phi \right) \zeta_j + \\ & + \sum_j C_{2j} \left(-\xi'_1 \sin 2\phi - \xi'_2 \cos 2\phi \right) \zeta_j \Bigg]. \end{aligned} \tag{4.23}$$

Comparing (4.23) with (4.22) we find

$$\begin{aligned} & C'_{0j}(\theta', \phi') = C_{0j}(\theta) \,, \qquad C'_{3j}(\theta', \phi') = C_{3j}(\theta), \\ & C'_{1j}(\theta', \phi') = -C_{1j}(\theta) \cos 2\phi - C_{2j}(\theta) \sin 2\phi, \\ & C'_{2j}(\theta', \phi') = C_{1j}(\theta) \sin 2\phi - C_{2j}(\theta', \phi') \cos 2\phi \,. \end{aligned} \tag{4.24}$$

To express correlation coefficients in the coordinate frame Fig. 2b as functions of the angles θ' and ϕ' one has to use (3.18).

5. Results for the dynamical parameters

In this section we give results for the dynamical parameters ξ, η, ζ, paying particular attention to the role of the retardation effects as compared to dipole contributions. As examples we use the $2p_{3/2}$ subshell of Carbon (Z = 6), Neon (Z = 10), Argon (Z =18), Iron (Z = 26) and Krypton (Z = 36). The parameters $\beta_{o\lambda}$ and $\beta_{1\lambda}$ can be expressed in terms of the cross-section coefficients B_λ discussed previously (Kim *et al.* 1980, Tseng *et al.* 1978, Bechler and Pratt 1990), and so we will not discuss them here in detail, but we plot them for the sake of completeness.

According to Table 1 the only dynamical parameters for which the dipole contributions do not vanish are $\xi_{31}, \xi_{22}, \eta_{22}, \eta_{02}, \zeta_{31}$, where in dipole approximation $\eta_{22}^{(d)} = \xi_{22}^{(d)}$. For these five parameters the first retardation correction vanishes except in the case of ξ_{22} and η_{22}, for which $\eta_{22}^{(r)} = -\xi_{22}^{(r)}$. The parameters for which the dipole contribution vanishes, and the first retardation contribution does not, are ξ_{32}, ξ_{23} and η_{23} (with $\eta_{23}^{(r)} = \xi_{23}^{(r)}$), η_{01}, η_{03}, ζ_{32} and ζ_{22}. In all there are seven independent nonvanishing first retardation terms in the dynamical parameters.

In Fig. 2 we show the four independent parameters $\xi_{31}, \xi_{22}, \eta_{02}, \zeta_{31}$, and also the parameter $\beta_{02}^{(d)}$ in the dipole approximation, for Z = 6, 10, 18, 26 and 36, and for photoelectron energies from threshold to 20 keV. Note the similar shapes of ξ_{22} and η_{02}, in agreement with formulas (B.7b) and (B.7c) in Appendix B. These are also the only dipole parameters having zeros in this energy region, corresponding to zeros of the phase shift difference Δ_{20} (c.f. also Kim, Goldberg and Pratt 1995). For Z = 6 the parameters ξ_{22} and η_{02} change sign once, and for the other atomic numbers they change sign twice. The parameters ξ_{31} and ζ_{31} are negative in the energy range; all four dynamical parameters in dipole approximation show, in general, a significant dependence on Z at given energy.

The seven independent retardation corrections to the dynamical parameters ξ, η, ζ, together with the cross section parameters $\beta_{01}^{(r)}$, $\beta_{03}^{(r)}$, are shown in Fig. 3. At low energies they are in general an order of magnitude smaller than the dipole contributions, but their values increase with increasing energy. For energies exceeding 1 keV the retardation corrections are of the order of 10^{-1}. At threshold $\xi_{32}^{(r)}$ and $\xi_{22}^{(r)}$ approach zero for all values of Z, while the remaining corrections to the dynamical parameters, i.e. $\xi_{23}^{(r)}$, $\eta_{01}^{(r)}$, $\eta_{03}^{(r)}$, $\zeta_{32}^{(r)}$ and $\zeta_{22}^{(r)}$, tend to zero for low values of Z (6, 10, 18), but do not vanish at threshold for higher atomic numbers.

The dynamical parameters were calculated using values of dipole and quadrupole radial matrix elements obtained from the numerical program PHOTO (Goldberg and Bergstrom, 1989). The same program calculates also, among other quantities, the dynamical parameters ξ, η, ζ, including as many multipoles as necessary at given value of energy. This allows us both to find the approximate (dipole + first retardation term) values of the dynamical parameters from formulas (4.28) and (4.29), and to compare them with exact values calculated numerically.

Table 2 contains comparison of our present results for the dynamical parameter ξ_{22} (the only one that has both dipole and first retardation contributions) with the exact values obtained numerically with the PHOTO-code. The comparison has been made for Z = 6 and Z = 36. The agreement is very good for low energies and low Z (Z = 6 in Table 3), and we can see that results which include both dipole and first retardation contributions compare much better with exact numerical values than those just from the dipole term, even at low energies. The agreement deteriorates with increasing energy, but the relative error does not exceed 10%. For higher atomic numbers (Z = 36 in Table 3) agreement between present calculations and exact numerical values is poorer than for Z = 6 in the whole energy rang. Including the first retardation contribution does not improve the agreement, indicating the importance of higher retardation corrections for higher atomic numbers.

6. Spin polarization of the photoelectron.

In this section we discuss consequences of the results of previous section for the spin and polarization correlations, using as examples transverse and longitudinal polarization of the photoelectron ejected by a circularly polarized photon from the $2p_{3/2}$ subshell.

The transverse polarization in the production plane of a photoelectron ejected by a circularly polarized photon (the Stokes parameters are $\xi_3 = 1,\ \xi_1 = \xi_2 = 0$) is given by[2]

$$P_1(\theta) = \frac{\sum_{\lambda\geq 1} \xi_{3\lambda} d^{\lambda}_{01}(\theta)}{F(\theta)}, \tag{6.1}$$

(cf. 4.20a and 4.21). In the dipole approximation this gives

$$P_1^{(d)}(\theta) = 2^{-1/2} \frac{\xi_{31}^{(d)} \sin\theta}{1 + B_2 P_2(\cos\theta)}, \tag{6.2}$$

and with the first retardation correction included

$$\begin{aligned} P_1^{(d+r)}(\theta) &= \frac{2^{-1/2}\xi_{31}^{(d)}\sin\theta + \frac{1}{2}(3/2)^{1/2}\xi_{32}^{(r)}\sin 2\theta}{1 - \frac{1}{2}\beta P_2(\cos\theta) + B_1 P_1(\cos\theta) + B_3 P_3(\cos\theta)} \approx \\ &\approx \frac{2^{-1/2}\xi_{31}^{(d)}\sin\theta}{1 - \frac{1}{2}\beta P_2(\cos\theta)}\left[1 - \frac{B_1 P_1(\cos\theta) + B_3 P_3(\cos\theta)}{1 - \frac{1}{2}\beta P_2(\cos\theta)}\right] + \frac{\frac{1}{2}(3/2)^{1/2}\xi_{32}^{(r)}\sin 2\theta}{1 - \frac{1}{2}\beta P_2(\cos\theta)}. \end{aligned} \tag{6.3}$$

