Relativistic total cross section and angular distribution for Rayleigh scattering by atomic hydrogen

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We study the total cross section and angular distribution in Rayleigh scattering by hydrogen atom in the ground state, within the framework of Dirac relativistic equation and second-order perturbation theory. The relativistic states used for the calculations are obtained by making use of the finite basis set method and expressed in terms of B-splines and B-polynomials. We pay particular attention to the effects that arise from higher (non-dipole) terms in the expansion of the electron-photon interaction. It is shown that the angular distribution of scattered photons, while it is symmetric with respect to the scattering angle $\theta=90^\circ$ within the electric dipole approximation, becomes asymmetric when higher multipoles are taken into account. The analytical expression of the angular distribution is parametrized in terms of Legendre polynomials. Detailed calculations are performed for photons in the energy range 0.5 to 10 keV. When possible, results are compared with previous calculations.

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I. INTRODUCTION

Rayleigh scattering (also called \textit{coherent scattering}) denotes the elastic scattering of photons by bound electrons and is usually mentioned in order to explain the blue sky and the red sunset \cite{1,2}.

Rayleigh scattering, apart from being a subject of theoretical study by itself, has also interesting applications to different fields. Recently, with the availability of X-Ray polarization detectors as well as synchrotron and FEL sources, new experimental information is emerging in the X-ray regime, and, consequently, the demand for accurate theoretical predictions is arising \cite{3,4}.

The total cross section for Rayleigh scattering has been widely investigated during the past decades, both within relativistic and non-relativistic frameworks \cite{5,10}. For instance, in 2007 Nganso and Njock have presented analytical results for Raman and Rayleigh scattering in hydrogenlike ions based on fully relativistic wavefunctions and the Sturmian expansions of the Dirac-Coulomb Green function \cite{11}. More recently, Costescu et al. have analyzed Rayleigh scattering amplitudes in ions and neutral atoms by using the independent particle model \cite{12}.

In contrast to the total cross section, less attention has been paid to the angular distribution of the scattered photons (i.e. the angle-differential cross section) as well as their polarization properties. To the best of our knowledge, a fully relativistic treatment of the angular distribution in Rayleigh scattering by hydrogen atom based on Dirac equation has not been performed yet \cite{13,17}. Hydrogen atom, although is not, perhaps, the best choice for experimental investigation, is the most abundant element in the Universe and therefore is of great interest in astrophysics. In the extended atmosphere around a giant star, for example, near-ultraviolet photons can be significantly scattered by atomic hydrogen \cite{18}.

In the present work, we study the total cross section and the angular distribution of the scattered photons in Rayleigh scattering by atomic hydrogen in the ground state. The calculations are carried out within a relativistic framework through the use of finite basis sets for the Dirac equation constructed from B-splines and B-polynomials. The angular distribution is furthermore parametrized in terms of Legendre polynomials and the resulting coefficients are plotted against the photon energy. The photon energy range we investigate is 0.5 to 10 keV. By comparing with previous works, good agreement is found in analyzing the total cross section in the whole energy range. We show that higher multipoles in the expansion of the electron-photon interaction operator play an important role both in the total cross section and, especially, in the angular distribution of the scattered photons. While, for the total cross section, the non-relativistic dipole approximation is adequate for energies below $\sim 3$ keV, in the angular distribution non-dipole effects become important already for photon energies $\gtrsim 500$ eV.

This article is structured as follows. In section \textsuperscript{III} we present the geometry we consider for the scattering process and the notation used. In section \textsuperscript{IV} the essential theoretical background needed for the calculations is presented together with a detailed explanation of the theoretical quantities that we intend to investigate, namely the total cross section and the angular distribution. In

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We explain the numerical method we use in order to obtain the total cross section and the angular distribution. In section III we present our results, by showing the impact that high multipoles in the expansion of the electron-photon interaction have. Finally, a summary is given in section IV together with a few perspectives for further theoretical studies.

II. ATOMIC SYSTEM AND GEOMETRY

To explore the cross section and the angular distribution in Rayleigh scattering, let us first introduce the atomic system and the geometry under which the distribution of scattered photons is considered.

