Retardation and multipole effects in Rayleigh scattering by hydrogenlike ions at low and x-ray photon energies

A. Costescu,[1,2] P. M. Bergstrom, Jr.,[1,*] C. Dinu,[2] and R. H. Pratt[1]
[1]*Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260*
[2]*Department of Physics, University of Bucharest, P.O. Box Mg-11, Bucharest, Romania*
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We investigate analytically multipole and retardation effects on Rayleigh scattering of photons from the ground state of a hydrogenic atom. Our approach, which goes beyond the usual form-factor approximation, simplifies the full nonrelativistic point-Coulombic amplitude considerably. We are able to express this simplified full multipole, fully retarded result as simple corrections to the nonrelativistic dipole amplitude. We demonstrate that these corrections are important, and larger than relativistic effects, for photon energies near the K-shell photoionization threshold. They are essential for accurately determining the angular distribution of scattered photons in this regime. We present numerical comparisons with relativistic S-matrix calculations that confirm the validity of our approach in this region for elements of low to moderate nuclear charge. For photon energies well above the K-shell threshold we show that retardation corrections are adequately given by the form factor, which has a greater variation with angles than the anomalous scattering factors. For still higher energies, we demonstrate that the full nonrelativistic result fails due to spurious poles in the imaginary part of the amplitude.

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I. INTRODUCTION

We seek to elucidate the nature of higher multipole and retardation contributions in Rayleigh scattering, studying the case of scattering from the K-shell electron of a hydrogenic system. By retardation contributions we mean the evaluation of multipoles beyond their long-wavelength limit. We evaluate these contributions simultaneously for all multipoles, for fixed orders in $k\alpha Z$ (where k is the photon energy divided by the nonrelativistic ground state binding energy). The approach that we use is nonrelativistic and follows logically from earlier work of Gavrila [1] and Gavrila and Costescu [2]. Making the dipole approximation to the point-Coulombic nonrelativistic Kramers-Heisenberg-Waller (KHW) matrix element, Gavrila derived an expression and presented results for the scattering from the ground state of a hydrogenic atom in terms of the Gauss hypergeometric function [1]. Gavrila and Costescu subsequently extended this result by including retardation and all multipoles, deriving a matrix element expressed in terms of Appell functions [2]. The resulting expressions were not evaluated numerically because relativistic corrections were expected to be of the same order as the higher multipole and retardation contributions. In fact we show that multipole and retardation contributions are more important than relativistic effects for photon energies above the photoionization threshold, but in a nonrelativistic domain, particularly for the determination of the angular distribution. The present work is based on the results of Gavrila and Costescu [2]. As the formalism is purely nonrelativistic, effects arising from relativity such as spin flip are not considered. Furthermore, we make use of a series expansion which limits the validity of our results to photon energies and angles $k\sin\frac{\theta}{2} \leq \frac{2}{\alpha Z}$. The highest energies are therefore restricted by the condition $k \leq (2/\alpha Z)$ when all angles are to be considered; higher energies can be discussed for forward scattering. We particularly wish to study the importance of higher multipole and retardation corrections in obtaining the shape of the angular distribution, as the nonretarded dipole result exhibits symmetry about 90° not found in the full result.

Fully relativistic numerical second-order S-matrix calculations of Rayleigh scattering have been reported by several authors [3–5]. These calculations include higher multipoles as well as retardation and relativistic contributions. However, the relative contributions of these corrections are not given explicitly in such an approach. Using the code of Kissel *et al.* [5], Roy and Pratt [6] examined the validity of the nonrelativistic and relativistic dipole treatments (their relativistic dipole results included retardation whereas their nonrelativistic results did not) for forward scattering and determined that a dipole treatment is useful below threshold and very near but above threshold. They found that a relativistic approach is necessary primarily for elements of high nuclear charge and that, for these high-Z elements, relativistic corrections can be roughly included by shifting the nonrelativistic energy levels (i.e., defining k as the ratio of the photon energy to the relativistic ground state en-

*Present address: Theoretical Physics, University of Tennessee, 200 South College, Knoxville, TN 37996-1501. Electronic address: pmb@utkvx.utk.edu

ergy). At higher energies, both the relativistic dipole and the nonrelativistic dipole treatments fail, even for forward scattering. Florescu *et al.* [7] investigated in more detail the importance of relativistic corrections to the dipole approximation below threshold, deriving a relativistic dipole approximation which retained all $p_{1/2}$ and $p_{3/2}$ intermediate states in the propagator. Their results confirm that relativistic effects are indeed important below threshold. These conclusions may be roughly understood for low photon energies in terms of (i) the parameters $\frac{\hbar\omega}{mc^2} = \frac{(Z\alpha)^2}{2}k$ and (ii) $(\alpha Z)^2$, which characterize the magnitude of relativistic corrections, and by the parameter $\frac{(k\alpha Z)^2}{4}$, which, as we show subsequently, may be used to characterize the magnitude of higher multipole and retardation effects for given scattering angle. At $k = 2$ all these parameters are the same, while for $k > 2$ (< 2) multipole and retardation (relativistic) parameters are larger. In Fig. 1, retardation corrections are larger than relativistic corrections in the region below the solid curve. The parameters that characterize relativistic effects are smaller than the parameter which characterizes higher multipole contributions and retardation corrections for photon energies above twice the K-shell threshold, though both grow with energy (and so a nonrelativistic approach cannot be used once the relativistic parameters are large). Relativistic corrections are significant for photon energies (nuclear charge) larger than those given by the vertical (horizontal) dashed lines. As will be discussed, our results are valid for all angles in the region where the retardation parameter is less than unity. This criterion is given by the lowest dotted curve. The other dotted curves correspond to the largest value of the retardation parameter considered in the numerical examples that we present and to a very small value of this parameter, where the dipole approximation should be valid.