In Fig. 4a we show plots of transverse polarization as function of the angle θ for Z = 26 and energies 3, 5, 10 and 20 keV, for which we may expect significant contributions from retardation. Deviations from the symmetric dipole angular dependence increase with increasing

[2] The symbols of the type $P_i(\theta)$, denoting the degree of polarisation, must not be confused with similarly looking symbols of the Legendre polynamials, appearing later in this section.

energy, and, in general, including the first retardation contribution gives quite satisfactory agreement with the results of exact numerical calculation (which include a sufficient number of multipoles at a given energy for convergence). An exception is the angle $\theta = \pi/2$, where the first retardation correction, proportional to $d^2_{01}(\theta) \propto \sin 2\theta$, vanishes, whereas the higher order terms in the multipole expansion contain contributions which are non-vanishing . Including the retardation correction removes the symmetry present in the $P_1(\theta)$ term around $\theta = \pi/2$, with the absolute values of polarizations increasing for forward, and decreasing for backward, angles. Depending on energy, $P_1(\theta)$ has two minima and one maximum (at lower energies), or one minimum and no maxima (at higher energies). This property can be qualitatively discussed in dipole approximation, where the θ-dependence of P_1 is given by a function of the type

$$P_1^{(d)}(\theta) = \frac{c \sin\theta}{a + b\cos^2\theta}. \tag{6.4}$$

Its derivative is

$$\frac{dP_1^{(d)}(\theta)}{d\theta} = c\cos\theta \frac{a + b\left(2 - \cos^2\theta\right)}{\left(a + b\cos^2\theta\right)^2}, \tag{6.5}$$

so that there is always an extremum for $\theta = \pi/2$. There will be two minima at $\theta \neq \pi/2$ (in which case the extremum at $\theta = \pi/2$ is a maximum), if the equation

$$\cos^2\theta = (a + 2b)/b \tag{6.6}$$

can be satisfied for some value of the angle θ. This depends on the values of the parameters $\xi_{31}^{(d)}$ and B_2, in terms of which a and b can be expressed.

The longitudinal polarization of the photoelectron ejected by a circularly polarized photon is described by formula (4.21c). For right-handed photon polarisation ($\xi_3 = 1$) we have

$$P_3(\theta) = \frac{\sum_{\lambda\geq 0} \zeta_{3\lambda} d^{\lambda}_{00}(\theta)}{1 + \sum_{\lambda\geq 1} \beta_{0\lambda} d^{\lambda}_{00}(\theta)}. \tag{6.7}$$

In the dipole approximation this gives

$$P_3^{(d)}(\theta) = \frac{\zeta_{31}^{(d)} P_1(\cos\theta)}{1 - \frac{1}{2}\beta P_2(\cos\theta)}, \tag{6.8}$$

and with the first retardation correction included

$$P_3^{(d+r)}(\theta) = \frac{\zeta_{31}^{(d)} P_1(\cos\theta) + \zeta_{32}^{(r)} P_2(\cos\theta)}{1 - \frac{1}{2}\beta P_2(\cos\theta) + B_1 P_1(\cos\theta) + B_3 P_3(\cos\theta)} \approx$$
$$\approx \frac{\zeta_{31}^{(d)} P_1(\cos\theta)}{1 - \frac{1}{2}\beta P_2(\cos\theta)} \left(1 - \frac{B_1 P_1(\cos\theta) + B_3 P_3(\cos\theta)}{1 - \frac{1}{2}\beta P_2(\cos\theta)}\right) + \frac{\zeta_{32}^{(r)} P_2(\cos\theta)}{1 - \frac{1}{2}\beta P_2(\cos\theta)} \quad . \tag{6.9}$$

Plots of the longitudinal polarization for Z = 26 as a function of the angle θ are shown in Fig. 4b. Again, deviations from the dipole approximation increase with increasing energy, and the beyond dipole contributions lead to a forward-backward asymmetry. The present approximate results (dipole and dipole with first retardation correction) satisfy, independent of energy, the properties

$$P_3(0) = -\tfrac{1}{2}, \qquad P_3(\pi) = \tfrac{1}{2}, \tag{6.10}$$

which follow from [cf. (4.9), (B.7d), (4.11) and (B.8f)]

$$1 - \frac{1}{2}\beta = -2\zeta_{31}^{(d)}, \qquad B_1 + B_3 = -2\zeta_{32}^{(r)}, \tag{6.11}$$

and from $P_\lambda(\pm 1) = (\pm 1)^\lambda$. It should be noted that (6.10) is not generally valid. The point is that the summation in the numerator of (6.7) starts from a term with $\lambda = 0$, which is independent of the angle, and it is only in the present approximation that $\zeta_{30} = 0$. Exact numerical calculations, including more multipoles and taking relativistic effects into account, show that $\zeta_{30} \neq 0$ and is of order 10^{-4} for $E = 3\,keV$, 10^{-2} for $E = 20\,keV$, giving increasing contributions with increasing energy. This is clearly visible at higher energies, where deviations of the exact numerical results from (6.10) can be noted. In general, the agreement between present calculation and exact numerical results is very good for lower energies, and at higher energies it is better for forward than for backward angles, where the deviation of the exact result from (6.10) is larger.

7. Final remarks

We have investigated in this paper higher multipole and retardation corrections to the spin and polarization correlations between incident photons and photoelectrons ejected from the $2p_J$ subshell. We used the nonrelativistic Pauli - Schrödinger approach and included the first term beyond nonrelativistic dipole approximation, describing the first retardation correction and corresponding to the long - wavelength limit of the electric quadrupole contribution. The spin correlations in the angular distributions of the photoelectrons, spin polarized in general, were described in terms of the correlation coefficients C_{ij}, depending on the momentum of the outgoing electron. An alternative description is given by expansions of the C_{ij} in a series of rotation group matrix elements, with series expansion coefficients called dynamical parameters. Relations between both types of description of the spin and polarization effects have been given.

In general, numerical values of the dynamical parameters obtained with the use of our formulas compare well with exact numerical calculations for Z = 6 - 36 in the energy range from close to threshold to a few keV. Including the retardation correction improves the agreement considerably as compared to the pure dipole results, for lower energies and lower values of Z.

The agreement deteriorates in the vicinity of energies for which the dynamical parameters go through zero and have very small values. Our formulas also lead to good agreement with exact numerical results for angular distributions of polarized photoelectrons.

The calculations presented in this paper were performed in the independent particle approximation, which is argued to give a useful first approximation except for energies close to threshold. Further work is desirable to confirm accuracy of this approximation.

