

Relativistic effects on low-frequency Rayleigh scattering including spin flip for hydrogenic atoms

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We present an approximate analytic expression for the low-frequency ground-state relativistic Rayleigh scattering matrix elements for hydrogenic atoms, including the possibility of electron spin flip as a result of the elastic photon atom scattering. Our expression is obtained by taking the long-wavelength approximation in the relativistic Coulomb matrix elements, without neglecting the photon frequency dependence in the Coulomb Green operator. By comparison with existing exact numerical calculations, we demonstrate that our approximation is appropriate for photon frequencies below the photoelectric threshold, at least for the non-spin-flip amplitude. Using our expressions, we investigate two issues: (i) the comparison of static and dynamical polarizabilities, and (ii) the behavior of the electron spin-flip amplitude, related to magnetic scattering.

I. INTRODUCTION

We wish to discuss relativistic features in the low-frequency Rayleigh (photon) scattering from hydrogenic atoms, including spin-orientation effects.

Rayleigh scattering by hydrogenic atoms in the ground state can be described by analytic equations. Three particular cases have been investigated in detail: (i) the nonrelativistic dipole approximation,¹ (ii) the nonrelativistic case with full inclusion of retardation,² and (iii) the relativistic high-frequency limit³ ($\omega \rightarrow \infty$, with finite momentum transfer). An earlier work on both nonrelativistic and relativistic cases remained unfinished,⁴ but stimulated the first numerical calculations.⁵ A very recent calculation⁶ expresses the relativistic matrix element by a series of some special functions, but does not explore in detail the numerical consequences. Exact numerical results are available in several particular cases from the Rayleigh scattering code designed for many electron atoms.⁷ There are several reviews of Rayleigh scattering⁸⁻¹⁰ emphasizing the x- and γ -ray regions. A study of relativistic dynamic polarizability of hydrogen is mentioned in Ref. 11, but its behavior is described only qualitatively.

Here we describe the approach to Rayleigh scattering representing the long-wavelength limit of the exact matrix element, suited in principle for photon energies much smaller than the electron rest energy multiplied by αZ (α is the fine-structure constant and Z is the nuclear charge). This does not involve (see Ref. 12) neglecting the dependence on the photon frequency in the Green's propagator (the static limit). We include the possibility of spin flip in the scattering process. The approach is presented in Sec. II, also giving the explicit expression of the analytic results. Some limiting cases are discussed in Sec. III. We show also that at low frequencies and for not-too-high- Z ions the relativistic corrections are more important than retardation effects. In Sec. IV, devoted to numerical re-

sults, we first compare in Table I our results with several exact results. We find that below the photoelectric threshold the relativistic effects are the main explanation for deviations from the nonrelativistic dipole approximation. We present then some of the predictions of our analytic formulas. In Table II we note a comparison between static and dynamic polarizabilities. In Table III we illustrate the behavior of the two scalar amplitudes in the transition matrix below the first resonance and in Table IV between the first two resonances.

II. RELATIVISTIC RAYLEIGH SCATTERING IN THE LONG-WAVELENGTH LIMIT

We consider the relativistic 2×2 matrix describing Rayleigh scattering by a ground-state electron in hydrogenic atoms:³

$$M_{mm'} = \sum_{j,k} s_{1j} s_{2k}^* \alpha_{kj}^{mm'}(\omega). \quad (1)$$

(If we are not taking the long-wavelength limit the α will also depend on the photon momenta \mathbf{k}_1 and \mathbf{k}_2 .) We denote by \mathbf{s}_1 and \mathbf{s}_2 the initial and scattered photon polarization vectors and by m and m' the values of the initial and, respectively, the final electron spin components on a fixed axis with unit vector \mathbf{e}_3 . If in the exact expression of the tensor α the exponentials $e^{i\mathbf{k}_1 \cdot \mathbf{r}}$ and $e^{-i\mathbf{k}_2 \cdot \mathbf{r}}$ are replaced by 1, one obtains

$$\alpha_{kj}^{mm'} = -m_e c^2 \langle 1m | \alpha_k G(\Omega_1) \alpha_j + \alpha_j G(\Omega_2) \alpha_k | 1m' \rangle. \quad (2)$$

Here $|1m\rangle$ is the ground-state bispinor with spin component m on the \mathbf{e}_3 axis, α are the Dirac matrices, G is the electron relativistic Coulomb resolvent, m_e is the electron mass, c is the velocity of light, and

$$\Omega_{\frac{1}{2}} = E_1 \pm \hbar\omega, \quad (3)$$

where E_1 is the ground-state relativistic energy and ω is the photon frequency.