Our system consists of a hydrogen atom in the ground state which is irradiated by light, as shown in Fig. 1. Incident (scattered) light has energy \( E_{\gamma(1,2)} = \hbar \omega_{\gamma(1,2)} \), propagation vector \( \mathbf{k}_{1(2)} \) and polarization vector \( \hat{\mathbf{e}}_{1(2)} \), where \( \hbar \) is the Planck constant and \( \omega \) is the angular frequency. Here and in the following, \( \hat{A} \) denotes the unit vector \( A/|A| \), for any vector \( A \).

We adopt the quantization \( z \) axis along the direction of the incident light \( \mathbf{k}_1 \). As we will see in Sec. III A, such a choice of quantization axis simplifies the multipole expansion of the electron-photon interaction operator. The scattered light propagates along the direction \( \mathbf{k}_2 \) at angle \( \theta \) with respect to the \( z \) axis. The scattering plane \( (xz) \) is defined by the incoming and outgoing photon directions.

Now that we have explained the adopted geometry and notation, we are ready to present the theory of Rayleigh scattering.

III. THEORY

A. Evaluation of the transition amplitude

There has been a lot of theoretical studies on the calculation of the transition amplitude in Rayleigh scattering both in non-relativistic and relativistic regimes. In those studies, the analysis of the scattering cross section is usually traced back to the second-order bound-bound transition amplitude. The procedures to derive such an amplitude are explained in standard textbooks of Quantum Mechanics [19, 20], and are based on second-order time-dependent perturbation theory. With some straightforward algebraic manipulation, the transition amplitude for Rayleigh (and Raman) scattering can be cast in the form

\[
\mathcal{M}^{\gamma \gamma}(i \rightarrow f) = \\
\sum_{\nu} \frac{\langle f | \alpha \cdot \hat{e}_2^* e^{-i\mathbf{k}_2 \mathbf{r}} | \nu \rangle \langle \nu | \alpha \cdot \hat{e}_1 e^{i\mathbf{k}_1 \mathbf{r}} | i \rangle}{\omega_{\nu f} - \omega_1} + \\
\sum_{\nu} \frac{\langle f | \alpha \cdot \hat{e}_1 e^{i\mathbf{k}_1 \mathbf{r}} | \nu \rangle \langle \nu | \alpha \cdot \hat{e}_2^* e^{-i\mathbf{k}_2 \mathbf{r}} | i \rangle}{\omega_{\nu f} + \omega_2},
\]  

(1)

where \( \omega_{\nu f} = (E_{\nu} - E_{f})/\hbar \) is the transition frequency between states \( |\nu\rangle \) and \( |i\rangle \), \( \alpha \) is the vector of Dirac matrices and \( E_{\nu(f)} \) is the energy of the intermediate (initial) atomic bound state. Here, the transition operator \( \hat{e}_{1,2} e^{i\mathbf{k}_{1,2} \mathbf{r}} \) describes the relativistic electron-photon interaction. As indicated in Eq. (1), the summation over the intermediate states runs over the complete one-particle spectrum \( |\nu\rangle \), including a summation over the discrete part of the spectrum as well as the integration over the positive and negative energy continua. The initial state \( |i\rangle \) and final state \( |f\rangle \) of atomic hydrogen have well-defined angular momentum \( j \), angular momentum projection \( m_j \) and parity \( (\pi^0) \), where \( l \) is the orbital angular momentum of the larger component of the Dirac spinor. In the following, we will rewrite them respectively as \( |\beta_{l,j,m_j}\rangle \) and \( |\beta_l j f, m_{j f}\rangle \), where \( \beta \) is a collective label used to denote all the additional quantum numbers needed to specify the atomic states but for \( j \) and \( m_j \). In particular, \( \beta \) refers to \( n \) (principal quantum number) and \( l \).

The transition amplitude in Eq. (1) can be interpreted in the language of Feynman diagrams from Quantum Electrodynamics theory. The whole scattering process can be described by the two Feynman diagrams shown in Fig. 2 which will be hereinafter called “absorption first” and “emission first”, respectively [21]. The middle lines in the diagrams refer to a set of virtual intermediate
states that represent both electron and positron states. Absorption first diagram corresponds to the first term of the transition amplitude (1) while emission first diagram corresponds to the second term.