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Appendix A

A1. Summation formulas for spherical spinors

The summation formulas for spherical spinors, analogous to the well known summation formulas for spherical harmonics, have the general form (Bechler 1993)

$$\sum_M \Omega_{JLM}(\hat{\mathbf{a}})\Omega^\dagger_{JLM}(\hat{\mathbf{b}}) = \frac{L}{4\pi} P_L(\hat{\mathbf{a}}\cdot\hat{\mathbf{b}}) + \frac{i}{4\pi} P'_L(\hat{\mathbf{a}}\cdot\hat{\mathbf{b}})(\hat{\mathbf{a}}\times\hat{\mathbf{b}})\cdot\boldsymbol{\sigma}, \tag{A.1}$$

for $J = L - 1/2$, and

$$\sum_M \Omega_{JLM}(\hat{\mathbf{a}})\Omega^\dagger_{JLM}(\hat{\mathbf{b}}) = \frac{L+1}{4\pi} P_L(\hat{\mathbf{a}}\cdot\hat{\mathbf{b}}) - \frac{i}{4\pi} P'_L(\hat{\mathbf{a}}\cdot\hat{\mathbf{b}})(\hat{\mathbf{a}}\times\hat{\mathbf{b}})\cdot\boldsymbol{\sigma}, \tag{A.2}$$

for $J = L + 1/2$. $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$ are unit vectors and $\boldsymbol{\sigma}$ the Pauli matrices. P_L denote the Legendre polynomials and P'_L the derivatives of the Legendre polynomials with respect to their arguments. For $p_{1/2}$ and $p_{3/2}$ cases we obtain from (A.1) and (A.2) respectively

$$\sum_M \Omega_{\frac{1}{2}1M}(\hat{\mathbf{a}})\Omega^\dagger_{\frac{1}{2}1M}(\hat{\mathbf{b}}) = \frac{1}{4\pi}\hat{\mathbf{a}}\cdot\hat{\mathbf{b}} + \frac{i}{4\pi}(\hat{\mathbf{a}}\times\hat{\mathbf{b}})\cdot\boldsymbol{\sigma}, \tag{A.3}$$

and

$$\sum_M \Omega_{\frac{3}{2}1M}(\hat{\mathbf{a}})\Omega^\dagger_{\frac{3}{2}1M}(\hat{\mathbf{b}}) = \frac{1}{2\pi}\hat{\mathbf{a}}\cdot\hat{\mathbf{b}} - \frac{i}{4\pi}(\hat{\mathbf{a}}\times\hat{\mathbf{b}})\cdot\boldsymbol{\sigma}. \tag{A.4}$$

A2. Auxiliary formulas.

The transition probability $\left|M_{fi}\right|^2$ has been calculated from (4.2) with the use of (3.12), (4.4) . It has been written in the final form (4.3) with the spin and polarization correlation coefficients given by (4.14) and (4.15). To express the transition probability in terms of the Stokes parameters ξ_i, photoelectron spin components ζ_i and the angle θ (Fig. 1) it is necessary to use the formulas relating invariants constructed from $\boldsymbol{\varepsilon}$ (the photon polarization vector), $\boldsymbol{\zeta}$ (electron spin), $\hat{\mathbf{p}}$ (electron direction) and $\hat{\mathbf{k}}$ (photon direction) to Stokes parameters, and the emission angle θ. These are

$$|\boldsymbol{\varepsilon}\cdot\hat{\mathbf{p}}|^2 = \frac{1}{2}(1+\xi_1)\sin^2\theta \tag{A.5}$$

$$\boldsymbol{\zeta}\cdot(\boldsymbol{\varepsilon}\times\boldsymbol{\varepsilon}^*) = i\xi_3(\zeta_1\sin\theta-\zeta_3\cos\theta) \tag{A.6}$$

$$(\boldsymbol{\varepsilon}^*\cdot\hat{\mathbf{p}})[\boldsymbol{\zeta}\cdot(\boldsymbol{\varepsilon}\times\hat{\mathbf{p}})] = -\frac{1}{2}(1+\xi_1)\zeta_2\sin\theta\cos\theta+\frac{1}{2}(\xi_2+i\xi_3)\zeta_1\sin\theta \tag{A.7}$$

$$(\boldsymbol{\varepsilon}^*\cdot\hat{\mathbf{p}})\left[\boldsymbol{\zeta}\cdot\left(\boldsymbol{\varepsilon}\times\hat{\mathbf{k}}\right)\right] = -\frac{1}{2}(1+\xi_1)\zeta_2\sin\theta+\frac{1}{2}(\xi_2+i\xi_3)\zeta_1\sin\theta\cos\theta+\frac{1}{2}(\xi_2+i\xi_3)\zeta_3\sin^2\theta \tag{A.8}$$

$$|\boldsymbol{\varepsilon}\cdot\hat{\mathbf{p}}|^2\left[\boldsymbol{\zeta}\cdot\left(\hat{\mathbf{p}}\times\hat{\mathbf{k}}\right)\right] = -\frac{1}{2}(1+\xi_1)\zeta_2\sin^3\theta \tag{A.9}$$

A3. Derivation of the correlation coefficients.

To outline the derivation of (4.14) and (4.15) we note that (4.2) give, after summation over initial magnetic substates (c.f. sections A1 and A2 of this Appendix);

$$\sum_M\left|M_{fi}\right|^2 \propto \left(D_0^2+2D_2^2\right)\sum_{i,j}c_{ij}\xi_i\zeta_j\,, \tag{A.10}$$

where the factor $D_0^2+2D_2^2$ has been extracted for later convenience. The differential cross-section for the emission of a polarized electron by a polarized photon has the form

$$\frac{d\sigma}{d\Omega}(\boldsymbol{\xi},\boldsymbol{\zeta}) = \frac{A}{2J+1}\left(D_0^2+2D_2^2\right)\sum_{ij}c_{ij}\xi_i\zeta_j\,, \tag{A.11}$$

where A is a kinematical factor. To obtain the unpolarized differential cross-section we average over incident photon polarizations and sum over spin states of the final electron:

, $$\left(\frac{d\sigma}{d\Omega}\right)_{unpol} = \frac{2A}{2J+1}\left(D_0^2+2D_2^2\right)c_{00}\,. \tag{A.12}$$

Explicit calculation, based on (A.10) and formulae of section A2, gives

$$c_{00}(\theta) = g(\theta) = 1 - \frac{1}{2}\beta P_2(\cos\theta) + B_1 P_1(\cos\theta) + B_3 P_3(\cos\theta), \tag{A.13}$$

in agreement with (4.8). The total cross-section can be now easily calculated as

$$\sigma = \int \left(\frac{d\sigma}{d\Omega}\right)_{unpol} d\Omega = \frac{8\pi A}{2J+1}\left(D_0^{\ 2} + 2D_2^{\ 2}\right), \tag{A.14}$$

so that

$$\left(\frac{d\sigma}{d\Omega}\right)_{unpol} = \frac{\sigma}{4\pi} g(\theta), \tag{A.15}$$

and formula (A.11) can be written as

$$\frac{d\sigma}{d\Omega}(\xi,\zeta) = \left(\frac{d\sigma}{d\Omega}\right)_{unpol} \frac{1}{2}\sum_{i,j=0}^{3} C_{ij}\xi_i\zeta_j\,, \tag{A.16}$$

with $C_{ij}(\theta) = c_{ij}(\theta)/g(\theta)$, $C_{00} = 1$ and $\xi_0 = \zeta_0 = 1$, in agreement with (1.1) and (4.3).

To obtain formulae (4.14) and (4.15) for the dipole and dipole plus first retardation approximations to the coefficients $c_{ij}(\theta)$, one has to identify terms containing products of the type $\xi_i\zeta_j$ (including $\xi_0 = 1$ and $\zeta_0 = 1$) in the first and second term of (4.2) respectively, using formulas of A2.

A4. Rotation group matrix elements.