By comparison with the exact matrix element for Rayleigh scattering, in which in an exact numerical calculation⁷ factors of the type $(\boldsymbol{\alpha} \cdot \mathbf{s})(e^{i\mathbf{k} \cdot \mathbf{r}})$ are expanded in multipole terms (electric and magnetic), Eq. (2) corresponds to the neglect of all multipoles, excepting the dipole electric term ($L=1$) together with the replacement of the spherical Bessel function j_0 by 1 and the neglect of the Bessel function j_1 (long-wavelength limit approximation). However the parameters Ω_1 and Ω_2 are not altered, which keeps the tensor matrix $\alpha_{jk}^{mm'}$ frequency dependent.

The approximate approach just described appears to have a rather large domain of validity. We shall report in Sec. III that at low frequencies and for small αZ the retardation correction to the non-spin-flip amplitude is smaller than the relativistic correction. A comparison with exact numerical results, described in Sec. IV, indicates that even for Z as high as 82 and for photon frequencies not too close to the photoelectric threshold, the relativistic corrections are predominant. Our approximation is also interesting because it gives information about the spin-flip process that can take place during the photon scattering. Such a process is the object of recent studies on x-ray scattering on solid targets. In general it originates from magnetic as well as from electric interactions.¹³

The tensor matrix α can be expressed in terms of two scalar amplitudes A and B :

$$\alpha_{jk}^{mm'}(\omega) = A(\omega)\delta_{jk}\delta_{mm'} + iB(\omega)\varepsilon_{jkl}(\sigma_l)_{mm'}, \quad (4)$$

where σ are Pauli matrices, $(\sigma_l)_{mm'}$ their matrix elements, and ε the Levi-Civita tensor. This expression is in agreement with the general structure of the dynamic polarizability tensor.^{14,15} Because of the spin character of the ground state only two invariant amplitudes characterize the transition.

For $m = m'$, we get the non-spin-flip amplitudes

$$M_{\pm\pm} = A(\omega)\mathbf{s}_1 \cdot \mathbf{s}_2^* \pm iB(\omega)(\mathbf{s}_2 \times \mathbf{s}_1) \cdot \boldsymbol{\xi}. \quad (5)$$

In the ground-state case we consider here, the second term does not appear in the nonrelativistic calculations, even when retardation is included.

For $m \neq m'$, the spin-flip amplitudes are

$$M_{\pm\mp} = iB(\omega)(\mathbf{s}_2^* \times \mathbf{s}_1) \cdot (\mathbf{e}_1 \mp i\mathbf{e}_2), \quad (6)$$

where \mathbf{e}_1 and \mathbf{e}_2 form, together with \mathbf{e}_3 already mentioned, an orthonormal basis in the geometrical space. To our knowledge the amplitude B has not been studied in the low-frequency regime. In the high-energy limit³ this amplitude survives in the same way as the non-spin-flip amplitude.

A characteristic of our approximation, like any long-wavelength approximation, is the independence of the

scalar amplitude A of the scattering angle. The amplitude B has the same property. Retardation effects change this behavior.

From the matrix elements (5) and (6) one constructs different observable quantities, referring to different types of experiments (polarized or unpolarized atomic hydrogen, polarized or unpolarized initial photons, etc.). The necessary formulas are easily obtained. We reproduce here only the quantities referring to unpolarized hydrogen:

$$\frac{1}{2} \sum_{m,m'} |M_{mm'}|^2 = (|A|^2 - |B|^2)|\mathbf{s}_1 \cdot \mathbf{s}_2|^2 + |B|^2, \quad (7)$$

$$\frac{1}{4} \sum_{s_1} \sum_{m,m'} |M_{mm'}|^2 = \frac{1}{2}(|A|^2 - |B|^2)(1 - |\mathbf{s}_2 \cdot \mathbf{v}_1|^2) + |B|^2, \quad (8)$$

$$\frac{1}{4} \sum_{s_1, s_2} \sum_{m,m'} |M_{mm'}|^2 = \frac{1}{2}(|A|^2 - |B|^2)(1 + \cos^2\theta) + 2|B|^2. \quad (9)$$

\mathbf{v}_1 and \mathbf{v}_2 are unit vectors along the initial and final photon momenta and θ denotes the angle between these vectors.

