Higher retardation and multipole corrections to the dipole angular distribution of 1s photoelectrons at low energies

A. Bechler* and R. H. Pratt
Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260
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We perform a nonrelativistic calculation of the first retardation and multipole corrections to the dipole angular distribution of 1s photoelectrons from light elements. A simple formula for this correction is obtained which compares well with the results of exact relativistic numerical calculations, for $Z \lesssim 40$ and final electron energies between 1 eV and 2 keV. These effects are small for the lightest Z, but their magnitude in general increases with increasing Z, reaching as much as 0.2–0.3 for $Z = 20$–30. The correction can change signs one or more times. The relatively large values of the first retardation-multipole correction to the $\sin^2\theta$ dipole angular distribution results in some tendency towards forward or backward peaking of the final electron angular distribution with respect to the direction of the incident photon.

I. INTRODUCTION

We present results of a calculation of the first retardation correction to the dipole angular distribution of 1s photoelectrons, for low-energy final electrons (1 eV–1 keV), in the framework of the independent-particle model. We understand the first retardation correction to be a contribution to the photoeffect amplitude corresponding to the term linear in $\mathbf{k}\cdot\mathbf{r}$ in the expansion of the photon plane wave. Replacing $\exp(i\mathbf{k}\cdot\mathbf{r})$ by unity gives, as is well known, the dipole approximation in the standard form.

It has been shown previously[1–3] that, contrary to common belief,[4] deviation from the dipole shape of the photoelectron angular distribution may persist down to threshold, especially for higher-Z elements. We find, as we discuss in this paper, that the magnitude of the first retardation correction is determined basically by a product of three factors. One of these is n_2/n_1, where n_l is the ratio of screened to point-Coulomb continuum normalization of the lth partial wave, in this case the d and p waves. Second is the cosine of the d- and p-wave phase-shift difference, $\cos(\delta_2-\delta_1)$; the third factor is $Z\alpha$. The retardation effect persists down to threshold when neither of the first two factors is small at small energies. On the other hand, the first retardation correction will be small at threshold when either $n_2/n_1 \ll 1$,[5] or $(\delta_2-\delta_1)\approx\pi/2$ (as in the Coulomb case, where $\delta_2-\delta_1\rightarrow-\pi/2$ at threshold).

Retardation corrections to the angular distribution of 1s photoelectrons in the point Coulomb case can be obtained from a formula derived long ago by Fisher[6] (cf. also Ref. 1),

$$\frac{d\sigma}{d\Omega} = A\sin^2\theta\left[1-\frac{2\mathbf{p}\cdot\mathbf{k}}{Z^2\alpha^2+\bar{p}^2}\right]^{-4}, \tag{1}$$

where $\mathbf{k}$ and $\mathbf{p}$ are, respectively, the incident photon and outgoing electron momenta, θ is the angle between $\mathbf{p}$ and $\mathbf{k}$, and A is independent of the angle θ [throughout the paper we use atomic units ($m_e=\hbar=c=1$)]. From conservation of energy we have $2pk/(Z^2\alpha^2+p^2)=v/c$, so that the first retardation correction describing deviations from the $\sin^2\theta$ dipole angular distribution is $\sim 4(v/c)\cos\theta$. The coefficient $4(v/c)$ is small ($\lesssim 0.1$) for most of the energies in the region considered in this paper and, of course, goes to zero at threshold.

This may be contrasted with the estimate obtained looking at the values of $\mathbf{k}\cdot\mathbf{r}$ that are relevant for the determination of the transition matrix element. For inner shells the bound-state wave function is basically Coulombic, i.e., screening effects do not have much influence on its shape. This means, for example, that for the 1s subshell the maximum distance which is relevant in the integral determining the matrix element is of the order a_B/Z, where a_B is the Bohr radius. (At higher energies the relevant distance may be significantly smaller, due to rapid oscillations of the continuum electron wave function.) Therefore the relevant values of $\mathbf{k}\cdot\mathbf{r}$ are $\sim ka_b/Z$, which near threshold is approximately given by $\frac{1}{2}Z\alpha$ in the Coulomb case and is smaller, particularly in light elements, when screening is present (since the binding energy, and so the threshold k, is then smaller). The values of $4(v/c)$ and $Z\alpha$ for energies from 0.2 eV to 2 keV and $Z=6,10,26,36$ are shown in Table I.