Expressions for the rotation group matrix elements were found with the use of general formulae quoted in Huang (1980) (Eqs 4.24 and 4.25 in that paper):

$$d^2_{20}(\theta) = \frac{1}{2}\left(\frac{3}{2}\right)^{1/2}\sin^2\theta,\ \ d^3_{20}(\theta) = \frac{1}{2}\left(\frac{15}{2}\right)^{1/2}\sin^2\theta\cos\theta,\ d^4_{20}(\theta) = \frac{1}{8}\left(\frac{5}{2}\right)^{1/2}(7\cos 2\theta + 5)\sin^2\theta,$$

$$d^1_{01}(\theta) = \left(\frac{1}{2}\right)^{1/2}\sin\theta,\ \ d^2_{01}(\theta) = \frac{1}{2}\left(\frac{3}{2}\right)^{1/2}\sin 2\theta,\ \ d^3_{01}(\theta) = \frac{3^{1/2}}{8}(5\cos 2\theta + 3)\sin\theta,$$

$$d^2_{21}(\theta) = -2\cos^3(\theta/2)\sin(\theta/2),\ \ d^3_{21}(\theta) = -\frac{1}{2}\left(\frac{5}{2}\right)^{1/2}\cos^3(\theta/2)\left[-5\sin(\theta/2) + 3\sin(3\theta/2)\right],$$

$$d^2_{2-1}(\theta) = -2\cos(\theta/2)\sin^3(\theta/2),\ \ d^3_{2-1}(\theta) = -\frac{1}{2}\left(\frac{5}{2}\right)^{1/2}\sin^3(\theta/2)\left[5\cos(\theta/2) + 3\cos(3\theta/2)\right].$$

Appendix B

To find a relation between (4.20), (4.21) and (4.19), and explicit expressions for the dynamical parameters, we use (4.7) and (4.13), from which it follows that

$$P_1(\theta)[g(\theta)+\xi_1 c_{10}(\theta)] = \xi_2 c_{21}(\theta)+\xi_3 c_{31}(\theta), \tag{B.1a}$$

$$P_2(\theta)[g(\theta)+\xi_1 c_{10}(\theta)] = c_{02}(\theta)+\xi_1 c_{12}(\theta), \tag{B.1b}$$

$$P_3(\theta)[g(\theta)+\xi_1 c_{10}(\theta)] = \xi_2 c_{23}(\theta)+\xi_3 c_{33}(\theta), \tag{B.1c}$$

so that

$$F(\theta) = g(\theta)+\xi_1 c_{10}(\theta), \tag{B.2}$$

and

$$c_{10} = -\sum_{l\geq 2} \beta_{1l} d^l_{20}, \tag{B.3a}$$

$$c_{21} = \sum_{l\geq 2}\left(\xi_{2l} d^l_{21} + \eta_{2l} d^l_{2-1}\right), \tag{B.3b}$$

$$c_{31} = \sum_{l\geq 1} \xi_{3l} d^l_{01}, \tag{B.3c}$$

$$c_{02} = \sum_{l\geq 1} \eta_{0l} d^l_{01}, \tag{B.3d}$$

$$c_{12} = -\sum_{l\geq 2}\left(\xi_{2l} d^l_{21} - \eta_{2l} d^l_{2-1}\right), \tag{B.3e}$$

$$c_{23} = \sum_{l\geq 2} \zeta_{2l} d^l_{20}, \tag{B.3f}$$

$$c_{33} = \sum_{l\geq 0} \zeta_{3l} d^l_{00}. \tag{B.3g}$$

The function

$$g(\theta) = 1 + \sum_{l\geq 1} \beta_{0l} d^l_{00}, \tag{B.4}$$

so that, according to (4.8)

$$\beta^{(d)}_{02} = -(1/2)\beta,\ \beta^{(d)}_{01} = B_1,\ \beta^{(d)}_{03} = B_3. \tag{B.5}$$

Comparing (B.3a) with (4.14a) and (4.15a), and using the explicit expressions for the rotation group matrix elements d^{λ}_{20}, given in Appendix A, we obtain

$$\beta^{(d)}_{12} = 6^{1/2} B_2 , \quad \beta^{(d)}_{13} = (10/3)^{1/2} B_3 . \tag{B.6}$$

Formulas (B.5) and (B.6) give the only cross section coefficients $\beta_{0\lambda}$ and $\beta_{1\lambda}$ that do not vanish in the present approximation.

Expressing (4.14 b-f) and (4.15 b-f) in terms of the rotation group matrix elements, and comparing with (B.3 b-g), we can obtain explicit expressions for the dynamical parameters $\xi_{3\lambda}$, $\xi_{2\lambda}$, $\eta_{2\lambda}$, $\eta_{0\lambda}$, $\zeta_{3\lambda}$, $\zeta_{2\lambda}$. Table 1 shows non-vanishing dipole and first retardation contributions to the dynamical parameters. The dipole contributions to the dynamical parameters for the $p_{1/2}$ initial subshell are

$$\xi^{(d)}_{31} = -2^{1/2} \frac{D_0{}^2 - 2D_2{}^2 - D_0 D_2 \cos\Delta_{20}}{D_0{}^2 + 2D_2{}^2} , \tag{B.7a}$$

$$\xi^{(d)}_{22} = \eta^{(d)}_{22} = 3 \frac{D_0 D_2 \sin\Delta_{20}}{D_0{}^2 + 2D_2{}^2} , \tag{B.7b}$$

$$\eta^{(d)}_{02} = 6^{1/2} \frac{D_0 D_2 \sin\Delta_{20}}{D_0{}^2 + 2D_2{}^2} , \tag{B.7c}$$

$$\zeta^{(d)}_{31} = \frac{D_0{}^2 + D_2{}^2 + 2D_0 D_2 \cos\Delta_{20}}{D_0{}^2 + 2D_2{}^2} .$$

(B.7d)

First retardation corrections to the dynamical parameters are given by

$$\xi^{(r)}_{32} = 6^{1/2} k \frac{-\frac{3}{10} F_{01} + \frac{1}{2} F_{23} + \frac{1}{5} F_{03}}{D_0{}^2 + 2D_2{}^2} , \tag{B.8a}$$

$$\xi^{(r)}_{22} = -\eta^{(r)}_{22} = 3k \frac{-\frac{1}{10} G_{01} + \frac{1}{15} G_{03} + \frac{1}{6} G_{23}}{D_0{}^2 + 2D_2{}^2} , \tag{B.8b}$$

$$\xi^{(r)}_{23} = \eta^{(r)}_{23} = 3\left(\frac{2}{5}\right)^{1/2} k \frac{\frac{1}{3} G_{03} + \frac{2}{5} G_{21} - \frac{1}{15} G_{23}}{D_0{}^2 + 2D_2{}^2} , \tag{B.8c}$$

$$\eta^{(r)}_{01} = 3 \cdot 2^{1/2} k \frac{-\frac{1}{10} G_{01} - \frac{2}{25} G_{21} - \frac{9}{50} G_{23}}{D_0{}^2 + 2D_2{}^2} , \tag{B.8d}$$

$$\eta_{03}^{(r)} = \frac{4 \cdot 3^{1/2}}{5} k \frac{\frac{1}{2} G_{03} - \frac{3}{5} G_{21} - \frac{1}{10} G_{23}}{D_0^{\ 2} + 2 D_2^{\ 2}}, \tag{B.8e}$$

$$\zeta_{32}^{(r)} = \frac{3}{5} k \frac{F_{01} + F_{03} + F_{21} + F_{23}}{D_0^{\ 2} + 2 D_2^{\ 2}}, \tag{B.8f}$$

$$\zeta_{22}^{(r)} = 3 \cdot \frac{6^{1/2}}{5} k \frac{G_{01} + G_{03} - G_{21} + G_{23}}{D_0^{\ 2} + 2 D_2^{\ 2}}, \tag{B.8g}$$

where $F_{\lambda\lambda'}$ are defined by (4.12) and $G_{\lambda\lambda'}$ by (4.16). It follows from (4.6) and (B.3a) and (B.4) that for the $p_{3/2}$ subshell

$$\beta_{0l}(p_{3/2}) = \beta_{0l}(p_{1/2}), \quad \beta_{1l}(p_{3/2}) = \beta_{1l}(p_{1/2}), \tag{B.9}$$

while from (4.6) and (B.3 b - g) we have

$$Z(p_{3/2}) = -\frac{1}{2} Z(p_{1/2}), \tag{B.10}$$

where Z denotes any of the coefficients ξ, η, ζ.

