Rayleigh Scattering Cross Section Redward of Ly$\alpha$ by Atomic Hydrogen

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ABSTRACT

We present a low energy expansion of the Kramers-Heisenberg formula for atomic hydrogen in terms of $(\omega/\omega_l)$, where $\omega$ and $\omega_l$ are the angular frequencies corresponding to the Lyman limit and the incident radiation, respectively. The leading term is proportional to $(\omega/\omega_l)^4$, which admits a well-known classical interpretation. With higher order terms we achieve accuracy with errors less than 4% of the scattering cross sections in the region $\omega/\omega_l \leq 0.6$. In the neighboring region around Ly$\alpha$ ($\omega/\omega_l > 0.6$), we also present an explicit expansion of the Kramers-Heisenberg formula in terms of $\Delta \omega \equiv (\omega - \omega_{Ly\alpha})/\omega_{Ly\alpha}$. The accuracy with errors less than 4 % can be attained for $\omega/\omega_l \geq 0.6$ with the expansion up to the fifth order of $\Delta \omega$. We expect that these formulae will be usefully applied to the radiative transfer in high neutral column density regions, including the Gunn-Peterson absorption troughs and Rayleigh scattering in the atmospheres of giants.

Key words: atomic data — atomic processes — radiative transfer — scattering

1 INTRODUCTION

Hydrogen is the most abundant element in the universe and therefore one may often encounter astronomical situations associated with the radiative transfer in a region with a very high neutral hydrogen column density $N_{HI}$. The extended atmosphere around a giant star is such an example, where near UV photons can be significantly scattered by atomic hydrogen (e.g. Isliker, Nussbaumer & Vogel 1989). Another example may be found in searches for the first objects that may be found in searches for the first objects that contributed to the reionization of the universe. When the universe is still partially neutral before the completion of the reionization process, radiation should go through regions with a very high neutral hydrogen column density $N_{HI}$.

In particular, the interactions with low energy electromagnetic waves with angular frequency $\omega$ are simply Rayleigh scattering, where the scattering cross section is known to be proportional to $\omega^4$ in the limiting case where $\omega$ is much smaller than the angular frequency $\omega_{Ly\alpha}$ corresponding to the Ly$\alpha$ transitions.

In quantum mechanics, the Rayleigh scattering process is described by a second-order time dependent perturbation theory, where the scattering atom suffers level transition twice, one associated with the annihilation of the incident photon and the other associated with the creation of the scattered photon. The scattering cross section is known as the Kramers-Heisenberg formula, which is obtained by combining an infinite sum over all the bound $np$ states with the energy $E = -E_0/n^2$ and an integral over all continuum states $n'p$ with the energy $E = E_0/n'^2$, where $E_0$ is the Rydberg energy (e.g. Sakurai 1967). Since the wave functions are analytically known for a single electron atom, the Kramers-Heisenberg formula for hydrogen can be written explicitly in a closed form.

However, the Kramers-Heisenberg formula is unwieldy due to the presence of the infinitely many atomic levels contributing to the cross section. In the case of a hydrogen atom in the ground state interacting with incident radiation with $\omega$ much less than $\omega_{Ly\alpha}$, this inconvenience can be overcome by expanding the Kramers-Heisenberg formula in terms of $\omega/\omega_{Ly\alpha}$. Devoid of any resonance in the red region of Ly$\alpha$, the scattering cross section is a well-behaved monotonic function of $\omega$, and the leading term is proportional to $\omega^4$, which admits an immediate classical interpretation. Because $\omega^4$ dependence is the limiting behaviour of $\omega/\omega_{Ly\alpha} \ll 1$, inclusion of higher order terms will be useful to obtain more accurate cross section values in the red vicinity of Ly$\alpha$. However, very near the Ly$\alpha$ resonance, the cross section is well approximated by a Lorentzian and hence a polynomic approximation becomes poor. Lee (2003) introduced an expansion of the Kramers-Heisenberg formula near Ly$\alpha$, by computing the deviation from the Lorentzian.