Here we report a calculation of the correction to the 1s photoelectron angular distribution, corresponding to the term linear in $\mathbf{k}\cdot\mathbf{r}$ in the expansion of the photon plane wave, which is the low-energy limit of the quadrupole term. This correction is basically and generally of the order $Z\alpha$ (contrary to the Coulomb result) and is therefore much bigger than the relativistic correction, which is $\sim(Z\alpha)^2$ or $(v/c)^2$. In the total cross section, however, this $Z\alpha$ term does not contribute (its integral over angles vanishes), and the first term beyond dipole approximation is $\sim(Z\alpha)^2$, i.e., of the same order as the first relativistic correction. It is thus plausible to calculate the retardation correction to the angular distribution using nonrelativistic electron wave functions, whereas in the case of

TABLE I. Values of the Coulomb retardation corrections $4(v/c)$ for energies 0.2–2 keV and of the parameter ka_B/Z for the same range of energies and $Z=6,10,26,36$.

E (keV)	$4\frac{v}{c}$	ka_b/Z ($Z=6$)	ka_b/Z ($Z=10$)	ka_b/Z ($Z=26$)	ka_b/Z ($Z=36$)
0.0002	3.54×10^{-3}	1.30×10^{-2}	2.30×10^{-2}	7.30×10^{-2}	1.06×10^{-1}
0.001	7.91×10^{-3}	1.30×10^{-2}	2.30×10^{-2}	7.31×10^{-2}	1.06×10^{-1}
0.005	1.77×10^{-2}	1.32×10^{-2}	2.31×10^{-2}	7.31×10^{-2}	1.06×10^{-2}
0.01	2.50×10^{-2}	1.34×10^{-2}	2.33×10^{-2}	7.31×10^{-2}	1.06×10^{-1}
0.02	3.54×10^{-2}	1.39×10^{-2}	2.35×10^{-2}	7.32×10^{-2}	1.06×10^{-1}
0.05	5.60×10^{-2}	1.52×10^{-2}	2.43×10^{-2}	7.36×10^{-2}	1.07×10^{-1}
0.1	7.91×10^{-2}	1.75×10^{-2}	2.57×10^{-2}	7.41×10^{-2}	1.07×10^{-1}
0.2	1.12×10^{-1}	2.19×10^{-2}	2.84×10^{-2}	7.51×10^{-2}	1.08×10^{-1}
1.0	2.50×10^{-1}	5.77×10^{-2}	4.98×10^{-2}	8.34×10^{-2}	1.14×10^{-1}
2.0	3.54×10^{-1}	1.02×10^{-1}	7.66×10^{-2}	9.37×10^{-2}	1.21×10^{-1}

the total cross section both types of corrections have to be considered simultaneously.

Our (approximate) analytic formula is described in Sec. II, while Sec. III contains a comparison of this formula with the results of numerical calculation and some discussion.

II. A FORMULA FOR THE FIRST RETARDATION CORRECTION

The nonrelativistic matrix element for the bound-free transition from an initial nl state of the atomic electron to a final continuum state characterized by asymptotic momentum $\mathbf{p}$ can be written as

$$M=\int d^3x\ \psi_{\mathbf{p}}^{*}e^{i\mathbf{k}\cdot\mathbf{r}}\boldsymbol{\epsilon}\cdot\mathbf{P}\psi_{nl}\ , \tag{2}$$

where $\psi_{\mathbf{p}}$ is the full continuum (outgoing) wave function of the final electron, ψ_{nl} is the bound-state wave function of the initial electron, $\boldsymbol{\epsilon}$ is the photon polarization vector and $\mathbf{k}$ its momentum, and $\mathbf{P}$ is the momentum operator. We want to find the amplitude (2) in the approximation in which only first two terms in the expansion of $\exp(i\mathbf{k}\cdot\mathbf{r})$ are kept, for the case that the initial electron is in the $1s$ state, i.e.,

$$\psi_{nl}(\mathbf{r})=R_{10}(r)\ , \tag{3}$$

where R_{10} is the $1s$ radial function.