Due to the conservation of energy, the quantities $E_{\gamma_1,2}$ and $E_{f,i}$ are simply related by the equation

$$E_f - E_i = E_{\gamma_1} - E_{\gamma_2}.$$  \hspace{1cm} (2)

Since Rayleigh scattering is an elastic process, the initial and final states are the same, $|i\rangle = |f\rangle$, and, thus, Eq. (2) simplifies to $E_{\gamma_1} = E_{\gamma_2} = E_{\gamma}$.

For gaining deeper insights in the transition amplitude (1), in the next subsection we shall decompose the electron-photon interaction operator in terms of its spherical tensor components.

B. Multipole decompositions of the photon fields

Since we want to study the angular properties of the scattered photons, we need to rewrite the vector plane wave $\hat{\epsilon} e^{ikr}$ in terms of elements with well defined angular momentum properties. This can be done by using the multipole decomposition of the vector plane wave in terms of spherical tensors [22]. Such a decomposition reads

$$\hat{\epsilon} e^{ikr} = \sqrt{2\pi} \sum_{L=1}^{\infty} \sum_{M=-L}^{L} \sum_{p=0,1} i^L [L]^{1/2}(i\lambda)^p \mathbf{a}_{LM}^p(k,r) \times D_{LM}^p(\hat{\epsilon} r, \theta_k, 0),$$  \hspace{1cm} (3)

where

$$\mathbf{a}_{LM}^p(k,r) = \begin{cases} \mathbf{A}_{LM}^{(m)}(k,r) & \text{if } p = 0, \\ \mathbf{A}_{LM}^{(e)}(k,r) & \text{if } p = 1, \end{cases}$$  \hspace{1cm} (4)

with $\lambda$ being the photon helicity. We have defined $[L_1, L_2, ..., L_n] = (2L_1 + 1)(2L_2 + 1)...(2L_n + 1)$ for the sake of simplicity. Each term $\mathbf{a}_{LM}^p(k,r)$ has angular momentum $L$, angular momentum projection $M$ and parity $(-1)^{L+1+p}$. The standard notation $\mathbf{A}_{LM}^{(e,m)}$ is used to denote the electric $(e)$ and magnetic $(m)$ multipole fields. Each of these multipoles can be expressed in terms of the spherical Bessel functions $j_L(kr)$ and the vector spherical harmonics $\mathbf{T}_{LL}^M(\hat{\epsilon})$ of rank $L$ as

$$\mathbf{A}_{LM}^{(m)}(k,r) = j_L(kr) \mathbf{T}_{LL}^M(\hat{\epsilon}),$$

$$\mathbf{A}_{LM}^{(e)}(k,r) = j_{L-1}(kr) \sqrt{\frac{L+1}{2L+1}} \mathbf{T}_{LL-1}^M(\hat{\epsilon})$$

$$- j_{L+1}(kr) \sqrt{\frac{L}{2L+1}} \mathbf{T}_{LL+1}^M(\hat{\epsilon}).$$  \hspace{1cm} (5)

where $\mathbf{T}_{JL}^M(\hat{\epsilon})$ is defined as

$$\mathbf{T}_{JL}^M(\hat{\epsilon}) = \sum_{m=-1}^{1} \langle L, M - m, 1, m|J, M\rangle Y_{LM}^{M-m}(\varphi_{\epsilon}, \theta_{\epsilon}) \hat{\epsilon}_m.$$  \hspace{1cm} (6)

The spin spherical tensor $\hat{\epsilon}_m$ is defined by

$$\hat{\epsilon}_m = \begin{cases} \frac{1}{\sqrt{2}}(\hat{x} - i\hat{y}) & \text{if } m = -1, \\ \hat{z} & \text{if } m = 0, \\ -\frac{1}{\sqrt{2}}(\hat{x} + i\hat{y}) & \text{if } m = +1. \end{cases}$$  \hspace{1cm} (7)