Retardation contributions are expected to become larger with increasing photon energies. However, we show that much of the retardation is given by the form factor for energies well above threshold. At still higher energies contributions from spurious poles [8] near the electron-positron pair production threshold in the nonrelativistic, fully retarded amplitude degrade this amplitude (and our results which are derived from it). The effects of these poles are known in photoeffect (which is related to the imaginary part of the forward Rayleigh scattering amplitude by the optical theorem). The nonrelativistic, nonretarded dipole approximation to the K-shell photoeffect due to Stobbe [9] may be written

$$\sigma_{\rm ph} = \frac{256\pi^2}{3}\alpha^5 Z^6 \left(\frac{mc^2}{\hbar\omega}\right)^4 \frac{e^{-4\nu \arctan\frac{1}{\nu}}}{1-e^{-2\pi\nu}}, \tag{1.1}$$

where

$$\nu = (k-1)^{-\frac{1}{2}}.$$

The corresponding result including all multipoles and retardation was obtained by Fischer [10]. It may be written

$$\sigma_{\rm ph} = \frac{256\pi^2}{3}\alpha^5 Z^6 \left(\frac{mc^2}{\hbar\omega}\right)^4 \frac{e^{-2\nu\chi}}{1-e^{-2\pi\nu}} \times \frac{1}{\left\{\left(1-\frac{\hbar\omega}{2mc^2}\right)^2 + \alpha^2 Z^2\right\}^2}, \tag{1.2}$$

where

$$\chi = \arctan\frac{2(k+1)^{\frac{1}{2}}}{2-k+(k\alpha Z/2)^2}.$$

The poles near the pair production threshold in this nonrelativistic retarded result cause substantial departures from the nonretarded dipole result at high energies, where the nonretarded dipole result is known to agree with calculations including retardation and relativity, implying a cancellation of these poles by relativistic contributions. This observation applies to both screened and Coulombic calculations of the total photoeffect cross section [11]. In contrast with the total photoeffect cross section, it is necessary to incorporate retardation effects in the ground state photoelectron angular distribution for all but the lightest elements down to the photoionization threshold. The parameter characterizing these corrections to the angular distribution is $\sim \alpha Z$ in the screened case and $\sim v/c$ in the point-Coulombic case [12].

We seek to complement analytically the numerical work of Kissel *et al.* [5] and of Roy and Pratt [6] in the region above the photoelectric threshold. We derive simple analytic formulas which include higher multipoles and retardation corrections for the elastic scattering of photons from a K-shell electron in a Coulombic field, starting from the nonrelativistic results of Gavrila and Costescu [2]. We expect good agreement with the results of a more exact treatment primarily for elements of low or moderate nuclear charge, where relativistic effects on the ground state are less important. The point-Coulombic approach that we use neglects screening and is expected to work best for the K shell. (However, very

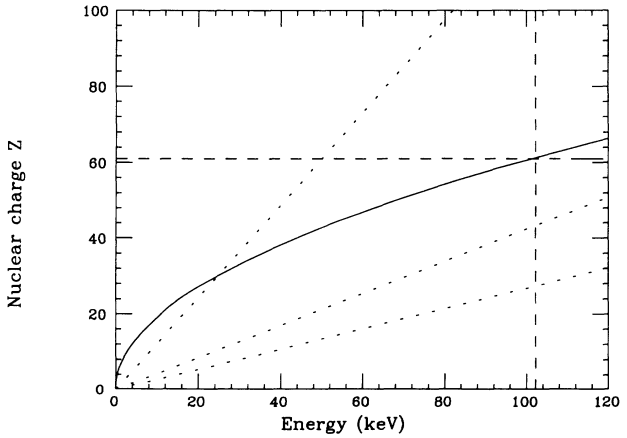

FIG. 1. The retardation parameter is equal to the relativistic parameters on the solid curve and larger below it. The vertical (horizontal) dashed line represents the photon energy (nuclear charge) where the relativistic parameter equals 0.2. The dotted curves represent the retardation parameter for values of (clockwise from top) 0.05, 0.4, and 1.0.

near threshold differences between the screened and the point-Coulombic results may be expected, as in the near threshold behavior of the K-shell photoionization cross section.) The formalism of our approach, our analytic results, and a discussion of the simple formulas obtained are presented in Sec. II. In Sec. III a comparison of numerical results obtained from these formulas with those calculated using the code of Kissel *et al.* [5] in a point-Coulombic potential and with results obtained using the form-factor approach [13] is given. We also compare photoelectric effect cross sections obtained from the imaginary part of our forward scattering amplitudes, using the optical theorem, to the nonrelativistic results given in Eqs. (1.1) and (1.2) as well as to the full multipole relativistic point-Coulombic results of Hultberg, Nagel, and Olsson [14] and to the full multipole relativistic screened calculations of Scofield [15].