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Table 1

Non vanishing dipole and first retardation contributions to the dynamical parameters

	$\beta_{0\lambda}$	$\beta_{1\lambda}$	$\xi_{3\lambda}$	$\xi_{2\lambda}$	$\eta_{2\lambda}$	$\eta_{0\lambda}$	$\zeta_{3\lambda}$	$\zeta_{2\lambda}$

λ (dipole)	2	2	1	2	2	2	1	-
λ (retardation)	1, 3	3	2	2, 3	2, 3	1, 3	2	2

Table 2

Comparison of the dipole, dipole with retardation and exact results for ξ_{22}

Z = 6

Energy (keV)	dipole (present calculation)	retardation correction (present calculation)	dipole plus retardation	exact	Relative error %	Relative error for dipole (%)
	a		b	c	Ib-cI/IcI	Ia-cI/IcI
$1.0\ 10^{-4}$	$-9.861\ 10^{-2}$	$9.647\ 10^{-4}$	$-9.764\ 10^{-2}$	$-9.757\ 10^{-2}$	$7.3\ 10^{-2}$	$1.1\ 10^{0}$
$1.0\ 10^{-3}$	$-2.072\ 10^{-1}$	$9.179\ 10^{-4}$	$-2.063\ 10^{-1}$	$-2.063\ 10^{-1}$	$1.1\ 10^{-2}$	$4.6\ 10^{-1}$
$5.0\ 10^{-3}$	$-2.258\ 10^{-1}$	$8.073\ 10^{-4}$	$-2.250\ 10^{-1}$	$-2.250\ 10^{-1}$	$2.1\ 10^{-2}$	$3.4\ 10^{-1}$
$1.0\ 10^{-2}$	$-1.764\ 10^{-1}$	$9.007\ 10^{-4}$	$-1.755\ 10^{-1}$	$-1.755\ 10^{-1}$	$1.7\ 10^{-2}$	$5.3\ 10^{-1}$
$5.0\ 10^{-2}$	$7.179\ 10^{-2}$	$3.273\ 10^{-3}$	$7.506\ 10^{-2}$	$7.493\ 10^{-2}$	$1.7\ 10^{-1}$	$4.2\ 10^{0}$
$1.0\ 10^{-1}$	$1.954\ 10^{-1}$	$3.273\ 10^{-3}$	$1.987\ 10^{-1}$	$2.007\ 10^{-1}$	$1.0\ 10^{0}$	$2.6\ 10^{0}$
$2.0\ 10^{-1}$	$2.808\ 10^{-1}$	$7.995\ 10^{-3}$	$2.888\ 10^{-1}$	$2.889\ 10^{-1}$	$2.6\ 10^{-2}$	$2.8\ 10^{0}$
$5.0\ 10^{-1}$	$2.961\ 10^{-1}$	$1.220\ 10^{-2}$	$3.083\ 10^{-1}$	$3.079\ 10^{-1}$	$1.2\ 10^{-1}$	$3.8\ 10^{0}$
$1.0\ 10^{0}$	$2.544\ 10^{-1}$	$1.552\ 10^{-2}$	$2.699\ 10^{-1}$	$2.687\ 10^{-1}$	$4.4\ 10^{-1}$	$5.3\ 10^{0}$
$2.0\ 10^{0}$	$2.155\ 10^{-1}$	$1.922\ 10^{-2}$	$2.347\ 10^{-1}$	$2.324\ 10^{-1}$	$9.9\ 10^{-1}$	$7.3\ 10^{0}$
$3.0\ 10^{0}$	$1.890\ 10^{-1}$	$1.943\ 10^{-2}$	$2.084\ 10^{-1}$	$2.057\ 10^{-1}$	$1.3\ 10^{0}$	$8.1\ 10^{0}$
$5.0\ 10^{0}$	$1.501\ 10^{-1}$	$2.047\ 10^{-2}$	$1.706\ 10^{-1}$	$1.657\ 10^{-1}$	$2.9\ 10^{0}$	$9.4\ 10^{0}$
$1.0\ 10^{+1}$	$1.182\ 10^{-1}$	$2.097\ 10^{-2}$	$1.392\ 10^{-1}$	$1.290\ 10^{-1}$	$7.9\ 10^{0}$	$8.4\ 10^{0}$
$2.0\ 10^{+1}$	$8.232\ 10^{-2}$	$2.268\ 10^{-2}$	$1.050\ 10^{-1}$	$9.894\ 10^{-2}$	$6.1\ 10^{0}$	$1.7\ 10^{+1}$

Z = 36

$1.0\ 10^{-4}$	$1.164\ 10^{-1}$	$3.308\ 10^{-4}$	$1.167\ 10^{-1}$	$1.142\ 10^{-1}$	$2.2\ 10^{0}$	$1.9\ 10^{0}$
$1.0\ 10^{-3}$	$1.820\ 10^{-1}$	$4.334\ 10^{-4}$	$1.824\ 10^{-1}$	$1.801\ 10^{-1}$	$1.3\ 10^{0}$	$1.0\ 10^{0}$
$5.0\ 10^{-3}$	$1.101\ 10^{-1}$	$2.435\ 10^{-4}$	$1.104\ 10^{-1}$	$1.067\ 10^{-1}$	$3.4\ 10^{0}$	$3.2\ 10^{0}$
$1.0\ 10^{-2}$	$1.925\ 10^{-2}$	6.997 10-05	$1.932\ 10^{-2}$	$1.565\ 10^{-2}$	$2.3\ 10^{+1}$	$2.3\ 10^{+1}$