As seen from Eq. (3), the angular dependence of the photon emission results from the Wigner (rotation) matrices. The Wigner matrices transform the multipole fields, with original quantization axis along the photon propagation direction, into the fields with quantization axis along the $\hat{z}||\hat{k}_2$ direction. Such a choice of quantization axis allows us to describe the second photon direction by means of a single polar angle $\theta$. On account of this, we will consider $D_{\lambda_1\lambda_2}^{L_2} (\hat{k}_2 \rightarrow \hat{z}) = d_{\lambda_1\lambda_2}^{L_2} (\theta)$ and $D_{\lambda_1\lambda_2}^{L_1} (\hat{k}_1 \rightarrow \hat{z}) = \delta_{\lambda_1\lambda_2}$ in evaluating the transition amplitude (1).

In the following subsection, by substituting the multipole decomposition (3) into the transition amplitude (1), we shall show how the total cross section and the angular distribution can be obtained in terms of the transition amplitude.

C. Total cross section and angular distribution

The general form of the relativistic transition amplitude for Rayleigh scattering is described by Eq. (1). Such an amplitude contains the whole information on the properties of the scattered radiation. For instance, the angular distribution function can be written in terms of the squared transition amplitude as (SI units)
\[
\frac{d\sigma}{d\Omega} = \frac{1}{2\pi} \frac{d\sigma}{d \cos \theta} = \frac{\alpha^2 c^2}{2(2j_i + 1)} \sum_{m_j, m_j} \left| \mathcal{M}^{-\gamma\gamma}(i \rightarrow f) \right|^2 , \tag{8}
\]

where \( \alpha (\alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c} \approx \frac{1}{137} ) \) is the electromagnetic coupling constant and \( c \) is the speed of light in vacuum. Since we do not investigate polarizations in the present article, in Eq. (8) we have summed over the final and averaged over the initial atom and photon polarizations. By combining Eqs. (1), (3) and (8) and by employing the Wigner-Eckart theorem, the transition amplitude can be written as

\[
\mathcal{M}^{-\gamma\gamma}(i \rightarrow f) = 2\pi \sum_{L_1, L_2, p_1, p_2} (i)^{L_1-L_2+p_1+p_2}[L_1, L_2]^{1/2}(-1)^{L_2}(\lambda_1)p_1(\lambda_2)p_2 d_{M_2-M_1}(\theta) \times \sum_{j_{\nu}} (-1)^{-j_{\nu}} \frac{1}{(2j_{\nu} + 1)^{1/2}} \left( \Theta^{j_{\nu}}(1,2)S^{j_{\nu}}(1,2) + \Theta^{j_{\nu}}(2,1)S^{j_{\nu}}(2,1) \right) . \tag{9}
\]

The reduced (second-order) matrix element is given by

\[
S^{j_{\nu}}(1,2) = \sum_{j_i} \frac{\langle \beta_i, j_i | \alpha \cdot a_{L_1}^{j_i}(k_1, r) | \beta_{\nu}, j_{\nu} \rangle \langle \beta_{\nu}, j_{\nu} | \alpha \cdot a_{L_2}^{j_{\nu}}(k_2, r) | \beta_i, j_i \rangle}{\omega_{j_i} + \omega_{j_{\nu}}} , \tag{10}
\]

and \( S^{j_{\nu}}(2,1) \) is obtained from Eq. (10) by i) interchanging the label 1 with 2 and ii) replacing the positive sign in the denominator with a negative sign. This latter replacement is given by the fact that, while the second photon is emitted, the first photon is absorbed by the atom.

Following the notation used in [24], we have furthermore defined

\[
\Theta^{j_{\nu}}(1,2) = \sum_{m_{j_{\nu}}} (-1)^{m_{j_{\nu}}+m_{j_{\nu}}} (2j_{\nu} + 1)^{1/2} \left( \begin{array}{ccc} j_i & j_{\nu} & L_1 \\ -m_{j_{\nu}} & m_{j_{\nu}} & \lambda_1 \end{array} \right) \left( \begin{array}{ccc} j_{\nu} & j_i & L_2 \\ -m_{j_{\nu}} & m_{j_{\nu}} & \lambda_2 \end{array} \right) , \tag{11}
\]

where \( \Theta^{j_{\nu}}(2,1) \) is obtained from Eq. (11) by replacing \( L_1 \leftrightarrow L_2 \) and \( \lambda_1 \leftrightarrow M_2 \).