Now we try to see how the new amplitude B affects the results. From Eq. (7) it follows that for orthogonal polarizations of the incident and final photon, the scattering cross section is determined only by B . Equation (8) shows that for unpolarized initial photons and final polarization orthogonal to the initial photon momentum ($\mathbf{s}_2 \cdot \mathbf{v}_1 = 0$), the scattering is also conditioned only by the fact that B is not zero.

If the hydrogenic results are extended to a many-electron atom (without including the electron interactions, a fairly good approximation in heavy elements) the K -shell contribution to the elastic photon scattering will be

$$M_K = \sum_m M_{mm} = 2A(\omega)\mathbf{s}_1 \cdot \mathbf{s}_2^*. \quad (10)$$

Now we describe the *analytic* results for the invariant amplitudes A and B in our approach. Due to the structure of Eq. (2), A and B are each constructed from two terms:

$$A(\omega) = a(\Omega_1) + a(\Omega_2), \quad (11)$$

$$B(\omega) = b(\Omega_1) - b(\Omega_2),$$

so analytic expressions of two functions, a and b , have to be described. These functions are given by radial integrals, which we are able to evaluate using previous results for the relativistic perturbed Coulomb $1s$ orbital in the long wavelength limit.¹⁶ We find that A and B are the combinations,

$$\begin{aligned} a(\Omega) &= \frac{1}{3\sqrt{3}}(I_1 + 2\sqrt{2}I_2), \\ b(\Omega) &= \frac{1}{3\sqrt{3}}(I_1 - \sqrt{2}I_2), \end{aligned} \quad (12)$$

of two quantities I_1 and I_2 representing, respectively, the contribution of all $p_{1/2}$ and all $p_{3/2}$ virtual intermediate states (bound and continuum) to Rayleigh scattering. Other intermediate states do not contribute in our approximation.

We first explain the parameters entering the expression of I_1 and I_2 :

$$\gamma_k = (k^2 - \alpha^2 Z^2)^{1/2} \quad (k=1,2)$$

$$\lambda = \alpha Z m_e c,$$

$$X = \left[m_e^2 c^2 - \frac{\Omega^2}{c^2} \right]^{1/2} \quad (\text{Re}X > 0),$$

$$Z = \frac{\lambda}{X} \frac{\Omega}{m_e c^2}.$$

The expression of I_1 is rather simple, containing an elementary function and a hypergeometric Gauss function

$$\begin{aligned} I_1 &= -\frac{1}{2\sqrt{3}} \left[1 + \frac{\Omega}{m_e c^2} \right]^{-1} \frac{(2\gamma_1 + 1)(1 + \lambda/X + \gamma_1 + Z)^2}{(1 + \gamma_1)(\gamma_1 + Z)(1 + \lambda/X)} \\ &\quad \times \left\{ \delta_1 + \delta_2 \frac{(4\lambda X)^{2\gamma_1 + 1}}{(X + \lambda)^{4\gamma_1 + 2}} {}_2F_1 \left[\gamma_1 - Z + 1, 2\gamma_1 + 2, \gamma_1 - Z + 2; \left[\frac{X - \lambda}{X + \lambda} \right]^2 \right] \right\}, \end{aligned} \quad (14)$$

with

$$\delta_1 = 2\gamma_1 + 1,$$

$$\delta_2 = -\frac{4}{\gamma_1 - \delta + 1} \left[\frac{(\lambda/X)(1 + \gamma_1) - Z}{1 + \frac{\lambda}{X}} \right]^2.$$