$5.0\ 10^{-2}$	$-1.469\ 10^{-1}$	3.048 10-05	$-1.468\ 10^{-1}$	$-1.515\ 10^{-1}$	$3.1\ 10^{0}$	$3.1\ 10^{0}$
$1.0\ 10^{-1}$	$-1.673\ 10^{-1}$	$4.056\ 10^{-3}$	$-1.633\ 10^{-1}$	$-1.690\ 10^{-1}$	$3.4\ 10^{0}$	$9.9\ 10^{-1}$
$2.0\ 10^{-1}$	$-1.528\ 10^{-1}$	$1.154\ 10^{-2}$	$-1.413\ 10^{-1}$	$-1.481\ 10^{-1}$	$4.6\ 10^{0}$	$3.2\ 10^{0}$
$5.0\ 10^{-1}$	$-8.875\ 10^{-2}$	$2.251\ 10^{-2}$	$-6.624\ 10^{-2}$	$-7.187\ 10^{-2}$	$7.8\ 10^{0}$	$2.3\ 10^{+1}$
$1.0\ 10^{0}$	$-6.789\ 10^{-3}$	$3.064\ 10^{-2}$	$2.385\ 10^{-2}$	$1.519\ 10^{-1}$	$8.4\ 10^{+1}$	$1.0\ 10^{+2}$
$2.0\ 10^{0}$	$8.740\ 10^{-2}$	$4.001\ 10^{-2}$	$1.274\ 10^{-1}$	$1.175\ 10^{-1}$	$8.4\ 10^{0}$	$2.6\ 10^{+1}$
$3.0\ 10^{0}$	$1.416\ 10^{-1}$	$4.616\ 10^{-2}$	$1.877\ 10^{-1}$	$1.796\ 10^{-1}$	$4.5\ 10^{0}$	$2.1\ 10^{+1}$
$5.0\ 10^{0}$	$2.087\ 10^{-1}$	$5.640\ 10^{-2}$	$2.651\ 10^{-1}$	$2.539\ 10^{-1}$	$4.4\ 10^{0}$	$1.8\ 10^{+1}$
$1.0\ 10^{+1}$	$2.793\ 10^{-1}$	$7.402\ 10^{-2}$	$3.533\ 10^{-1}$	$3.326\ 10^{-1}$	$6.2\ 10^{0}$	$1.6\ 10^{+1}$
$2.0\ 10^{+1}$	$3.140\ 10^{-1}$	$9.492\ 10^{-2}$	$4.089\ 10^{-1}$	$3.676\ 10^{-1}$	$1.1\ 10^{+1}$	$1.5\ 10^{0}$

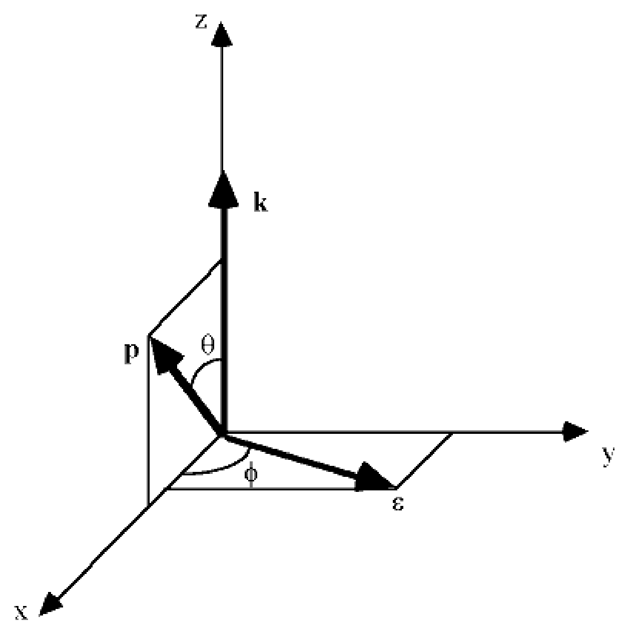
Figure captions

Fig. 1 Coordinate systems used for the description of spin and polarization correlations.

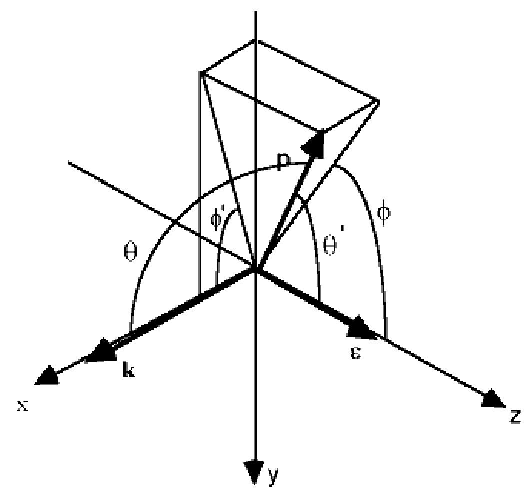
Fig. 2 Plots of four independent, non-vanishing dynamical parameters, and the cross section parameter $\beta_{02}^{(d)}$, in the dipole approximation versus photoelectron energy for Z = 6 ———— , Z = 10 ---------------- , Z = 18 – – – – – – – , Z = 26 — - — - — - — , and Z = 36 — - - — - - — - -

Fig. 3 First retardation contributions to the dynamical parameters, and the cross section parameters $\beta_{01}^{(r)}$, $\beta_{03}^{(r)}$ versus photoelectron energy for the same values of Z as in Fig. 3.

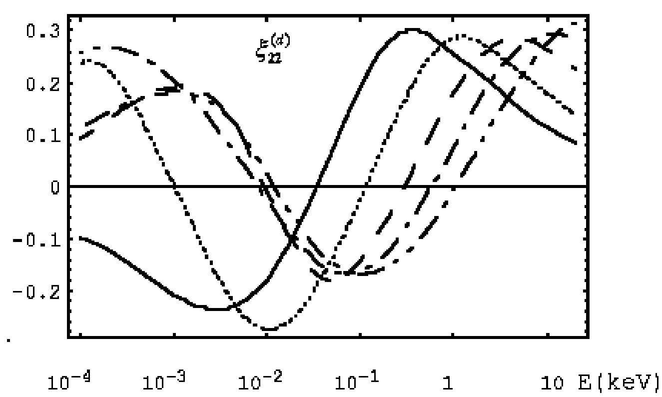
Fig. 4 Transverse (a) and longitudinal (b) polarizations of the $2p_{3/2}$ photoelectron ejected by circularly polarized photon from Iron (Z = 26), as functions of the angle between electron and photon momenta.



1a



1b



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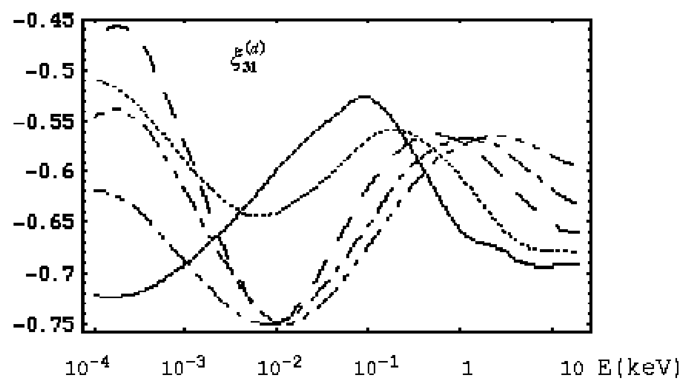