The angular distribution of final electrons can be simply determined with the use of the partial-wave expansion of the continuum wave function $\psi_{\mathbf{p}}$ and photon plane wave (i.e., not a true multipole expansion),

$$\psi_{\mathbf{p}}=\sum_{l=0}^{\infty}(2l+1)i^{l}e^{-i\delta_l}R_l(r)P_l(\hat{\mathbf{p}}\cdot\hat{\mathbf{r}}\cdot)\ , \tag{4a}$$

$$e^{i\mathbf{k}\cdot\mathbf{r}}=\sum_{L=0}^{\infty}(2L+1)i^{L}j_L(kr)P_L(\hat{\mathbf{k}}\cdot\hat{\mathbf{r}})\ , \tag{4b}$$

where δ_l is the phase shift, R_l the continuum radial function, and P_l the Legendre polynomial. Substituting (4) into (2) we find

$$M=\sum_{l,L}(2L+1)(2l+1)i^{L-l}e^{i\delta_l}\times\int_0^{\infty}dr\,r^2R_l(r)j_L(kr)\frac{dR_{10}(r)}{dr}\times\int d\Omega_{\mathbf{r}}P_l(\hat{\mathbf{p}}\cdot\hat{\mathbf{r}})\hat{\boldsymbol{\epsilon}}\cdot\hat{\mathbf{r}}P_L(\hat{\mathbf{p}}\cdot\hat{\mathbf{r}})\ . \tag{5}$$

Performing the angular integration

$$M=4\pi i\frac{\boldsymbol{\epsilon}\cdot\mathbf{p}}{\sin^2\theta}\times\sum_{l}\frac{l(l+1)}{2l+1}e^{i\delta_l}[P_{l+1}(\hat{\mathbf{p}}\cdot\hat{\mathbf{k}})-P_{l-1}(\hat{\mathbf{p}}\cdot\hat{\mathbf{k}})]\times\int_0^{\infty}dr\,r^2R_l(r)\frac{dR_{10}(r)}{dr}\times[j_{l+1}(kr)+j_{l-1}(kr)]\ , \tag{6}$$

where θ is the angle between $\mathbf{p}$ and $\mathbf{k}$. Using recursion formulas for the spherical Bessel functions and Legendre polynominals,[7] we can write (6) in the simpler form

$$M=4\pi i(\boldsymbol{\epsilon}\cdot\mathbf{p})\sum_{l=1}^{\infty}(2l+1)e^{i\delta_l}\frac{a_l(k)}{k}P_l'(\hat{\mathbf{p}}\cdot\hat{\mathbf{k}})\ , \tag{7}$$

where the radial matrix element

$$a_l(k)=\int_0^{\infty}dr\,rR_l(r)\frac{dR_{10}(r)}{dr}j_l(kr)\ . \tag{8}$$

Formula (7) is suitable for the analysis of successive terms in the retardation expansion. To obtain the dipole approximation in the standard form one has to take the limit $k\to0$. This leaves only first term in (7), with the radial matrix element

$$M_{\text{rad}}^{\text{dipole}}=\int_0^{\infty}dr\,r^2R_l(r)\frac{dR_{10}(r)}{dr}\ . \tag{9}$$