The transition amplitude formally includes the infinite summation over all the multipoles combinations \( p_1 L_1 p_2 L_2 \), where \( p = 1 \) (0) refers to \( E \) (\( M \)). Using standard notation, we may write

\[
\mathcal{M}^{-\gamma\gamma}(i \rightarrow f) \simeq E1E1 + E1M1 + M1M1 + M1E1 + E2E1 + ... . \tag{12}
\]

However, according to parity and angular momentum selection rules, the number of allowed (i.e. non-zero) terms in the summation is restricted to certain combinations of the indices \( L_1, L_2, p_1 \) and \( p_2 \). Since the atomic (initial and final) state that we consider for the calculations is 1s1/2 (the ground state), the allowed multipole terms are the ones with equal parity and \( |L_1 - L_2| \leq 1 \). More explicitly, the multipoles that must be considered are \( E1E1, E1M1, E1M2, M2E1, ... \).

Finally, integrating (8) over the second photon directions, we get the total cross section as (SI units)

\[
\sigma = \frac{\alpha^2 c^2}{2(2j_i + 1)} \sum_{L_1, L_2} \sum_{\lambda_1, \lambda_2} \left| \mathcal{M}^{-\gamma\gamma}(i \rightarrow f) \right|^2 , \tag{13}
\]

where

\[
\tilde{\mathcal{M}}^{-\gamma\gamma}(i \rightarrow f) = 4\pi \sqrt{\pi} \sum_{L_1, p_1, p_2} (i)^{L_1+p_1+p_2}[L_1]^{1/2}(\lambda_1)p_1(\lambda_2)p_2 \times \sum_{j_{\nu}} (-1)^{-j_{\nu}} \frac{1}{(2j_{\nu} + 1)^{1/2}} \left( \Theta^{j_{\nu}}(1,2)S^{j_{\nu}}(1,2) + \Theta^{j_{\nu}}(2,1)S^{j_{\nu}}(2,1) \right) . \tag{14}
\]

Comparing Eqs. (13) and (8), we note that the summation over the multipoles of the outgoing photon \( (L_2, M_2) \), while is inside the modulus squared in the angu-
lar distribution, comes outside the modulus squared in the total cross section. By using the notation introduced in Eq. (12), we may better underline the consequences of this fact: Interference terms of the type \((E1E1)(M1M1)^*\) or \((M1M1)(E1E1)^*\) are forbidden in the calculation of the total cross section, while they are allowed in the calculation of the angular distribution. Thus, higher (non-dipole) multipoles will start giving non-zero contributions in the angular distribution at lower photon energies than in the total cross section. This effect will be analyzed in detail in Sec. V where expressions (8) and (14) will be used to explore the total cross section as well as the angular distribution in the Rayleigh scattering by hydrogen atom. However, prior to doing that, we shall explain how the reduced matrix elements 10 are calculated in the present work.

IV. COMPUTATION

During the last decade, various methods have been investigated for calculating the reduced second order amplitude 10 as well as the transition amplitude 11–12, 23, 27. In practice, of course, the summation over the complete spectrum contained in 10 is difficult to be performed explicitly. Several approaches and approximation techniques have been proposed to perform such a summation. Among them, the Coulomb-Green function approach has been widely used for investigating both decay of and scattering by atoms and ions 28, 29.

An alternative approach is the finite basis set method 30, 31. The finite basis set method is based on the supposition that the ion (or atom) is enclosed in a finite cavity with a radius \(R\) large enough to get a good approximation for the wave functions. Such a restriction leads to a “discretized” continuum part of the atomic or ionic spectrum, and hence to a representation of the Dirac wavefunctions in terms of pseudo basis set functions. This basis set forms a complete set of orthonormal functions 31.