The expression of I_2 is more complicated:

$$\begin{aligned} I_2 &= \frac{1}{2\sqrt{6}} \left[1 + \frac{\Omega}{m_e c^2} \right] \frac{\lambda}{2X + \lambda} \frac{1}{1 + \gamma_1} \frac{1}{\Gamma(2\gamma_1 + 1)} \\ &\quad \times \left[\left[\frac{2X}{X + \lambda} \right]^{2\gamma_2} \left[\frac{2\lambda}{X + \lambda} \right]^{2\gamma_1 + 2} \frac{\Gamma^2(\gamma_1 + \gamma_2 + 1)}{\Gamma(2\gamma_2 + 1)} T - \Gamma(2\gamma_1 + 2) \right], \end{aligned} \quad (15)$$

where T is the series

$$\begin{aligned} T &\equiv \frac{1}{\gamma_2 - Z} \sum_m \frac{(\gamma_2 - Z)_m (2\gamma_2 + 1)_m}{(\gamma_2 - Z + 1)_m j_m} \left[\left(1 + \frac{\lambda}{X} - \gamma_1 - \delta \right) {}_2F_1 \left[-m, \gamma_1 + \gamma_2 + 1, 2\gamma_2 + 1; \frac{2X}{X + \delta} \right] \right. \\ &\quad \left. + (\gamma_1 + \gamma_2 + 1) {}_2F_1 \left[-m, \gamma_1 + \gamma_2 + 1, 2\gamma_2 + 1; \frac{2X}{X + \lambda} \right] \right]^2. \end{aligned} \quad (16)$$

For photon frequencies below the photoelectric threshold all the quantities involved in our equations are real. Due to the neglect of higher multipoles, the scattering amplitude does not incorporate all the resonances of the relativistic hydrogenic atom, but only those which correspond to transitions from the ground state to the fine-structure levels with total angular momentum number $j=1/2$ and $3/2$. The position of these resonances is exactly the same as in an exact treatment of the problem and, of course, it is different from the positions in the nonrelativistic approximation, the difference increasing with Z .

III. THE NONRELATIVISTIC LIMIT: RELATIVISTIC EFFECTS ON THE DYNAMIC DIPOLE POLARIZABILITY

It is first interesting to see how the nonrelativistic limit is contained in our equations. By replacing γ_1 by 1 and γ_2 by 2, and considering also that $\hbar\omega/m_e c^2 \ll 1$, we get the results

$$I_1^{\text{NR}} = -\frac{3\sqrt{3}}{2} + \sqrt{3}P(\Omega^{\text{NR}}),$$

$$I_2^{\text{NR}} = \sqrt{\frac{3}{2}}P(\Omega^{\text{NR}}), \quad (17)$$

where $P(\Omega^{\text{NR}})$ is Gavrila's amplitude [Eq. (54) of Ref. 1]. In the limit considered here the parameters in Eq. (13) take their nonrelativistic meaning. We mention only the connection $\Omega = m_e c^2 + \Omega^{\text{NR}}$, a relation valid if one neglects terms of the order $(\alpha Z)^4$. Then, from Eq. (12) we get

$$\begin{aligned} a^{\text{NR}}(\Omega) &= -\frac{1}{2} + P(\Omega^{\text{NR}}), \\ b^{\text{NR}}(\Omega) &= -\frac{1}{2}. \end{aligned} \quad (18)$$

These results together with Eq. (11) lead to

$$\begin{aligned} A^{\text{NR}}(\omega) &= -[1 - P(\Omega_1^{\text{NR}}) - P(\Omega_2^{\text{NR}})], \\ B^{\text{NR}}(\omega) &= 0. \end{aligned} \quad (19)$$

In this way Gavrila's result is recovered, and we also have a direct proof that the nonrelativistic limit of the spin-flip amplitude is zero.

It is interesting to note that the first term in $A^{\text{NR}}(\omega)$, which is equal to -1 , comes only from $p_{1/2}$ intermediate states; on the other hand it is known (Ref. 12) that this term, which in the nonrelativistic case represents the \mathbf{A}^2 term contribution (\mathbf{A} the potential vector of the electromagnetic field) comes from negative continuum (positron) states. The $p_{1/2}$ states contribute one third and the $p_{3/2}$ states contribute two thirds of the other terms in the total amplitude.