II. FORMALISM

In a purely nonrelativistic formalism, where the electron is assumed to be a spinless particle, the matrix element for the elastic scattering of photons may be written

$$M_{\vec{\varepsilon}_1\vec{\varepsilon}_2} = (\vec{\varepsilon}_1 \cdot \vec{\varepsilon}_2)M + (\vec{\varepsilon}_1 \cdot \vec{k}_2)(\vec{\varepsilon}_2 \cdot \vec{k}_1)N, \tag{2.1}$$

where $\vec{\varepsilon}_1$ and $\vec{\varepsilon}_2$ are the initial and final photon polarizations and $\vec{k}_1$ and $\vec{k}_2$ are unit vectors in the directions of the initial and final photon momenta. M and N are functions of the photon energy, the scattering angle, and the nuclear charge. Gavrila and Costescu [2] derived nonrelativistic retarded multipole expressions (valid for all $k\alpha Z$) for M and N of a hydrogenlike system in terms of two Appell functions F_1:

$$M = O - P(\tau_1, k\alpha Z, \theta) - P(\tau_2, k\alpha Z, \theta), \tag{2.2}$$

$$N = -[Q(\tau_1, k\alpha Z, \theta) + Q(\tau_2, k\alpha Z, \theta)],$$

$$\tau_1 = \begin{cases} i(k-1)^{-\frac{1}{2}}, & k > 1 \\ (1-k)^{-\frac{1}{2}}, & k < 1, \end{cases} \quad \tau_2 = (k+1)^{-\frac{1}{2}},$$

$$k = 2\hbar\omega/(\alpha Z)^2 mc^2,$$

where $\hbar\omega$ is the photon energy and

$$O = \left\{1 + \frac{(k\alpha Z)^2}{4}\sin^2\frac{\theta}{2}\right\}^{-2}, \tag{2.3}$$

$$P(\tau, k\alpha Z, \theta) = \frac{128\tau^5}{\left[(\tau+1)^2 + \tau^2(k\alpha Z)^2/4\right]^4} \times \frac{F_1(2-\tau; 2, 2; 3-\tau; x_1, x_2)}{2-\tau}, \tag{2.4}$$

$$Q(\tau, k\alpha Z, \theta) = \frac{512\tau^7}{\left[(\tau+1)^2 + \tau^2(k\alpha Z)^2/4\right]^6} \times \frac{(k\alpha Z)^2 F_1(3-\tau; 3, 3; 4-\tau; x_1, x_2)}{3-\tau}. \tag{2.5}$$

Here x_1 and x_2 are defined by

$$x_1 x_2 = p = \left[\frac{(\tau-1)^2 + \tau^2(k\alpha Z)^2/4}{(\tau+1)^2 + \tau^2(k\alpha Z)^2/4}\right]^2, \tag{2.6}$$

$$x_1 + x_2 = 2\sqrt{p} - \frac{4\tau^2(k\alpha Z)^2\sin^2\frac{\theta}{2}}{(\tau+1)^2 + \tau^2(k\alpha Z)^2/4},$$

and θ is the photon scattering angle. One may recognize Eq. (2.3) as the well known hydrogenic form factor [13]. This means that a generalization of the real and imaginary anomalous scattering factors, which include their angular dependence, are determined by the real and imaginary parts of the amplitudes P and Q.

It is possible to compute numerically the amplitudes P and Q using Eqs. (2.4) and (2.5). However, in order to achieve a better understanding of higher multipole contributions and retardation effects in Rayleigh scattering, we wish to obtain simple formulas which make clear the energy, angle, and charge dependence of the amplitudes and how P and Q depend on k and on αZ. Our procedure is to expand the amplitudes P and Q in powers of αZ at fixed k, i.e., at fixed τ. We may do this by first using series expansions for the angular functions F_1 that occur in the invariant amplitudes P and Q (valid due to the degeneracy of the second and third parameters in the Appell functions); one obtains the expansions [2]

$$P(\tau; k\alpha Z, \theta) = \frac{2\tau^2}{(\tau+1)^2 + \tau^2(k\alpha Z)^2/4} \times \sum_{t=0}^{\infty}(t+1)\left[-\frac{(k\alpha Z)^2}{4}\sin^2\frac{\theta}{2}\right]^t \times \frac{{}_2F_1(1, -1-t-\tau, 3-t-\tau; \sqrt{p})}{2+t-\tau} \tag{2.7}$$

and

$$Q(\tau; k\alpha Z, \theta) = \frac{\tau^2}{(\tau+1)^2 + \tau^2(k\alpha Z)^2/4}\frac{(k\alpha Z)^2}{4} \times \sum_{t=0}^{\infty}(t+1)(t+2)\left[-\frac{(k\alpha Z)^2}{4}\sin^2\frac{\theta}{2}\right]^t \times \frac{{}_2F_1(1, -2-t-\tau, 4-t-\tau; \sqrt{p})}{3+t-\tau}. \tag{2.8}$$

Here ${}_2F_1(a, b; c; u)$ is the Gauss hypergeometric function. The series of Equations (2.7) and (2.8) converge for any angle θ when the condition $\frac{(k\alpha Z)^2}{4} < 1$ (or $\hbar\omega < \alpha Z mc^2$)

is met; note that they are even in $(k\alpha Z)\sin\frac{\theta}{2}$.