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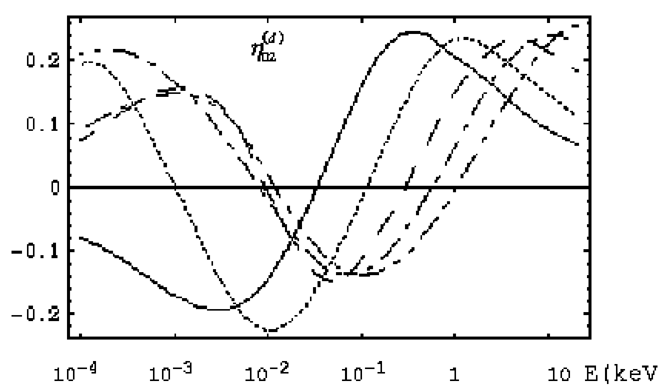
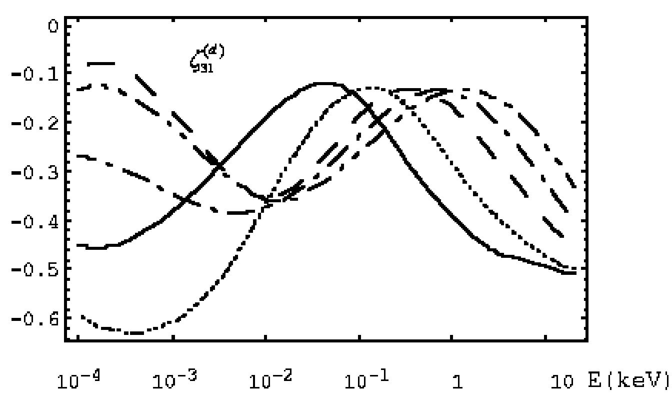
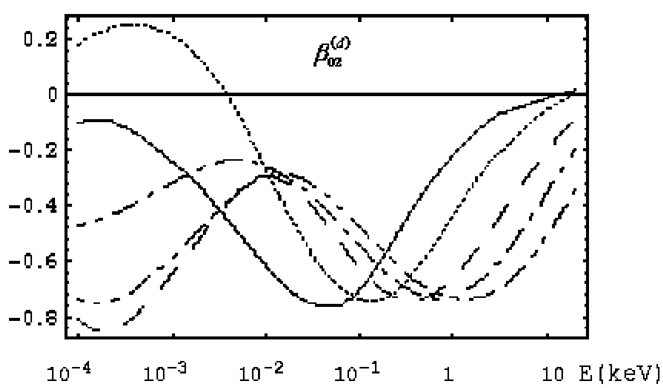


2c



2d



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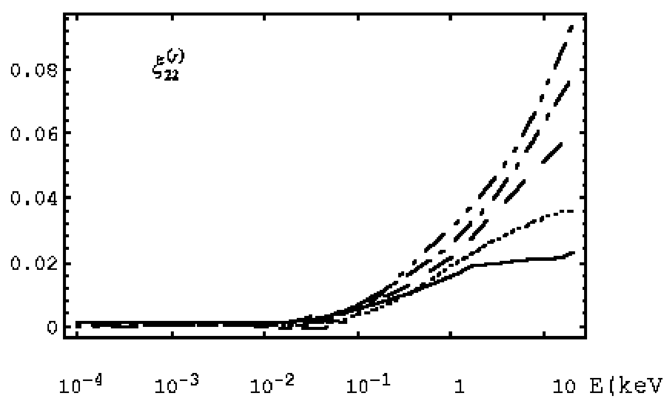
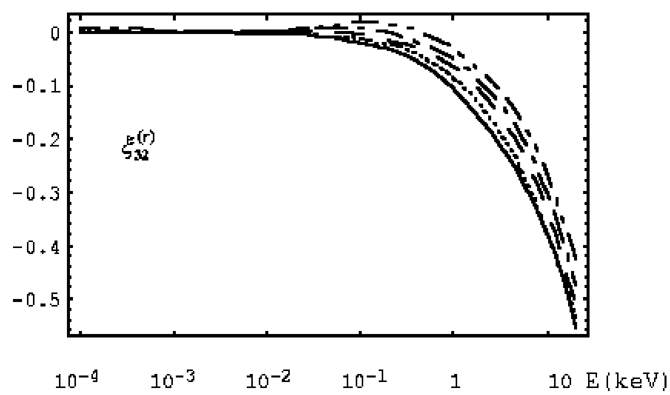
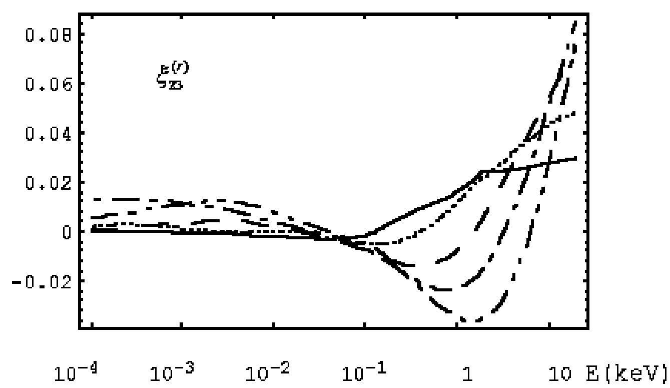


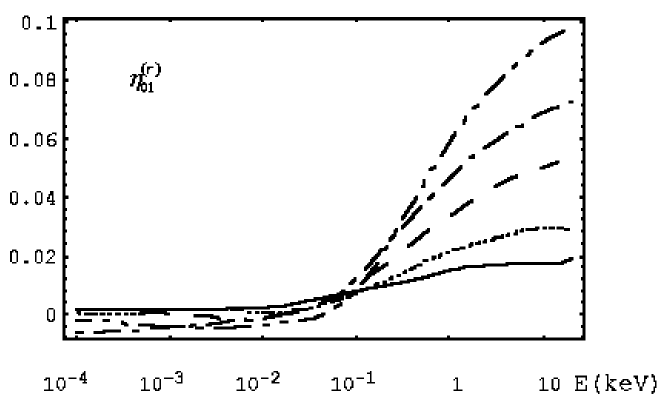
3a



3b



3c



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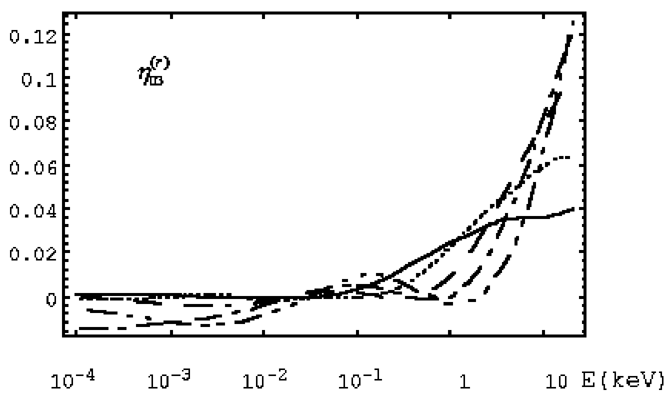

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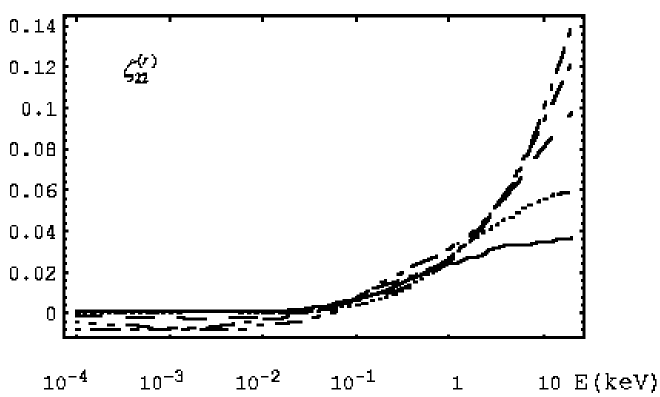