This can be reduced to the standard expression by using the relation $ip_r=[r,H]$, where p_r is the radial component of the momentum operator

$$p_r=i^{-1}(\partial/\partial r+r^{-1})\ .$$

We are interested in the expression for the amplitude M including first retardation corrections, which corresponds to keeping terms at most linear in k in (7). It is easy to see that in this case only the first two terms in (7) survive. We obtain

$$M \approx 4\pi i(\boldsymbol{\epsilon}\cdot\mathbf{p})(\alpha_1 e^{i\delta_1} + \alpha_2 e^{i\delta_2} k\cos\theta) , \tag{10}$$

where

$$\alpha_l = \int_0^\infty dr\, r^{l+1} R_l(r) \frac{dR_{10}(r)}{dr} . \tag{11}$$

In general, the expansion in powers of k (which we call the retardation expansion) will cause mixing of various multipoles in the multipole expansion of the amplitude, i.e., a term of given order in k will contain contributions from many multipoles. The only exceptions are the first two terms, where the contribution of zeroth-order corresponds to the small-k limit of the dipole terms and the contribution of order one to the small-k limit of the quadrupole amplitude. By contrast, the term proportional to k^2 contains a next-to-leading term of the dipole amplitude as well as the leading term of the octupole. The number of multipoles contributing to a term of given order in k increases with increasing powers of the photon momentum.

It proves convenient to parametrize the correction to the amplitude in terms of the velocity of the final electron, in analogy to the point-Coulomb matrix-element case. This can be done using the energy conservation equation, from which it follows that

$$\frac{v}{c} = \frac{pk}{E+\epsilon_B} , \tag{12}$$

where E is the energy of the continuum electron and ϵ_B is the (positive) binding energy of the initial electron. We write now (10) as

$$M = 4\pi i(\boldsymbol{\epsilon}\cdot\mathbf{p})\alpha_1 e^{i\delta_1}\left[1+\frac{\alpha_2}{\alpha_1}\frac{E+\epsilon_B}{p}e^{i(\delta_2-\delta_1)}\frac{v}{c}\cos\theta\right] . \tag{13}$$

Deviations from the dipole angular distribution are measured by the product of v/c, $\cos(\delta_2-\delta_1)$, and b, where b is defined as

$$b = \frac{\alpha_2}{\alpha_1}\frac{E+\epsilon_B}{p} . \tag{14}$$

The real radial integrals α_l are proportional to the continuum normalizations[8] N_l. This allows us to express b in terms of the ratios of screened to point-Coulomb normalizations $n_l \equiv N_l/N_l^c$ as

$$b = b^c b^{\rm scr}\frac{n_2}{n_1} , \tag{15}$$

where b^c is the limit of b when screening is removed and $b^{\rm scr}$, which goes to unity in the limit of vanishing screening, describes the screening effects in b beyond the screening correction to point-Coulomb normalizations. Now, b^c is given by

$$b^c = (\nu^2+4)^{1/2} , \tag{16}$$

where $\nu = Z\alpha/p$. Note that at threshold $b^c(v/c) = Z\alpha$.

We have performed an analytic calculation of $b^{\rm scr}$ based on the analytic perturbation theory (APT) for screened Coulomb potentials, in which the screening effects are treated perturbatively.[9] We have also considered numerical calculations. We find that screening effects in $b^{\rm scr}$ are small in the case that an electron is ejected from an inner shell, so that for qualitative purposes $b^{\rm scr}$ can be approximated by unity. The main screening effects in the retardation correction are due to the continuum normalizations (n_2/n_1 is significantly different from 1 though usually not small) and to the phase shifts.

We can write the amplitude (10) as

$$M \approx 4\pi i(\boldsymbol{\epsilon}\cdot\hat{\mathbf{p}})\alpha_1 e^{i\delta_1} \times\left[1+\frac{n_2}{n_1}(\nu^2+4)^{1/2}\frac{v}{c}e^{i(\delta_2-\delta_1)}\cos\theta\right] , \tag{17}$$

where we have put $b^{\rm scr}=1$. The unpolarized differential cross section calculated up to and including the first retardation correction is then given by

$$\frac{d\sigma}{d\Omega} \approx A\sin^2\theta(1+\kappa\cos\theta) , \tag{18}$$

where

$$\kappa = 2\frac{n_2}{n_1}(\nu^2+4)^{1/2}\frac{v}{c}\cos(\delta_2-\delta_1) , \tag{19}$$

and A is independent of the angle θ, and is equal to $(3/8\pi)\sigma_{\rm tot}^{\rm dipole}$.