Now we discuss the behavior of the matrix element for $\omega \rightarrow 0$. For this purpose it is useful to transform each term in Eq. (2) as follows:

$$\begin{aligned} &\langle 1m | \alpha_j G(\Omega) \alpha_k | 1m' \rangle \\ &= \frac{1}{i\hbar} \langle 1m | x_j \alpha_k | 1m' \rangle + \frac{\Omega - E_1}{\hbar c} \langle 1m | x_j x_k | 1m' \rangle \\ &\quad + \frac{(\Omega - E_1)^2}{\hbar^2 c^2} \langle 1m | x_j x_k G(\Omega) | 1m' \rangle. \end{aligned} \quad (20)$$

The identity is based on the successive use of the relation $\langle k | \alpha | n \rangle = (1/i\hbar c)(E_n - E_k) \langle k | \mathbf{r} | n \rangle$ between the matrix elements of the Dirac matrices α and of the position vector \mathbf{r} , taken between Dirac energy eigenstates. The first two terms in (20) have simple expressions; since according to (3) $\Omega_{1/2} = E_1 \pm \hbar\omega$, one can obtain the first term in the low-frequency expansion of the functions $a(\Omega)$ and $b(\Omega)$.

We express the low-frequency results with photon energy measured in $Z^2 x \text{ Ry}$:

$$k \equiv \frac{2\hbar\omega}{(\alpha Z)^2 m_e c^2}. \quad (21)$$

We have in this way

$$a(\Omega_1) \simeq \pm \frac{k}{12} (1 + \gamma_1)(2\gamma_1 + 1) - \frac{1}{8} \alpha_0 k^2, \quad (22)$$

$$b(\Omega_1) \simeq -\frac{1}{6} (2\gamma_1 + 1) + \beta_0 k^2. \quad (23)$$

Then, from Eq. (11) we obtain

$$A(\omega) \simeq -\frac{1}{4} \alpha_0 k^2 + O(k^4), \quad (24)$$

$$B(\omega) \simeq O(k^3), \quad (25)$$

in agreement with the general properties (see Ref. 15)

$$A(-\omega) = A(\omega), \quad B(-\omega) = -B(\omega).$$

The coefficient α_0 in Eqs. (22) and (24) is the *relativistic static dipole polarizability* of the ground state (up to the dimensional factor a_0^3 , with a_0 the Bohr radius). This quantity has been studied by many authors. The simplest expression for α_0 is that given by Zon, Manakov, and Rapaport.¹⁷ Precise numerical values were also presented by these authors. A more complicated expression together with numerical results has been given by Shestakov and Khristenko,¹⁸ and recently a very precise numerical evaluation of α_0 was published by Goldman.¹⁹

The first term in the expansion of the static polarizability α_0 in terms of $(\alpha Z)^2$ has been known for a long time.²⁰ Using it in combination with Eq. (24) one has

$$A(\omega) \simeq -\frac{9}{8} k^2 [1 - \frac{28}{27} (\alpha Z)^2]. \quad (26)$$

The first term is the nonrelativistic term¹ and the second is the first relativistic correction in the low-frequency regime. The neglected terms are of orders k^4 and $k^2(\Omega)^4$. Equation (26) offers a first argument in favor of including relativistic effects in comparison with retardation effects, in the low-frequency, low- αZ cases: it has been proven recently²¹ that retardation effects in the nonrelativistic regime lead to the behavior

$$A^{\text{NR,ret}} \simeq -\frac{9}{8} k^2 [1 - \frac{1}{9} (\alpha Z)^2]. \quad (27)$$

The first retardation correction in (27) and the first relativistic correction in (26) are both of the order $k^2(\alpha Z)^2$, but the coefficient of the retardation correction is smaller than that of the relativistic correction. Our numerical evaluation based on our analytic results in Sec. II will emphasize where relativistic corrections become important.

IV. NUMERICAL RESULTS

We present representative numerical data for frequencies below the K -shell photoelectric threshold.

We mention that in the numerical evaluation of I_2 [Eqs. (15) and (16)], some care has to be taken in evaluating the series T . The convergence of this series is not too fast, especially for increasing Z and k . Precise evaluation is required, especially at low values of k , because there are cancellations between the two terms in Eq. (11). The quantity B is the most sensitive to this. Also, a simple evaluation of the polynomial ${}_2F_1$ in Eq. (16) for large values of m ($m > 20$) usually can lead to errors, now because of cancellations in the polynomial itself. We have chosen appropriate methods, like analytic continuations of the Gauss function, for evaluating these polynomials.