In this paper, we will provide and compute the accuracy...
of the expansions that provide the Rayleigh scattering cross section redward of Lyα.

2 CALCULATION

2.1 The Kramers-Heisenberg Formula

The interaction of electromagnetic waves with an atomic electron is described using the Kramers-Heisenberg formula that is obtained from the fully quantum mechanical second-order time dependent theory (e.g. Sakurai 1969, Merzbacher 1970). In terms of the matrix elements of the dipole operator, the Kramers-Heisenberg formula can be written as

$$\frac{d\sigma}{d\Omega} = r_0^2 \left[ \frac{1}{m_e h} \sum_i \left( \frac{\omega(p \cdot e^{(\alpha)})_{IA} (p \cdot e^{(\alpha)})_{AI}}{\omega_A - \omega} \right) \right]^2 r$$

$$= \left( \frac{r_0 \omega}{m_e h} \right)^2 \left[ \sum_i \left( \frac{\omega(p \cdot e^{(\alpha)})_{IA} (p \cdot e^{(\alpha)})_{AI}}{\omega_A^2 (1 - \omega/\omega_A)} \right) \right]^2,$$

(1)

where $m_e$ is the electron mass, $r_0 = e^2/m_e c^2$ is the classical electron radius, and $e^{\alpha}$, $e^{\alpha'}$ are polarization vectors of incident and scattered radiation respectively. Here, $\omega_A$ is the angular frequency between the intermediate state $I$ and the ground state $A = 1s$. The intermediate state $I$ includes all the bound np and free n'p states, and therefore the summation notation should be interpreted as a sum over all bound np states plus an integration over all continuum n'p states.

The Wigner-Eckart theorem allows one to separate the matrix elements of the rank 1 tensor operator $p$ into the angular part and the radial part, where the radial part is given by the reduced matrix elements $< f \parallel p \parallel i >$. (e.g. Merzbacher 1970). Applying the Wigner-Eckart theorem, we obtain

$$\sum_i \langle f \parallel p \parallel A \rangle^2 = \sum_i < f \parallel p \parallel A >^2 e^{(\alpha)} \cdot e^{(\alpha')}.$$  

(2)

The dot product of the polarization gives rise to the same dipole type angular distribution as that for Thomson scattering or classical Rayleigh scattering (e.g. Lee & Ahn 1998, Lee & Lee 1997, Schmid 1989).

Bluelow of Lyα the cross section shows singular behaviours at resonances with bound excited states, which can be avoided introducing damping terms associated with the finite life times of excited states. However, redward of Lyα, there is no resonance and the cross section is a well-behaved monotonic function of $\omega$. We have $\omega < \omega_A$ for any intermediate state $I$ redward of Lyα, which allows the expansion

$$\left( 1 \pm \frac{\omega}{\omega_A} \right)^{-1} = 1 \mp \frac{\omega}{\omega_A} + \frac{\omega^2}{\omega_A^2} \mp \cdots.$$  

(3)

Substituting these relations into Eq. (1), we have

$$\sum_i \left[ \frac{\langle f \parallel A \parallel I >^2}{\omega_A} \right] \left( 1 + \frac{\omega}{\omega_A} \right)^{-1} = \sum_i \left| \frac{\omega(p \cdot e^{(\alpha)})_{IA} (p \cdot e^{(\alpha)})_{AI}}{\omega_A (1 - \omega/\omega_A)} \right|^2$$

$$+ \left| \frac{\omega(p \cdot e^{(\alpha)})_{IA} (p \cdot e^{(\alpha)})_{AI}}{\omega_A^2 (1 - \omega/\omega_A)} \right|^2.$$  

(4)

Here, we used a commutation relation

$$< A | p I > = i m_n \omega_A,< A | x I >,$$  

(5)

which results from the commutation relation $p = m_n x / i \hbar$ with $H_0$ being the Hamiltonian. The leading term is proportional to $\omega^4$, which is well-known result for the Rayleigh scattering cross section in the low energy limit.