In the point-Coulomb case $\delta_{c_2}-\delta_{c_1} = -\tan^{-1}(2/\nu)$ and at low energies when $\nu \gg 1$, $\delta_{c_2}-\delta_{c_1} \approx -\pi/2 - 2/\nu$, so that $\cos(\delta_{c_2}-\delta_{c_1}) \approx 2/\nu$ and $\kappa \sim v/c$ in agreement with (1). If, however, screening is present then $\delta_2-\delta_1$ often differs significantly from $-\pi/2$, so that $|\cos(\delta_2-\delta_1)| \sim 1$. It follows then from (19) that at low energies $\kappa \sim Z\alpha$ rather then $\kappa \sim v/c$.

III. COMPARISON WITH NUMERICAL RESULTS AND DISCUSSION

To begin the discussion of formulas (18) and (19) we again note that there are three main factors which determine the magnitude of the first retardation correction to the dipole $\sin^2\theta$ angular distribution of $1s$ photoelectrons. These are $\cos(\delta_2-\delta_1)$, n_2/n_1, and $(\nu^2+4)^{1/2}(v/c)$. According to the discussion in the preceding section we have set $b^{\rm scr}=1$, which is justified for qualitative purposes for inner shells where screening effects in $b^{\rm scr}$ are not large. We may expect $b^{\rm scr}$ to differ significantly from unity for outer-shell photoelectrons.

We show in Table II values of these three factors for $Z=6,10,26,36$ and energies ranging from 0.2 eV to 1 keV. This table contains also values of the retardation correction κ as calculated from formula (19) and its exact values obtained with the use of the numerical program

FOTO, calculating parameters characterizing the photoelectric effect.[10] The shape of κ as a function of the continuum electron energy for $Z=6,10,26,36$ is shown in Fig. 1, together with the point-Coulomb result $\kappa=4(v/c)$ which is independent of Z.

For low values of Z ($Z=6$ and 10) the first retardation correction at low energies (0.2 eV to $\sim$20 eV) is of the order of $4(v/c)$ or smaller. This is due to small values of the ratio n_2/n_1 ($\sim 10^{-2}$) in this case and to small values of $(\nu^2+4)^{1/2}(v/c)$, which at low energies is $\approx Z\alpha$. The parameter κ is negative close to threshold, then its absolute value increases with increasing energy toward a minimum (maximum of the absolute value). The absolute value of κ then decreases toward a zero and at higher energies the screened and point-Coulomb values of the first retardation correction converge, with the screened result smaller than the Coulomb one. The position of both the minimum and of the zero of κ increases with increasing

TABLE II. First retardation correction as a function of energy as obtained from formula (19) and from the numerical program FOTO. The intermediate columns contain values of the three factors which determine κ for inner-shell photoelectrons.