First we present, in Table I, a comparison between the values of the amplitude A and its values taken from the literature^{7,22} or calculated recently,²³ representing "exact" results, i.e., including "all" multipoles in a relativistic treatment. The results in Table I refer to several values of the nuclear charge Z . The photon energy is

TABLE I. Comparison between the values of the amplitude A in Eq. (5) in our calculations (RDPLWL), exact calculation (RMP), and the approximations RDP and NRDPA (from references described in the text) as functions of the photon energy, for different values of Z .

Z	$\hbar\omega$ (keV)	k	RMP	RDP	RDPLWL	NRDPA	Σ
13		0.3	-0.115 85		-0.115 843	-0.117 02	0.006
		0.5	-0.452 87		-0.452 70	-0.458 45	0.04
		0.7	-3.069 51		-3.0532	-3.1771	0.5
		0.74	-13.6315		-13.2205	-15.764	3.0
30		0.1012	-0.011 06		-0.111 22	-0.011 705	0.6
		0.3037	-0.113 29		-0.113 96	-0.120 383	0.6
		0.5061	-0.442 81		-0.445 924	-0.477 669	0.7
		0.7491	-13.833		-13.969	-170.833	1.0
47	5.41	0.1800	-0.033	-0.0335	-0.033 576	-0.038 29	1.7
	17.43	0.5799	-0.646	-0.649	-0.658 13	-0.8089	1.9
	22.10	0.7353	-3.711	-3.713	-3.7967	-10.77	2.3
	26.0	0.8650	0.890	0.895	0.952 26	-0.4015	7.0
82	5.41	0.059 14	-0.002 45	-0.002 54	-0.002 544 3	-0.003 955	3.8
	17.43	0.1905	-0.0265	-0.027	-0.027 484	-0.043 16	3.7
	40.85	0.4469	-0.183	-0.1865	-0.190 75	-0.323 33	4.2
	59.5	0.6504	-0.627		-0.655 06	-1.537	4.5
	74.96	0.8194	-10.53	-10.535	-10.450	1.6559	0.8
	84.26	0.9210	1.2115	1.2155	1.4277	0.7290	18.0
90		0.1140	-0.008 194		-0.008 533 8	-0.014 912	4.1
		0.3421	-0.083 473		-0.087 221	-0.159 75	4.5
		0.5701	-0.320 40		-0.337 60	-0.750 15	5.4
		0.8437	-25.766		-24.307	0.709 43	5.7

given in both keV and Z^2x Ry for the cases in which the calculation in the literature corresponds to a photon energy given in keV. The column RMP gives the exact results (relativistic multipole). For $Z=13, 30$, and 90 we reproduce numbers given by Zhou.²³ The values for $Z=47$ are taken from Ref. 22, together with the values for $Z=82$, with two exceptions: the result for photon energy 59.5 keV comes from Ref. 7 and that for $Z=82$ and the energy 5.41 keV is the one recalculated recently²³ with increased precision compared to Ref. 22. The column RDP represents the contribution of the relativis-

tic electric dipole term with retardation included, as calculated in the literature,²² but the value for $Z=82$ and photon energy 5.41 keV is one calculated with higher precision by Zhou.²³ Following the phase convention in Ref. 1 the signs of RMP and RDP are the opposite of those in Refs. 7 and 22. Our results are presented in the column RDPLWL (relativistic dipole in the long-wavelength limit). The next column (NRDPA) presents numbers calculated by us from the nonrelativistic dipole approximation formula of Gavrilă. The last column gives the modulus of the relative error ϵ of our approach

TABLE II. Ratio between the non-spin amplitude A in our calculation and in the nonrelativistic dipole approximation. The values in the first line represent the same ratio for the static polarizabilities from Refs. 17 ($Z=1, 3, 30, 50$, and 70) and 18 ($Z=13$ and 92).