By comparing Eqs. (2.3) and (2.6)–(2.8) with the dipole approximation expression of Gavrila [1], one may see that the dipole approximation is equivalent to setting αZ to zero everywhere in the retarded results except in k or τ. In this case O and Q become one and zero, respectively, and P becomes

$$P_{DA}(\tau) = \frac{2\tau^2}{(\tau+1)^2(2-\tau)} \times {}_2F_1\left(1,-1-\tau;3-\tau;\frac{(\tau-1)^2}{(\tau+1)^2}\right), \quad (2.9)$$

which is the nonretarded dipole approximation result obtained by Gavrila [1]. P_{DA} depends only on k (or τ), whereas the full multipole, retarded result depends separately on k and on αZ.

We then apply recursion relationships for the Gauss hypergeometric function. Keeping all terms of order $(\alpha Z)^2$ and $(\alpha Z)^4$, both above and below the photoelectric threshold, we obtain

$$M = 1 - C_0\left(k^2,\alpha Z\right) - \left(\frac{(k\alpha Z)^2}{2} + C_1\left(k^2,\alpha Z\right)\right)\sin^2\frac{\theta}{2} + \left(\frac{3(k\alpha Z)^4}{16} - C_2\left(k^2,\alpha Z\right)\right)\sin^4\frac{\theta}{2} \quad (2.10)$$

and

$$N = -\left(D_0\left(k^2,\alpha Z\right) + D_1\left(k^2,\alpha Z\right)\sin^2\frac{\theta}{2}\right), \quad (2.11)$$

where the anomalous terms are given by the C_i and D_i as

$$C_0\left(k^2,\alpha Z\right) = \left[1-(\alpha Z)^2 + \left(\frac{5}{8}k^2+1\right)(\alpha Z)^4\right]\left[P_{DA}(\tau_1)+P_{DA}(\tau_2)\right] + k(\alpha Z)^2\left[1-\frac{7}{4}(\alpha Z)^2\right]\left[P_{DA}(\tau_1)-P_{DA}(\tau_2)\right] + (\alpha Z)^2 - (\alpha Z)^4, \quad (2.12)$$

$$C_1\left(k^2,\alpha Z\right) = -\frac{6}{5}(\alpha Z)^2\left[1-2\left(k^2+1\right)(\alpha Z)^2\right]\left[1-P_{DA}(\tau_1)-P_{DA}(\tau_2)\right] - \frac{k}{5}(\alpha Z)^2\left[8-25(\alpha Z)^2\right]\left[P_{DA}(\tau_1)-P_{DA}(\tau_2)\right] - \frac{23}{10}k^2(\alpha Z)^4, \quad (2.13)$$

$$C_2\left(k^2,\alpha Z\right) = \frac{2(\alpha Z)^4}{35}\left\{12\left(3k^2+2\right)\left[P_{DA}(\tau_1)+P_{DA}(\tau_2)\right] - 59k\left[P_{DA}(\tau_1)-P_{DA}(\tau_2)\right] - 4\left(k^2+6\right)\right\}, \quad (2.14)$$

and, from Eqs. (2.7) and (2.8),

$$D_0 = -C_1/2, \quad D_1 = -C_2. \quad (2.15)$$

The other terms in Eq. (2.10) result from expanding the form factor. As we have used Eqs. (2.7) and (2.8) our results are valid for all angles only if $k \le 2/(\alpha Z)$. Equations (2.10) – (2.15) are our main results, and we shall show in Sec. III that they represent well exact numerical S-matrix data.

We note that the leading retardation corrections in the anomalous terms are proportional to the sum and difference of the nonrelativistic point-Coulombic dipole amplitudes P_{DA}, which have been shown by Gavrila [1] to be significant below the photoeffect threshold and above the photoelectric threshold to nearly 10 times the nonrelativistic binding energy.

It is interesting to point out how symmetry requirements are operating in Rayleigh scattering. The time reversal invariance of quantum mechanics implies that the Rayleigh matrix elements and the amplitudes are unchanged if the photon energy changes sign. Indeed, $\tau_1(-k) = \tau_2(k)$ so $P(\tau_1(-k)) = P(\tau_2(k))$ and $Q(\tau_1(-k)) = Q(\tau_2(k))$. This means that the sums $P(\tau_1,k\alpha Z)+P(\tau_2,k\alpha Z)$ and $Q(\tau_1,k\alpha Z)+Q(\tau_2,k\alpha Z)$ are invariant under the transformation $k \to -k$. This also means that $P(\tau_1,k\alpha Z)-P(\tau_2,k\alpha Z)$ and $Q(\tau_1,k\alpha Z)-Q(\tau_2,k\alpha Z)$ change sign under the same transformation. Thus all of the coefficients C_i must be even functions of k. Equations (2.12)–(2.14) show explicitly that this happens. In fact, the dominant terms, which are present separately in $P(\tau_1,k\alpha Z)$ and $P(\tau_2,k\alpha Z)$, cancel when these amplitudes are summed because they are odd functions of the photon energy. Such cancellations must involve the dominant dipole and some of the retardation corrections which are present in P and in Q, but disappear from the sums of these amplitudes.