E (keV)	$\cos(\delta_2-\delta_1)$	n_2/n_1	$(\nu^2+4)^{1/2}\frac{v}{c}$	κ (num.)	κ [Eq. (19)]
			$Z=6$		
0.0002	-1.00×10^{0}	7.22×10^{-2}	4.38×10^{-2}	-5.89×10^{-3}	-6.33×10^{-3}
0.001	-9.52×10^{-1}	8.27×10^{-2}	4.40×10^{-2}	-6.44×10^{-3}	-6.93×10^{-3}
0.005	-6.67×10^{-1}	1.32×10^{-1}	4.47×10^{-2}	-7.35×10^{-3}	-7.89×10^{-3}
0.01	-4.05×10^{-1}	1.90×10^{-1}	4.55×10^{-2}	-6.54×10^{-3}	-7.02×10^{-3}
0.02	-4.04×10^{-2}	2.86×10^{-1}	4.72×10^{-2}	-1.02×10^{-3}	-1.09×10^{-3}
0.04	3.45×10^{-1}	4.01×10^{-1}	5.04×10^{-2}	1.30×10^{-2}	1.39×10^{-2}
0.1	6.48×10^{-1}	5.67×10^{-1}	5.90×10^{-2}	4.06×10^{-2}	4.33×10^{-1}
0.6	9.16×10^{-1}	8.65×10^{-1}	1.06×10^{-1}	1.62×10^{-1}	1.69×10^{-1}
1.0	9.47×10^{-1}	9.12×10^{-1}	1.33×10^{-1}	2.22×10^{-1}	2.29×10^{-1}
2.0	9.72×10^{-1}	9.21×10^{-1}	1.82×10^{-1}	3.31×10^{-1}	3.27×10^{-1}
			$Z=10$		
0.0002	-7.99×10^{-1}	2.86×10^{-2}	7.30×10^{-2}	-3.15×10^{-3}	-3.34×10^{-3}
0.001	-9.35×10^{-1}	3.24×10^{-2}	7.31×10^{-2}	-4.18×10^{-3}	-4.43×10^{-3}
0.005	-9.92×10^{-1}	5.01×10^{-2}	7.35×10^{-2}	-6.92×10^{-3}	-7.32×10^{-2}
0.01	-9.24×10^{-1}	7.15×10^{-2}	7.41×10^{-2}	-9.26×10^{-3}	-9.79×10^{-3}
0.02	-7.60×10^{-1}	1.14×10^{-1}	7.51×10^{-2}	-1.24×10^{-2}	-1.31×10^{-2}
0.05	-3.22×10^{-1}	2.34×10^{-1}	7.82×10^{-2}	-1.12×10^{-2}	-1.18×10^{-2}
0.1	1.23×10^{-1}	3.63×10^{-1}	8.30×10^{-2}	6.94×10^{-3}	7.42×10^{-2}
0.2	4.64×10^{-1}	5.11×10^{-1}	9.20×10^{-2}	4.14×10^{-2}	4.36×10^{-2}
1.0	8.60×10^{-1}	8.09×10^{-1}	1.45×10^{-1}	1.94×10^{-1}	2.02×10^{-1}
2.0	9.24×10^{-1}	8.90×10^{-1}	1.92×10^{-1}	3.06×10^{-1}	3.15×10^{-1}
			$Z=26$		
0.0002	-9.01×10^{-2}	2.77×10^{-1}	1.90×10^{-1}	-8.38×10^{-3}	-9.48×10^{-3}
0.001	-3.56×10^{-1}	3.00×10^{-1}	1.90×10^{-1}	-3.85×10^{-2}	-4.05×10^{-2}
0.005	-7.42×10^{-1}	3.77×10^{-1}	1.90×10^{-1}	-1.03×10^{-1}	-1.06×10^{-1}
0.01	-9.00×10^{-1}	4.30×10^{-1}	1.90×10^{-1}	-1.43×10^{-1}	-1.47×10^{-1}
0.02	-9.95×10^{-1}	4.69×10^{-1}	1.91×10^{-1}	-1.73×10^{-1}	-1.78×10^{-1}
0.05	-9.32×10^{-1}	4.73×10^{-1}	1.92×10^{-1}	-1.65×10^{-1}	-1.69×10^{-1}
0.1	-7.42×10^{-1}	4.88×10^{-1}	1.94×10^{-1}	-1.37×10^{-1}	-1.40×10^{-1}
0.5	1.86×10^{-2}	5.78×10^{-1}	2.09×10^{-1}	2.82×10^{-3}	4.50×10^{-3}
1.0	3.43×10^{-1}	6.50×10^{-1}	2.27×10^{-1}	9.73×10^{-2}	1.01×10^{-1}
2.0	5.95×10^{-1}	7.36×10^{-1}	2.60×10^{-1}	2.20×10^{-1}	2.27×10^{-1}
			$Z=36$		
0.0002	9.27×10^{-1}	3.92×10^{-1}	2.63×10^{-1}	1.86×10^{-1}	1.91×10^{-1}
0.001	6.81×10^{-1}	4.47×10^{-1}	2.63×10^{-1}	1.59×10^{-1}	1.60×10^{-1}
0.005	-2.28×10^{-1}	5.91×10^{-1}	2.63×10^{-1}	-6.71×10^{-2}	-7.11×10^{-2}
0.01	-7.36×10^{-1}	5.89×10^{-1}	2.63×10^{-1}	-2.21×10^{-1}	-2.28×10^{-1}
0.02	-9.66×10^{-1}	5.36×10^{-1}	2.63×10^{-1}	-2.66×10^{-1}	-2.73×10^{-1}
0.05	-9.83×10^{-1}	5.28×10^{-1}	2.64×10^{-1}	-2.69×10^{-1}	-2.74×10^{-1}
0.1	-8.63×10^{-1}	5.43×10^{-1}	2.66×10^{-1}	-2.46×10^{-1}	-2.49×10^{-1}
0.5	-2.72×10^{-1}	5.90×10^{-1}	2.77×10^{-1}	-8.91×10^{-2}	-9.09×10^{-2}
1.0	5.93×10^{-2}	6.35×10^{-1}	2.91×10^{-1}	1.55×10^{-2}	2.01×10^{-2}
2.0	3.59×10^{-1}	6.97×10^{-1}	3.17×10^{-1}	1.51×10^{-1}	1.59×10^{-1}