Z	1	3	13	30	50	70	92
k							
0.0	0.999 945	0.999 503	0.990 69	0.950 569	0.864 040	0.737 525	0.557 04
0.001	0.999 945	0.999 503	0.990 68	0.950 57	0.863 99	0.737 28	0.557 10
0.1	0.999 944	0.999 499	0.990 606	0.950 206	0.863 111	0.735 935	0.554 821
0.2	0.999 443	0.999 487	0.990 377	0.949 031	0.860 121	0.730 872	0.548 096
0.3	0.999 440	0.999 463	0.989 927	0.946 731	0.854 317	0.721 153	0.535 351
0.4	0.999 935	0.999 418	0.989 098	0.942 527	0.843 863	0.704 037	0.513 633
0.5	0.999 925	0.999 329	0.987 452	0.934 288	0.823 945	0.672 711	0.476 086
0.6	0.999 900	0.999 104	0.983 310	0.914 151	0.778 088	0.606 180	0.404 285
0.7	0.999 761	0.997 857	0.960 991	0.817 650	0.599 172	0.399 302	0.228 496
0.74	0.999 863	0.989 878	0.838 671	0.489 856	0.246 186	0.129 063	0.063 070

TABLE III. Values of the amplitudes A and B [see Eq. (5)] for several values of Z and k . Quantities in square brackets represent powers of 10 by which the numbers are to be multiplied.

k	Z	1	3	13	30	50	70	92
0.1	A	-1.141 82[-2]	-1.141 32[-2]	-1.131 16[-2]	-1.085 03[-2]	-9.855 76[-3]	-8.403 56[-3]	-6.335 43[-3]
	B	4.1505[-9]	3.7337[-8]	6.9458[-7]	3.5404[-6]	8.8858[-6]	1.4702[-5]	1.8592[-5]
0.2	A	-4.784 03[-2]	-4.781 85[-2]	-4.738 26[-2]	-4.540 45[-2]	-4.115 08[-2]	-3.496 71[-2]	-2.622 25[-2]
	B	3.1605[-8]	2.8432[-7]	5.2906[-6]	2.7006[-5]	6.8015[-5]	1.1327[-4]	1.4632[-4]
0.3	A	-1.170 15[-1]	-1.169 59[-1]	-1.158 43[-1]	-1.107 88[-1]	-9.997 37[-2]	-8.439 06[-2]	-6.264 77[-2]
	B	9.3822[-8]	8.4406[-7]	1.5722[-5]	8.0610[-5]	2.0498[-4]	3.4621[-4]	4.5668[-4]
0.4	A	-2.376 52[-1]	-2.375 29[-1]	-2.350 76[-1]	-2.240 07[-1]	-2.005 58[-1]	-1.673 26[-1]	-1.220 74[-1]
	B	1.4942[-7]	1.3446[-6]	2.5173[-5]	1.3202[-4]	3.5135[-4]	6.2984[-4]	8.9431[-4]
0.5	A	-4.584 14[-1]	-4.581 41[-1]	-4.526 96[-1]	-4.283 23[-1]	-3.777 36[-1]	-3.084 03[-1]	-2.182 61[-1]
	B	-1.0265[-7]	-9.2020[-7]	-1.5919[-4]	-2.0912[-3]	4.4522[-6]	3.1964[-4]	9.2316[-4]
0.6	A	-9.506 55[-1]	-9.498 98[-1]	-9.348 82[-1]	-8.691 29[-1]	-7.397 67[-1]	-5.763 26[-1]	-3.843 74[-1]
	B	-2.8398[-6]	-2.5513[-5]	-8.9674[-3]	-5.3955[-5]	-3.9992[-3]	-4.2036[-3]	-2.0842[-3]
0.7	A	-3.176 38[0]	-3.170 33[0]	-3.053 20[0]	-2.597 79[0]	-1.903 66[0]	-1.268 64[0]	-7.259 63[-1]
	B	-5.7298[-5]	-5.1378[-4]	-8.9674[-3]	-3.4824[-2]	-5.2228[-2]	-4.4976[-2]	-2.3795[-2]
0.74	A	-1.574 57[1]	-1.560 41[1]	-1.322 05[-1]	-7.721 89[0]	-3.880 78[0]	-2.034 49[0]	-9.942 12[-1]
	B	-1.6855[-3]	-1.4910[-2]	-2.0363[-1]	-3.7954[-1]	-2.6893[-1]	-1.4409[-1]	-5.7404[-2]

(RDPLWL) compared with the exact number results (RMP). As pointed out by Roy and Pratt²² the differences between RDP and RMP are generally small. The difference between RDPLWL and RDP gives an idea about the magnitude of the retardation corrections in the electric dipole term. Relativistic effects become visible for $Z=47$ and the differences between relativistic and nonrelativistic results increase with increasing k because of the different position of the resonances.