Finally we note that, at high photon energies (but still where $k \le 2/\alpha Z$) [1], the sum

$$P_{DA}(\tau_1)+P_{DA}(\tau_2) = -\frac{16}{3k^2} + \frac{32}{3}\frac{1+i}{k^{2.5}} - \frac{32}{3}\frac{i\pi}{k^3} + \cdots.$$

$P_{DA}(\tau)$ and $P_{DA}(\tau_1)-P_{DA}(\tau_2)$ behave as $1/k$. Thus the coefficients C_i become independent of k and are smaller than the corresponding form-factor contributions. This means the anomalous scattering factors vary less with

energy than the form factor. This explains the use of the form factor with angle-independent anomalous scattering factors in the characterization of Rayleigh scattering [16]. Thus, in the nonrelativistic high-energy limit, retardation corrections are given adequately by the form factor.

As has been stated, our results are valid for any $k < 2/(\alpha Z)$, so we can use them both above and below the photoelectric threshold. Further simplification is possible below the first resonance ($k < 3/4$) where we can make use of expansions in k of the sum and difference of $P_{DA}(\tau_1)$ and $P_{DA}(\tau_2)$ so that

$$P_{DA}(\tau_1) + P_{DA}(\tau_2) = \sum_{t=0}^{\infty} S(-2t)\, k^{2t} \tag{2.16}$$

and

$$P_{DA}(\tau_1) - P_{DA}(\tau_2) = k \sum_{t=0}^{\infty} S(-2t-1)\, k^{2t}, \tag{2.17}$$

where $S(-r)$ are the negative order sum rules obtained by Dalgarno and Kingston [17] for $r \leq 6$ and by Gavrila [1] for $7 \leq r \leq 10$:

$$S(0) = S(-1) = 1, \quad S(-2) = 9/8,$$

$$S(-3) = 43/32, \quad S(-4) = 319/192, \ldots .$$

Note that the use of Eqs. (2.16) and (2.17) eliminates the need to calculate hypergeometric functions to obtain the amplitudes.

To fourth order in k the result in the region below the resonances is

$$C_0(k^2, (\alpha Z)^2) = 1 + \frac{k^2}{8}\left[9 - (\alpha Z)^2\right] + \frac{k^4}{192}\left[319 - 61(\alpha Z)^2 + \frac{5}{2}(\alpha Z)^4\right] + O\left[k^6 (\alpha Z)^2\right], \tag{2.18}$$

$$C_1(k^2, (\alpha Z)^2) = -\frac{(k\alpha Z)^2}{4}\left[1 + \frac{5}{8}k^2 - \frac{1}{8}(k\alpha Z)^2\right] + O\left[k^6 (\alpha Z)^2\right], \tag{2.19}$$

$$C_2(k^2, (\alpha Z)^2) = \frac{(k\alpha Z)^4}{16} + O\left[k^6 (\alpha Z)^2\right]. \tag{2.20}$$

Equation (2.18) was obtained previously, using an independent method, in connection with an extensive discussion of electrical, magnetic, and toroidal polarizabilities [18].

In the case of the K-shell Rayleigh forward scattering at low energies, the amplitudes are

$$M = 1 - C_0 = -\frac{k^2}{8}\left[9 - (\alpha Z)^2\right] - \frac{k^4}{192}\left[319 - 61(\alpha Z)^2 + \frac{5}{2}(\alpha Z)^4\right] \tag{2.21}$$

and

$$N = -D_0 = \frac{C_1}{2}. \tag{2.22}$$

It is worth noting that the main retardation term in the forward scattering amplitude gives the well known Langevin diamagnetic susceptibility [18]. Equation (2.21) shows that, in the low-energy limit, the largest correction due to retardation and higher multipoles for forward Rayleigh scattering is $(k\alpha Z)^2/8$, which is small compared with the dipole contribution $9k^2/8$ and is also smaller than relativistic corrections [which are $\frac{7}{8}(k\alpha Z)^2$ [19]]. While our results are valid for all angles, the corrections to the dipole angular distribution are small in this low-energy region as the leading corrections to the dipole angular dependence are of higher order in k.

III. NUMERICAL RESULTS

For purposes of comparison with the results of Kissel's S-matrix code [5] we rewrite the KHW matrix element M in terms of the two complex invariant amplitudes $A_{||}$ and $A_{\perp}$, the subscript indicating that, if the photon polarization is initially parallel or perpendicular to the scattering plane, it continues to have that property after scattering. We have

$$M_{\vec{\varepsilon}_1 \vec{\varepsilon}_2} = \vec{\varepsilon}_1^{\,||} \vec{\varepsilon}_2^{\,||} A_{||} + \vec{\varepsilon}_1^{\,\perp} \vec{\varepsilon}_2^{\,\perp} A_{\perp}, \tag{3.1}$$

where

$$A_{||} = M\cos\theta - N\sin^2\theta, \qquad A_{\perp} = M. \tag{3.2}$$

For unpolarized incident photons, the differential cross section for Rayleigh scattering is given by an average over incident photon polarization and a sum over scattered photon polarizations:

$$\frac{d\sigma_{\text{unpol}}}{d\Omega} = \frac{{r_0}^2}{2} \sum_{\vec{\varepsilon}_1} \sum_{\vec{\varepsilon}_2} |M_{\vec{\varepsilon}_1 \vec{\varepsilon}_2}|^2 = \frac{{r_0}^2}{2}\left(|A_{||}|^2 + |A_{\perp}|^2\right). \tag{3.3}$$