By performing the angular integration for unpolarized incident radiation and averaging over the polarization for an outgoing radiation, we have $|d\Omega| e^{(\alpha')} \cdot e^{(\alpha)} | = \omega^6 / h$. We define the dimensionless angular frequencies

$$\omega_{IA} \equiv \omega_A / \omega_0,$$  

(6)

where $\omega_0$ is the angular frequency corresponding to the Lyman limit. From this we have $\omega_{np 1s} = 1 - n^{-2}$ and $\omega_{np 1s} = 1 + (n')^{-2}$ for a bound np state and a continuum n'p state, respectively. In a similar way, we define a dimensionless position operator

$r = \frac{r}{a_0}$  

(7)

where $a_0 = \hbar^2 / (m_e c^2) = 0.53 \text{Å}$ is the Bohr radius for hydrogen.

With these definitions we may write the total scattering cross section

$$\sigma(\omega) = \sigma_T \left( \frac{\omega}{\omega_0} \right)^4 \sum_i \left| \frac{\omega(p \cdot e^{(\alpha)})_{IA} (p \cdot e^{(\alpha)})_{AI}}{\omega_{IA}^2} \right|^2$$

$$\left[ 1 + \frac{1}{\omega_{IA}^4} \left( \frac{\omega}{\omega_{IA}} \right)^2 + \frac{1}{\omega_{IA}^2} \left( \frac{\omega_{IA}}{\omega} \right)^4 + \cdots \right]^{-2}.$$  

(8)

Here, $\sigma_T = 8 \pi r_0^2 / 3 = 0.665 \times 10^{-24} \text{cm}^2$ is the Thomson scattering cross section. We note that the leading term is proportional to $\omega^4$, which is a well-known result for Rayleigh scattering. We are interested in the higher order terms of $\omega / \omega_0$ for better approximation redward of Lyα.

The matrix elements of the dipole operators $< np \parallel \tilde{r} \parallel 1s >$, $< n'p \parallel x \parallel 1s >$ are easily found in textbooks on quantum mechanics (e.g. Berestetskii, Lifshitz & Pitaevskii 1971, Saslow & Mills 1969, Bethe & Salpeter 1967). The matrix elements are given by

$$< np \parallel \tilde{r} \parallel 1s > = \left[ \frac{2^{8} n^7 (n-1)^{2n-5}}{3(n+1)^{2n+5}} \right]^{1/2}$$  

(9)

for the bound states. For the continuum states, the corresponding values are given by

$$< n'p \parallel \tilde{r} \parallel 1s > = \left[ \frac{2^{8} (n')^7 (n'-1)^{n-1}(1/n')}{3[(n')^2 + 1]^2 [1 - e^{-2(n')^2}]} \right]^{1/2}.$$  

(10)
Here, the normalization condition for continuum wavefunctions is

$$\int_0^\infty R_{n'p}(r)R_{n''p'}r^2dr = \delta(n' - n''),$$

where $\delta(n')$ is the Dirac delta function.

With these matrix elements we may divide the terms involving bound states and continuum states and write the scattering cross section as a sum of two power series of $\omega/\omega_l$

$$\frac{\sigma(\omega)}{\sigma_f} = \left(\frac{\omega}{\omega_l}\right)^4 \left[ \sum_{p=0}^\infty a_p \left(\frac{\omega}{\omega_l}\right)^{2p} + \sum_{p=0}^\infty b_p \left(\frac{\omega}{\omega_l}\right)^{2p+1} \right]^2. \quad (12)$$

Here, the coefficients $a_p, b_p$ are given by

$$a_p = \sum_{n=2}^{\infty} \frac{2^8\pi^7(n-1)^{2n-5}}{3(n+1)^{2n+5}} \frac{(1 - \frac{1}{n^2})^{-2p-1}}{2},$$

$$b_p = \int_0^\infty dn' \frac{2^8(n')^7e^{-4n'\tan^{-1}(1/n')}}{3([n']^2 + 1)^3} \frac{(1 + \frac{1}{n'^2})^{-2p-1}}{2}. \quad (13)$$