Our conclusion concerning the low-frequency behavior, based on Table I and on the arguments presented in proceeding sections, is that our RDPLWL approach gives the main features of the Rayleigh scattering amplitude at photon energies below the photoelectric threshold. In fact, because we miss some of the resonances (those corresponding to energies of transitions from the ground state to states with $j > \frac{3}{2}$), we cannot go beyond the fourth resonance (frequency corresponding to the transition from $1s$ to $n=3, j = \frac{3}{2}$ states).

We present numerical results based on our equations in Sec. II for the following quantities: (i) the ratio between the amplitude A in (4) and its nonrelativistic dipole approximation limit in Eq. (19); (ii) the values of the amplitudes A and B in Eq. (4) for several values of Z and values of k below the first resonance; (iii) the values of the amplitudes A and B between the first two resonances.

According to the discussion in Sec. III, when the photon frequency goes to zero, the ratio between the amplitude A in the relativistic and nonrelativistic dipole approximation treatments should go to the ratio between the relativistic and nonrelativistic static dipole polarizabilities. When the frequency increases, deviations from this ratio should become observable. The situation is illustrated in Table II. The first line, corresponding to $k=0$, represents the static ratio $\alpha_0/\alpha_0^{\text{NR}}$ taken from Ref. 17. For $Z=13$ and 92 the values are from Ref. 18. The numbers in Ref. 17 and 18 agree with those in Ref. 19, within the limit of the published number of significant figures. Analysis of our values for A in the relativistic and nonrelativistic approaches indicates that their ratio is changing more slowly with increasing photon energy than the two amplitudes themselves.

In Table III we give some values for the amplitudes A and B for photon energies below the first resonance. For the amplitude B we have no previous information. The amplitude B has very small values at low frequencies compared to the amplitude A : Eqs. (19) and (25) show that the amplitude B is a quantity of the order $(\alpha Z)^4 k^3$. But the amplitude B varies rather abruptly with k , goes to a maximum, decreases, and goes through zero for a value of k around 0.5 , then, becoming negative, increases in magnitude. It remains to be seen in further studies how much retardation effects affect this amplitude.

We illustrate the behavior of the amplitudes A and B between the first two resonances in Table IV, for $Z=47$.

TABLE IV. Behavior of the amplitudes A and B , for $Z=47$, between the first two resonances.

k	A	B
0.771	-119.19	-100.71
0.7712	-197.95	-179.03
0.7713	-305.64	-286.49
0.7714	-710.84	-691.45
0.771 44	-1575.2	-1555.7
0.771 47	resonance	
0.7715	1808.1	1827.8
0.7716	381.79	401.67
0.772	81.601	102.55
0.774	0.8277	29.454
0.775	-9.1320	25.945
0.776	-19.113	26.196
0.778	-65.170	44.101
0.779	-243.19	131.57
0.7792	-480.21	249.82
0.779 41	resonance	
0.7795	1156.8	-569.04
0.78	179.85	-81.133
0.782	44.216	-15.004

The first resonance is located at $k=0.77147$ and the second at $k=0.77941$. The two correspond respectively to transitions from the ground state to the $2p_{1/2}$ and $2p_{3/2}$ states. They replace a single resonance located at $k=0.75$ in the nonrelativistic model. The amplitude A vanishes at a particular energy between the two resonances. In the region investigated the amplitudes A and B become comparable.

In conclusion, we have presented in Sec. II analytical equations, including the lowest electric multipole in its long-wavelength limit, which lead to the structure (5) for the matrix element of Rayleigh scattering from the ground state of hydrogenic atoms, with or without spin flip. We have shown, by comparison with exact numerical results, that our approach is meaningful for photon frequencies below the fourth resonance. However, for very precise predictions retardation corrections should also be included.

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