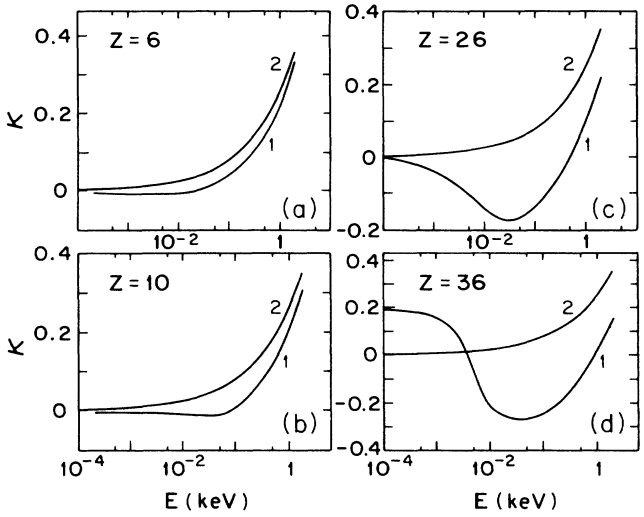

FIG. 1. Numerical values of the first retardation correction (curve 1) for (a) $Z=6$, (b) $Z=10$, (c) $Z=26$, and (d) $Z=36$, as a function of photoelectron energy E. The Coulomb retardation correction $4(v/c)$ (curve 2) is also shown for comparison with the screened case.

TABLE III. First retardation correction at threshold, as a function of Z.

Z	κ
6	-5.77×10^{-3}
8	-4.19×10^{-3}
10	-2.92×10^{-3}
12	-1.30×10^{-3}
14	1.21×10^{-2}
16	3.37×10^{-2}
18	5.08×10^{-2}
20	-2.60×10^{-2}
22	-1.72×10^{-2}
24	-3.24×10^{-2}
26	-1.24×10^{-2}
28	5.39×10^{-3}
30	1.10×10^{-2}
32	7.98×10^{-2}
34	1.36×10^{-1}
36	1.89×10^{-1}
38	-4.54×10^{-2}
40	-3.58×10^{-2}

Z. In general, for low atomic numbers the first retardation correction at lower energies is smaller than v/c. Its value increases after passing through zero and at higher energies (1–2 keV) approaches the point-Coulomb result.