In Fig. 2 we present results obtained using Eqs. (2.10)–(2.15) for the scattering of 1.38, 8.04, and 22.1 keV photons from the K-shell electron of an aluminum ion (unless otherwise noted, all quantities in this section are calculated in a point-Coulomb potential). These energies are 0.6 (below the first resonance), 3.5, and 9.6 times the K-shell binding energy. We also give the nonrelativistic point-Coulombic dipole results, the nonrelativistic form-factor results, and results obtained using Kissel's S-matrix code. At the lowest photon energy considered here, below the photoionization threshold, the S-matrix results are adequately reproduced both by our calculations and by the dipole result. This indicates that retardation corrections are unimportant here, as discussed above. The need for further multipoles and for retardation corrections is evident in the remaining cases considered for scattering from aluminum. For photon energies 3.5 and 9.6 times the photoionization threshold the dipole result is no longer adequate for predicting the whole angular distribution. While most of these multipole and

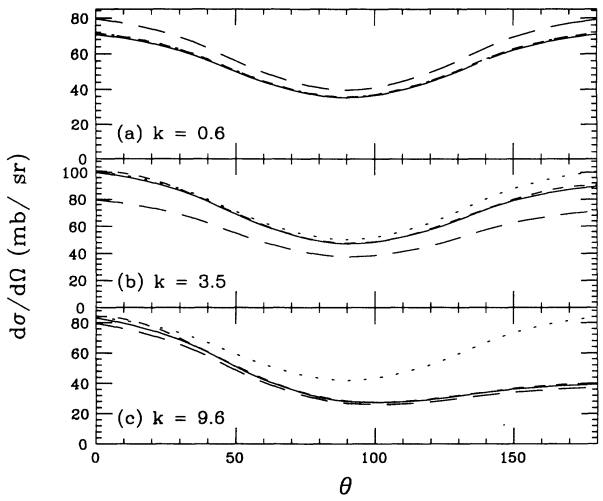

FIG. 2. Comparison of Rayleigh scattering cross section from our calculations (small dashed line), the nonrelativistic dipole result (dots), and the hydrogenic form factor (large dashed line) [13] with the second-order S-matrix code of Kissel *et al.* [5] (solid line) for the K shell of aluminum at photon energies of (a) 1.38, (b) 8.04, and (c) 22.1 keV.

retardation contributions are given by the form factor at the highest applied energy, the form factor is inadequate in the near and below threshold cases. As expected relativistic contributions are not important in any of these cases. The level of agreement between our approach and the second-order S-matrix may be seen in detail in Tables I and II. Differences between the approaches, which are quite small in general, become larger at higher energies and also where the amplitudes are small (for example at 90° in the amplitude $A_{||}$). These differences, though small, reflect the onset of the overestimation of the amplitude due to the spurious poles discussed above. We note that we have also compared our calculations with screened S-matrix calculations (not given here). While our results differ more from these screened calculations than from point-Coulombic calculations at the same photon energy, differences to the real part of the scattering amplitudes remain small ($< 5\%$) and relative differences to the imaginary parts of these amplitudes are nearly constant.

Figure 3 presents cross sections calculated within the same approaches as in Fig. 2 for the scattering of 18.0 ($k = 0.6$), 40.3 ($k = 1.3$), and 90.5 ($k = 3.0$) keV photons from the K-shell electrons of silver (Z=47). Below the K-shell photoionization threshold, no approximate theory accurately reproduces the S-matrix results, reflecting the need to include relativistic effects. Above threshold the S-matrix results are most adequately reproduced by our retarded results, particularly the asymmetric nature of the angular distribution. As with scattering from aluminum, the form-factor result fails at low energy above threshold. It reproduces some of the asymmetric nature of the angular distribution and works best for increasing photon energies.

These figures have shown that for low and intermediate Z, and for energies somewhat above the photoelectric effect threshold, our results [based on Eqs. (2.10)–(2.15)] are quite reasonable and are particularly useful in understanding the angular distribution of the scattered radiation. For elements of high nuclear charge there is a small region above threshold and far from the spurious poles where our results are valid. However, as discussed above, in this region and below threshold relativistic cor-

TABLE I. Comparison of the Rayleigh scattering amplitude $A_{||}$ obtained within our approach (NR) to the relativistic S-matrix results of Kissel *et al.* [5] (REL) for photons of energies 1.38, 8.04, and 22.1 keV incident on the K-shell electrons of aluminum.