We rewrite Eq. (12) as a single power series

$$\frac{\sigma(\omega)}{\sigma_f} = \left(\frac{\omega}{\omega_l}\right)^4 \left[ c_0 + c_1 \left(\frac{\omega}{\omega_l}\right)^2 + c_2 \left(\frac{\omega}{\omega_l}\right)^4 + \cdots \right]$$

$$= \left(\frac{\omega}{\omega_l}\right)^4 \sum_{p=0}^{\infty} c_p \left(\frac{\omega}{\omega_l}\right)^{2p}, \quad (14)$$

which forms a low energy expansion of the Kramers-Heisenberg formula. The coefficients $c_p$ are obtained from the coefficients $a_p$ and $b_p$ by the relation

$$c_p = \sum_{q=0}^{p} (a_q + b_q)(a_{p-q} + b_{p-q}). \quad (15)$$

In Table 1, we listed the numerical values of the coefficients $a_p, b_p$ and $c_p$ up to $p = 9$. It is noted that the continuum contribution represented by $b_p$ is small for high orders, but not negligible for low orders and must be included for accurate calculations.

### 3 RESULT

#### 3.1 Low Energy Expansion

In Fig. 1, we show our result for the low energy expansion in Eq. (14) up to $p = 9$ by a long dashed line. In the figure, we also show the result from the fully quantum mechanical computation, which was numerically obtained by performing the summation and integration appearing in the Kramers-Heisenberg formula. The exact cross section of Rayleigh scattering by atomic hydrogen was presented by Gavrila (1967), who computed the Green function in momentum space and provided the cross section in a tabular form. The crosses in the figure mark the result from the work of Gavrila (1967). It is noted that the cross marks are found on the solid line indicating excellent agreement.

Because the Ly$\alpha$ resonance is located at $\omega/\omega_l = 0.75$, the coverage is rather slow for $\omega/\omega_l \approx 0.6$, which requires a large number of terms in the expansion. This behaviour is natural because the scattering cross section changes too steeply near resonance for any polynomial approximation to be suitable. On the other hand, in the region with $\omega/\omega_l < 0.5$ the agreement is almost perfect and the two results are not distinguished in the figure.

For comparison purpose, we make a plot for the polynomial fit to the result of Gavrila (1967) obtained by Ferland (2001). He incorporated it in his photoionization code ‘Cloudy,’ in which the formula is quoted to be useful for radiation with $\lambda > 1410 \ \text{Å}$, corresponding to $\omega/\omega_l = 0.647$. He used the Lorentzian function instead for $\lambda < 1410 \ \text{Å}$, where the resonance of Ly$\alpha$ dominates. The polynomial fit to the scattering cross section obtained by Ferland (2001) is

$$\sigma_{CL}(\omega) = \left[ 8.41 \times 10^{-25} \left(\frac{\omega}{\omega_l}\right)^4 + 3.37 \times 10^{-24} \left(\frac{\omega}{\omega_l}\right)^6 + 4.71 \times 10^{-22} \left(\frac{\omega}{\omega_l}\right)^{14} \right] \text{cm}^2, \quad (16)$$

which shows the same $\omega^4$ dependence in the leading term. In Fig. 1, we also show the values obtained from this polynomial fit by a dotted line.

Because the coefficients $a_p, b_p$ and $c_p$ are all positive,
any finite expansion of Eq. (14) gives smaller values than the true ones obtained from the full Kramers-Heisenberg formula. Therefore, the long dashed line is always located under the solid line. However, such a behaviour cannot be seen in the case of the polynomial fit given by Eq. (16), for which it crosses the solid line at $\omega/\omega_l \sim 0.54$.