In the present work, we calculate the transition amplitude 10 by using B-splines and B-polynomials as finite basis sets. The B-splines are one of the most commonly used family of piecewise polynomials, since they are well adapted to numerical tasks 31. The B-polynomials, or the Bernestein polynomials 32, are a good alternative to the B-splines since they allow for analytical finite basis set calculations. These are polynomial functions of \(n\)th degree that are used to obtain the solution of some linear and nonlinear differential equations 32. The details of these basis sets, as well as a comparison between them, can be found in Ref. 32. Thus, we restrict ourselves to describe the characteristic parameters used in this work. The parameters of the B-splines basis set are the radius of the cavity \(R_{bs}\), the number of B-splines \(n_{bs}\) and their degree \(k\). As for the B-polynomials, the parameters are the radius of the cavity \(R_{bp}\) and the number of B-polynomials \(n_{bp}\) (the degree of the B-polynomials is \(n_{bp} - 1\)).

The parameters used in both basis sets were optimized in order to obtain stability and agreement of six digits between the results of both basis sets. The optimal parameters are: \(R_{bs} = 60\) a.u., \(n_{bs} = 60, k = 9, R_{bp} = 50\) a.u. and \(n_{bp} = 40\). Such set of parameters was already obtained for the case of two photon emission in Refs. [37, 38].

The finite basis set method has been widely used during the past years to explore the two-photon decay of the metastable \(2s_{1/2}\) state in heavy hydrogenlike ions 24, 50. In contrast to the two photon decay process, to our knowledge no one has ever applied this method to calculate the transition rate for Rayleigh scattering.

V. RESULTS AND DISCUSSION

With the formalism developed above, we can now adequately analyze the total cross section and the angular distribution in Rayleigh scattering by hydrogen atom. The initial and final state considered for the calculations is \(1s_{1/2}/2s_{1/2}\).

In Fig. 3 we plot the total cross section in the photon energy range 0.5 to 10 keV as given by Eq. (13). Calculations obtained within the electric dipole approximation \((E1E1)\) and by including all multipoles are separately displayed. Furthermore, results from Veigele’s work 39 have been interpolated and are also shown. Our cross sec-

![Graph of total cross section](image-url)
tion practically coincides with Veigele’s, indicating that there is good agreement between the two calculations. Moreover, it can be seen that for high photon energies the electric dipole approximation deviates from the results of Veigele and of us obtained with the account of all multipoles. For photon energy \( \approx 3 \) keV, the electric dipole approximation underestimates the cross section by about 3%, while, for photon energy \( \gtrsim 6 \) keV, it is lower by a factor of two or more. Indeed, this result is not unexpected: in low photon energy range, the first (dipole) term \( E1E1 \) dominates the transition amplitude, while, for higher photon energy (such that \( kr \gtrsim 1 \), where \( r \) is the atomic radius), higher multipoles play an important role, as it is evident from Eqs. (3) and (5). For a detailed comparison, our results for the total cross section in the whole energy range, we make an expansion of \( d\sigma/d\Omega \) in terms of Legendre polynomials and we normalize it to the total cross section \( \sigma \):

\[
\frac{d\sigma}{d\Omega} = \sigma \left( \beta_0 P_0(\cos \theta) + \beta_1 P_1(\cos \theta) + \ldots \right),
\]

where \( \beta_i \) are real numbers called \textit{anisotropy coefficients} [11].

The results for the \( \beta \) coefficients are displayed in Fig. 4 within the considered energy range. The first coefficient

| \( E_\gamma \) (eV) | Veigele | NIST | This calculation |
|----------------|-------|-----|----------------|
| 500            | 0.642 | n.a. | 0.6465         |
| 1000           | 0.579 | 0.5805 | 0.5812         |
| 2000           | 0.414 | 0.4141 | 0.4142         |
| 3000           | 0.277 | 0.2760 | 0.2764         |
| 5000           | 0.135 | 0.1341 | 0.1341         |
| 8000           | 0.0618 | 0.0612 | 0.0609         |
| 10000          | 0.0416 | 0.04121 | 0.04030        |

FIG. 4: (Color online) Angular distribution in Rayleigh scattering by atomic hydrogen in the ground state as a function of the scattering angle \( \theta \). Results are calculated within the exact relativistic theory (solid-black line) and within the electric dipole approximation (red-dashed line), for three selected photon energies.
\[ \beta_i \approx 0.0796. \]
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