		Real			Imaginary		
k	θ	NR	REL	%	NR	REL	%
0.6	0	0.949	0.944	0.58			
	30	0.822	0.817	0.59			
	60	0.474	0.472	0.59			
	90	-5.4×10^{-4}	-5.3×10^{-4}	1.8			
	120	-0.475	-0.473	0.58			
	150	-0.823	-0.818	0.58			
	180	-0.950	-0.944	0.58			
3.5	0	-1.120	-1.113	0.56	0.128	0.125	2.0
	30	-0.966	-0.960	0.59	0.110	0.107	2.1
	60	-0.550	-0.547	0.7	0.061	0.060	2.2
	90	3.13×10^{-3}	3.14×10^{-3}	0.3	-2.46×10^{-3}	-2.43×10^{-3}	1.2
	120	0.539	0.537	0.34	-0.064	-0.063	1.6
	150	0.923	0.918	0.49	-0.107	-0.104	2.0
	180	1.061	1.055	0.52	-0.123	-0.120	2.1
9.6	0	-1.031	-1.023	0.73	0.017	0.016	7.6
	30	-0.867	-0.861	0.70	0.014	0.013	7.9
	60	-0.463	-0.460	0.65	7.44×10^{-3}	6.91×10^{-3}	7.7
	90	-3.7×10^{-3}	-3.7×10^{-3}	0.0	-1.0×10^{-3}	-9.4×10^{-4}	7.0
	120	0.389	0.387	0.51	-8.5×10^{-3}	-7.8×10^{-3}	8.9
	150	0.629	0.625	0.22	-0.013	-0.012	7.3
	180	0.709	0.704	0.6	-0.015	-0.014	7.6

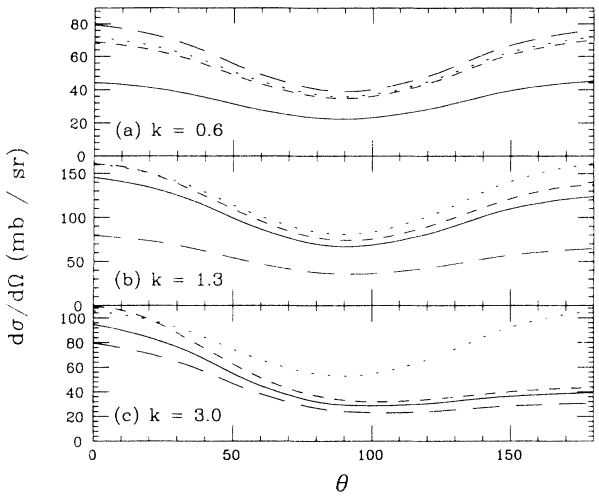

FIG. 3. Same as Fig. 2, for the K shell of silver at photon energies of (a) 18.0, (b) 40.3, and (c) 90.5 keV.

rections are at least as important as retardation corrections. While we are not primarily interested in this region, in Table III we present (as a test of our simple formulas) a comparison between our calculations using the simple formulas [Eqs. (2.18) and (2.19)], the results of Florescu *et al.* [7], and the S-matrix predictions for forward scattering. Note that we follow the method of Roy and Pratt [6], using k to denote the ratio of the photon energy to the relativistic Coulombic K-shell binding energy in using the nonrelativistic theories. (We give the nonrelativistic values of k for reference.) This shift takes account of some relativistic corrections to the binding energy. It cannot be expected to work too near to resonance, where the detailed resonant structure may only be described relativistically (this is because the shift that we have applied, which is appropriate for the K shell, overestimates the shift of the L-shell binding energy). Because neglected terms are of order k^2 times the highest order terms retained in our expansion, these terms are negligible only at low photon energies. This may be seen to be true for $k \leq 0.4$ where our simple formulas are sufficient to accurately describe the nonrelativistic result which differs from the relativistic prediction, as expected.

TABLE II. Comparison of the Rayleigh scattering amplitude $A_\perp$ obtained within our approach (NR) to the relativistic S-matrix results of Kissel *et al.* [5] (REL) for photons of energies 1.38, 8.04, and 22.1 keV incident on the K-shell electrons of aluminum.

		Real			Imaginary		
k	θ	NR	REL	%	NR	REL	%
0.6	0	0.949	0.944	0.58			
	30	0.949	0.944	0.58			
	60	0.949	0.944	0.58			
	90	0.949	0.944	0.58			
	120	0.950	0.944	0.58			
	150	0.950	0.944	0.58			
	180	0.950	0.944	0.58			
3.5	0	-1.120	-1.114	0.56	0.128	0.125	2.0
	30	-1.116	-1.110	0.56	0.127	0.125	2.0
	60	-1.105	-1.099	0.56	0.126	0.124	2.0
	90	-1.090	-1.084	0.55	0.125	0.122	2.1
	120	-1.075	-1.069	0.54	0.124	0.121	2.1
	150	-1.064	-1.059	0.53	0.123	0.120	2.1
	180	-1.061	-1.055	0.53	0.123	0.120	2.1
9.6	0	-1.031	-1.023	0.73	0.017	0.016	7.6
	30	-1.002	-0.995	0.73	0.017	0.016	7.6
	60	-0.932	-0.925	0.73	0.016	0.015	7.7
	90	-0.847	-0.841	0.7	0.016	0.015	7.7
	120	-0.774	-0.768	0.66	0.015	0.014	7.7
	150	-0.726	-0.721	0.62	0.015	0.014	7.7
	180	-0.709	-0.704	0.6	0.015	0.014	7.7