### 3.2 Near-Resonance Behavior

Lee (2003) discussed the deviation of the scattering cross section from the Lorentzian near Ly$\alpha$ resonance. The deviation is attributed to contributions from infinitely many other states than $2p$. According to him, near resonance, the Kramers-Heisenberg formula can be expanded in terms of $\Delta \omega = \omega - \omega_{21}$, where $\omega_{21} = 0.75\omega_l$ is the angular frequency corresponding to the Ly$\alpha$ transition. Explicitly, the expansion can be written as

$$
\sigma(\omega) = \sigma_T \left( \frac{\omega_{21}}{\Delta \omega} \right)^2 \left| A_0 + A_1 \left( \frac{\Delta \omega}{\omega_{21}} \right) \right|^2 + A_2 \left( \frac{\Delta \omega}{\omega_{21}} \right)^2 + \cdots \right|^2.
$$

(17)

The coefficients up to $A_5$ are given by

$$
A_0 = f_{12}/2 = 0.2081
$$

$$
A_1/A_0 = -0.8961
$$

$$
A_2/A_0 = -1.222 \times 10^4
$$

$$
A_3/A_0 = -5.252 \times 10^4
$$

$$
A_4/A_0 = -2.438 \times 10^2
$$

$$
A_5/A_0 = -1.210 \times 10^3,
$$

(18)

where $f_{12} = 0.4162$ is the oscillator strength for the Ly$\alpha$ transition.

With these coefficients, the Rayleigh scattering cross section near Ly$\alpha$ can be written explicitly up to the fifth order

$$
\frac{\sigma_L(\tilde{\omega})}{\sigma_T} = \frac{0.0433056}{\tilde{\omega}^2} (1 - 1.792\tilde{\omega} - 23.637\tilde{\omega}^2 - 83.1393\tilde{\omega}^3 - 244.1453\tilde{\omega}^4 - 699.473\tilde{\omega}^5)
$$

(19)

where we define $\tilde{\omega} \equiv (\omega - 0.75)/0.75 = \Delta \omega/\omega_{21}$.

In Fig. 2 we make a plot of this expansion up to the fifth order represented by a dotted line. We also compare this result with the results from the full Kramers-Heisenberg formula and approximations with lower order corrections. In this figure, the cross marks from the result of Gavrila (1969) fall on the solid line representing the full Kramers-Heisenberg formula as seen in Fig. 1. The agreement with the fifth order correction to the Lorentzian is excellent.

It is very interesting to note that the approximation of the first order correction to the Lorentzian depicted by a dashed line is poorer than just the Lorentzian without any correction terms in the region $\omega/\omega_l \sim 0.7$ represented by a dot-dash line. However, the first order approximation is excellent and better than the Lorentzian very near the resonance, i.e., $\frac{\Delta \omega}{\omega_l} > 0.70$, which is not plotted here (see Lee 2003). This behaviour is explained by the alternating nature of the series given in Eq. (19).

As is done in the photoionization code ‘Cloudy’ by Ferland (2001), the Rayleigh scattering cross section is approx-

| $p$ | $a_p$ | $b_p$ | $c_p$ | $a_p$ | $b_p$ | $c_p$ | $a_p$ | $b_p$ |
|-----|-------|-------|-------|-------|-------|-------|-------|-------|
| 0   | 1.26537 | 0.9157 | 0.2092 | 5      | 81.1018 | 13.5826 | 0.0571 |
| 1   | 3.73766 | 1.52456 | 0.1368 | 6      | 161.896 | 23.9  | 0.04983 |
| 2   | 8.8127 | 2.58886 | 0.1015 | 7      | 319.001 | 42.19 | 0.0442 |
| 3   | 19.1515 | 4.4587 | 0.08061 | 8      | 622.229 | 74.641 | 0.03971 |
| 4   | 39.919 | 7.75546 | 0.06685 | 9      | 1203.82 | 132.251 | 0.03605 |

Table 1. Numerical Values of the Coefficients $a_p$, $b_p$, and $c_p$
imated by the Lorentzian near resonance \( \omega/\omega_1 > 0.647 \) and Eq. (16) for \( \omega/\omega_1 < 0.647 \), which gives accurate results within errors not exceeding 5%. In a similar way, the combination of Eq. (14) up to \( p = 9 \) for \( \omega/\omega_1 < 0.6 \) and Eq. (19) for \( \omega/\omega_1 > 0.6 \) is accurate within errors less than 4%. In particular, it should be emphasized that significant errors are found only near the boundary region dividing the two expansions.