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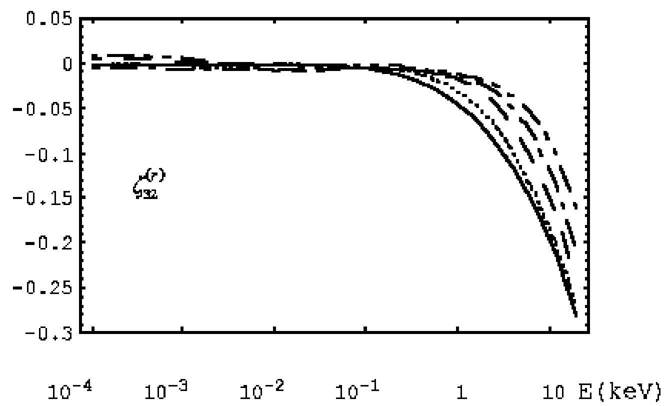

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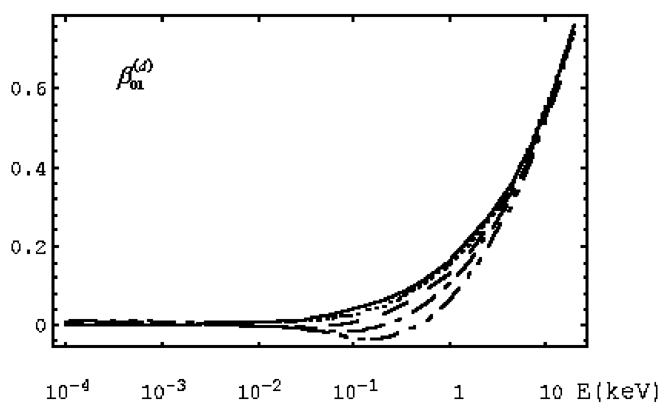

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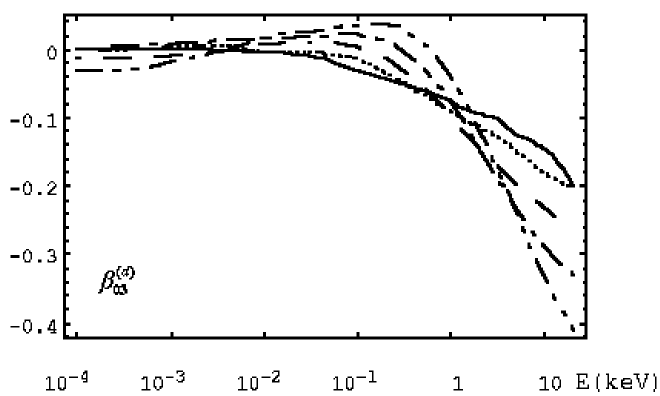

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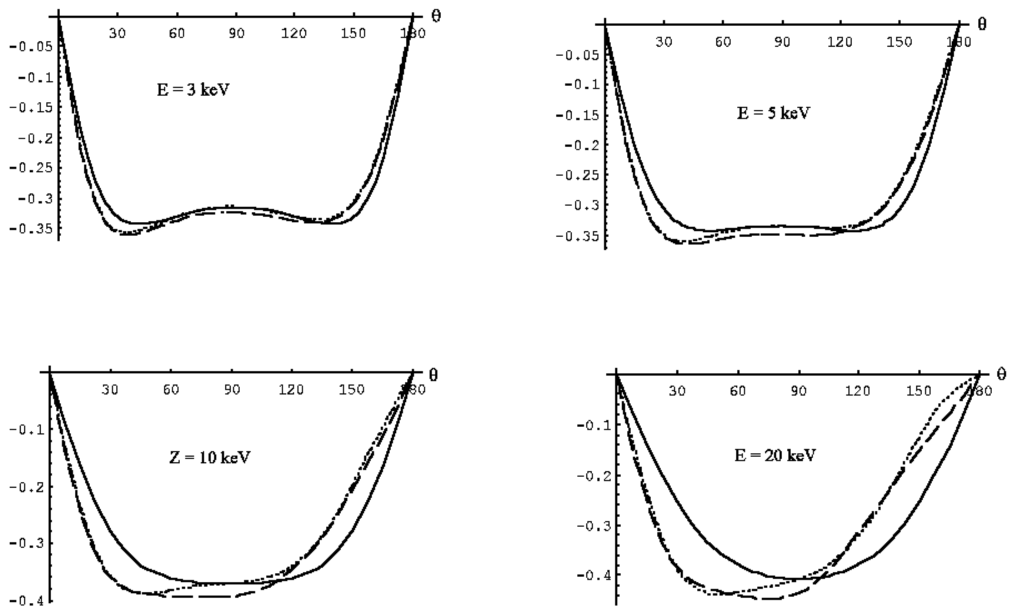
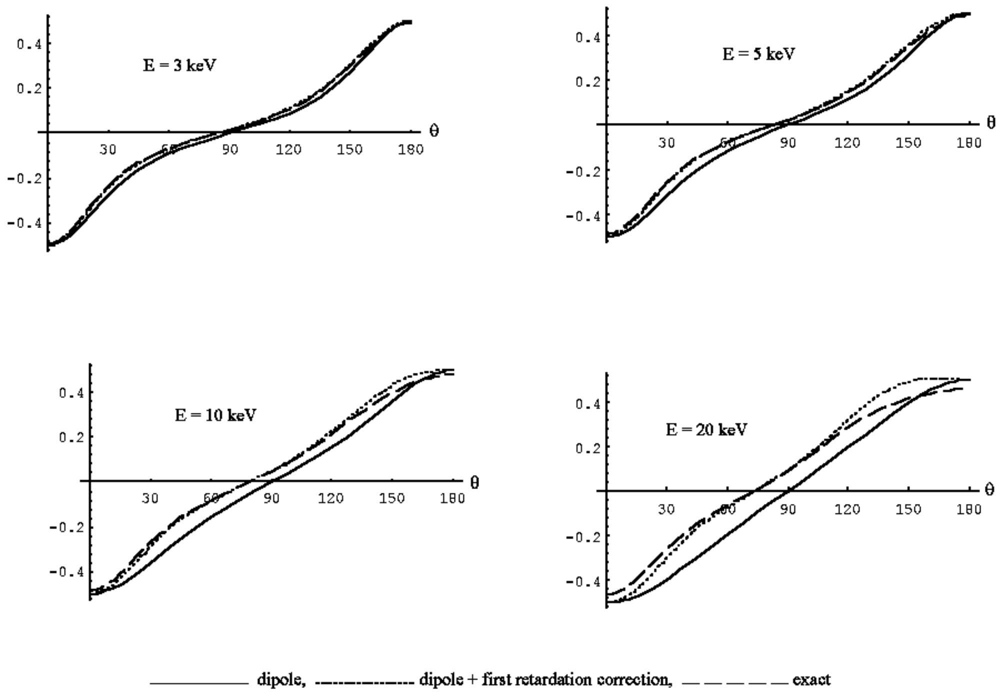


θ
30
60
90
120
150
180
-0.05
-0.1
-0.15
-0.2
-0.25
-0.3
-0.35
E = 3 keV
E = 5 keV
-0.4
Z = 10 keV
E = 20 keV

4a


E = 3 keV
E = 5 keV
E = 10 keV
E = 20 keV
θ
0.4
0.2
-0.2
-0.4
30
60
90
120
150
180
dipole,
dipole + first retardation correction,
exact

4b