The optical theorem gives the following relationship between the total photoeffect cross section and the imaginary part of the forward Rayleigh amplitude

$$\sigma_{\rm ph} = \frac{4\pi mc^2}{\alpha\omega} |{\rm Im}A_\perp(\omega, \theta = 0)| , \tag{3.4}$$

where we have neglected the contributions of bound-bound transitions to the inelastic photon-atom interaction. In Fig. 4 we compare photoeffect cross sections by inserting the imaginary part of the forward scattering amplitude given in Eqs. (2.10)–(2.15) into Eq. (3.4) with the nonrelativistic dipole results of Eq. (1.1), with the full nonrelativistic results of Eq. (1.2), with the relativistic Coulombic photoeffect calculations of Hultberg *et al.* [14] and with the relativistic screened results of Scofield [15]. While the calculations of Hultberg *et al.* and Scofield are relativistic, we do not expect the region above the K-shell photoelectric threshold to be a region where relativistic effects dominate higher multipole and retardation corrections. For aluminum, agreement between all of the approaches is rather good. The screened calculations agree reasonably well, confirming expectations, at least for forward scattering, that screen-

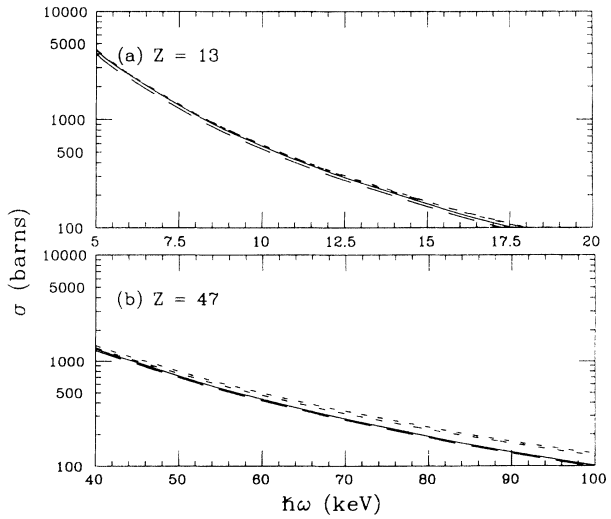

FIG. 4. Comparison of photoeffect cross section from our calculations (small dashed line) to screened relativistic results of Scofield [15] (large dashed line) and to the relativistic Coulombic results of Hultberg *et al.* [14], for the K shell of (a) aluminum and (b) silver. Also shown are results obtained using Eqs. (1.1) and (1.2).

TABLE III. A comparison between results obtained using our simple formula (NRET), the nonrelativistic dipole approximation (NRDPA), and the relativistic S-matrix result (RMP) for the forward scattering of photons at energies below threshold from lead (Z=82). Also shown are the relativistic dipole results of Florescu *et al.* [7] (RDLWL) and the relativistic dipole result of Roy and Pratt [6] (RDP) where available.

ω_{keV}	k_{NR}	k_{rel}	NRD	RMP	RDLWL	RDP	NRET
0.1	0.0011	0.00098					-1.05×10^{-6}
0.5	0.0055	0.0049					-2.62×10^{-6}
1.0	0.0109	0.0098					-1.05×10^{-4}
5.4	0.0591	0.0533	-0.00245	-0.00254	-0.00254	-0.00396	-0.00307
17.4	0.1905	0.1716	-0.0265	-0.027	-0.0275	-0.0432	-0.0332
40.9	0.4469	0.4021	-0.183	-0.187	-0.191	-0.323	-0.215
59.5	0.6504	0.5857	-0.627		-0.655	-1.537	-0.553

ing effects are not particularly large for K-shell scattering away from threshold (as we know for photoeffect at these energies). The silver results agree fairly well at low photon energies, but the results computed using our forward Rayleigh amplitudes and Eq. (3.4) are substantially larger at higher photon energies from both the relativistic (screened or Coulombic) calculations. Here the full multipole nonrelativistic approach with retardation reaches the limits of its validity due to the spurious poles mentioned above. The nonrelativistic, nonretarded dipole results agree reasonably well with the fully relativistic results at all energies in this case, implying a cancellation of the poles by relativistic contributions (as will be demonstrated explicitly in a subsequent paper [8]). We have calculated, but have not shown, results for lead because, at this high Z, the spurious poles in the retarded result cause large discrepancies with the relativistic calculations.

IV. CONCLUSIONS

In this work we have considerably simplified the nonrelativistic full multipole retarded amplitude for Coulombic K-shell Rayleigh scattering obtained by Gavrila and Costescu [2]. We express the result, including multipole and retardation effects, in terms of corrections to the nonretarded dipole result of Gavrila [1]. For very low photon energies, below the K-shell photoelectric threshold, we obtain particularly simple formulas for the amplitude. We show that the corrections due to retardation are smaller than those due to relativistic effects in this region and demonstrate that the angular distribution is well described by the dipole approximation. Above the photoelectric threshold, corrections due to including higher multipoles and retardation start to dominate relativistic corrections. Here we find that our results are significantly better than the form factor at low energies. The leading retardation corrections to the dipole form factor (which is unity) are of order $(k\alpha Z^2)$, which is of the order of our corrections to the remaining terms of the nonrelativistic amplitude (and angular distribution). We accurately predict the asymmetric angular distribution. The nonrelativistic retarded approach starts to fail at higher energies, however, where spurious poles in the full nonrelativistic results cause our results to overestimate the amplitude. As will be discussed in a subsequent paper, these spurious poles are canceled when relativistic corrections are included. As a result, the formalism presented here is useful only for energies where the contributions of these poles are not significant.

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