4 DISCUSSION AND OBSERVATIONAL RAMIFICATIONS

In this paper, we obtained an expansion in terms of \( \omega/\omega_1 \) of the Rayleigh scattering cross section by atomic hydrogen, which is applied in the low energy regime with \( \omega/\omega_1 < 0.6 \). By combining this with another expansion of the Kramers-Heisenberg formula around the Ly \( \alpha \) resonance in terms of \( \Delta \omega = (\omega - \omega_{\text{Ly} \alpha})/\omega_{\text{Ly} \alpha} \), we may have a wieldy and useful approximate formula for the Rayleigh scattering process redward of Ly \( \alpha \) by atomic hydrogen, which can be made arbitrarily accurate by inclusion of higher order terms directly calculated from the Kramers-Heisenberg formula.

Rayleigh scattering by atomic hydrogen is important only in the presence of a scattering region with a very high neutral hydrogen column density \( N_{\text{HI}} \). Such high column density media may be found in an extended atmosphere of a giant star where the mass loss process is already very important. Isliker et al. (1989) considered the effect of Rayleigh scattering in binary systems containing a giant star. In these systems, for a given inclination and density distribution, the scattering optical depth is dependent on the wavelength, and therefore light curves differ according to the observed wavelength. This information may be quite important to investigate the mass loss process from a giant star.

In their analysis, Isliker et al. (1989) presented the Rayleigh scattering cross section given by

\[
\sigma(\omega) = \sigma_T \left[ \sum_{k=2}^{\infty} \frac{f_{1k}}{(2k+1)^2 - 1} \right]^2, \tag{20}
\]

where \( f_{1k} \) is the oscillator strength between \( 1s \) and \( kp \) states. In their work, they neglected the contribution from the continuum states. However, as is noted in the previous section, the contribution from the continuum states to the low energy regime is not negligible, and hence caution should be exercised.

In more than half of the symbiotic stars, Raman scattered O VI 6827, 7088 features are seen, which are formed via Raman scattering of O VI 1032, 1038 resonance doublet by atomic hydrogen. Being slightly less energetic than Ly \( \beta \), O VI 1032, 1038 doublet may excite a hydrogen atom that can subsequently de-excite to excited 2s state re-emitting an optical photon redward of H \( \alpha \). This process was first identified by Schmid (1989), where the scattering cross section is of similar order to that for Rayleigh scattering (e.g. Lee & Lee 1997, Nussbaumer, Schmid, & Vogel 1989).

A very high column density media may be found in an early universe when the reionization of intergalactic medium initiated by the first objects was not completed. In this partially ionized universe, a significant extinction around Ly \( \alpha \) is expected, which will result in a big absorption trough known as the Gunn-Peterson effect (Gunn & Peterson 1965, Scheuer 1965). Thus far several quasars with redshift \( z > 6.2 \) have been identified with Gunn-Peterson troughs (Becker et al. 2001, Fan et al. 2003). It appears that the H I column density that is responsible for these Gunn-Peterson troughs are not sufficiently high for applications of our current work, but may be high enough to see the deviation from the Lorentzian approximation of the scattering cross section (see Lee 2003, Miralda-Escudé 1998). Deeper IR search for higher redshifted objects may exhibit extremely high neutral hydrogen column density, where an accurate calculation of the cross section is required.

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Rayleigh scattering cross section
Fig. 1

Gavrila
- Full calculation
- Hazy
- Low Energy Expansion
Fig. 2

- Gavrila
- Full Calculation
- Lorentzian
- Lorentzian + 1st Order Correction
- Lorentzian + 5th Order Correction

vs.

\frac{\sigma}{\sigma_T}

vs.

\frac{\omega}{\omega_i}