For $Z=26$, which is the next case considered in detail in this paper, the value of the first retardation correction is also small close to threshold. However, this is now due to $\delta_2-\delta_1$ having values close to $\pi/2$ for very low energies (cf. also Ref. 11). With increasing energy $|\kappa|$ increases rapidly toward a minimum of κ (maximum of the absolute value) at $E\approx20$ eV. The value of κ at the minimum is about -0.18. For $Z=36$ the first retardation correction to the angular distribution is positive at threshold and of the order of 0.2. It has two zeros now—the first for $E\approx3$ eV and the second one between 0.9 and 1 keV. The value of κ at the minimum is ≈-0.27. In general, when the parameter κ is not small it is of the order of ka_B/Z.

The values of κ as obtained from formula (19) compare well with the exact numerical values and reflect the same type of behavior with energy. The error of Eq. (19) does not exceed 10%.

The sign of the first retardation correction depends on the sign of $\cos(\delta_2-\delta_1)$. Whether the number of zeros of κ is odd or even depends on its sign at threshold and at high energy. As we have seen, the first retardation correction approaches the positive point-Coulomb result as energy increases, so that what matters is the sign at threshold, determined by $\cos(\delta_2-\delta_1)$. If κ is positive for $E\rightarrow0^+$ it will have an even number of zeros (e.g., two for $Z=36$), while if $\cos(\delta_2-\delta_1)$ is negative at threshold κ will pass through zero at least once. The values of the first retardation correction at threshold are shown in Table III. We see that the sign of κ at threshold changes several times when going from lower to higher values of Z.

The value of this non-Coulombic part of the phase shift at threshold

$$\Delta_l(0)=\delta_l(0)-\delta_l^c(0)\ , \tag{20}$$

where $\delta_l^c(p)$ is the Coulomb phase corresponding to the long-range Coulombic tail of the potential, can be related to the number of bound states N_l, with the angular momentum l, below some (small) energy $-\varepsilon$ with $\epsilon>0$. The expression is[12]

$$N_l=E((1/\pi)\Delta_l(0)+\omega)\ ,\quad 0\le\omega<1 \tag{21}$$

where $E(x)$ is the largest integer not exceeding x. When the number of bound states increases by one, the phase shift at threshold, $\delta_l(0)$, increases by π. These changes occur at different Z for different l,[11] so that the difference of phase shifts oscillates.

The first threshold sign change of κ, in the vicinity of $Z=10$ (neon), corresponds to the increase of the number of bound states with $l=1$, when the $3p$ level dives deeply enough and starts to be filled. The next change of sign occurs near the next rare gas ($Z=18$), when the $3d$ level becomes bound by the short-range part of the potential with the $2p$ and $3p$ subshells already filled. The third change of sign takes place when the $4p$ subshell becomes bound by the short-range potential well, and the last change displayed in Table III corresponds to the situation when the $4d$ level dives deeply enough.

We cannot be *a priori* sure that, performing an expansion in powers of $\mathbf{k}\cdot\mathbf{r}$, we have obtained the entire leading correction to the dipole cross section, since we have no bound on the magnitude of contributions from successive terms in an expansion in $\mathbf{k}\cdot\mathbf{r}$. A perturbative calculation of the next term [i.e., the one proportional to $(\mathbf{k}\cdot\mathbf{r})^2$]

yields a result an order of magnitude smaller than that discussed here,[9] but we lack a proof that there are no other terms of a similar or greater order of magnitude.

To summarize, we have obtained a simple semianalytic formula which can be used to find the value of the first retardation correction to the 1*s*-photoelectron angular distribution at low energies and for lighter elements. This formula shows also the role of various factors in determining this correction. Results of our calculations can be checked experimentally, since in the cases when κ is not small, the retardation effect cause a significant forward or backward peaking of the angular distribution, depending on whether κ is positive or negative.

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*Permanent address: Institute of Physics, University of Szczecin, Wielkopolska 15, 70-451 Szczecin, Poland.

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