Journal of Quantitative Spectroscopy & Radiative Transfer 189 (2017) 339–343

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

Rayleigh scattering and the internal coupling parameter for arbitrary particle shapes

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ARTICLE INFO

Article history:
Received 29 September 2016
Received in revised form
2 December 2016
Accepted 5 December 2016
Available online 9 December 2016

Keywords:
Light scattering
Rayleigh differential cross section
Q-space
Internal coupling parameter

ABSTRACT

A general method for calculating the Rayleigh scattering by a particle of arbitrary shape is introduced. Although analytical solutions for Rayleigh scattering exist for spheres and ellipsoids, analytical solutions for more complicated shapes don't exist. We find that in general the Rayleigh differential cross section goes as $k^4V^2|\alpha(m)|^2$ where $k = 2\pi/\lambda$ and λ is the wavelength, V is the volume of the particle and $\alpha(m)$ the average volume polarizability which is dependent on the shape and the complex index of refraction, m. We use existing computational techniques, the discrete dipole approximation (DDA) and the T-matrix method, to calculate the differential scattering cross section divided by k^4 and plot it vs V^2 to determine $|\alpha(m)|^2$. Furthermore, we show that this leads to a general description of the internal coupling parameter $\rho'_{arbitrary}=2\pi k\frac{V}{A}|\alpha(m)|$ where A is the average projected area of the particle in the direction of incident light. It is shown that this general method makes significant changes in the analysis of scattering by particles of any size and shape.

1. Introduction

The light scattering by regularly and irregularly shaped particles has been the subject of a great deal of theoretical, computational, and experimental work. This work not only advances our knowledge in general, but also plays an important role in climate models. The advancements of computers and computational techniques over the last three decades have made the calculation of light scattering quantities from non-spherical particles more practical as well and greatly increased the speed at which the calculations from spherical particles (Mie scattering) can be calculated. The most common way of presenting the angular patterns of the light scattered intensity from particles is to plot them vs the scattering angle θ, but these are generally not amenable to quantitative description or differentiation for different shapes. Over the past years, we have developed a unique approach that provides quantitative descriptions of angular light scattering patterns produced by particles, Q-space analysis (see Section 2).

The Rayleigh differential cross section for a sphere has a well-known analytical solution which can be found in numerous locations, [1–4] are but a few. An analytical solution for the Rayleigh differential cross section of ellipsoids can also be found in [2,4]. As the shape of the particle begins to become more complicated, finding an analytical solution becomes nearly if not completely impossible. The focus of this work is to present a general description for the Rayleigh scattering cross section of an arbitrary shape and a straightforward method by which it can be calculated using existing computational techniques. It will also be shown that the general definition of the Rayleigh scattering cross section leads to a general definition of the internal coupling parameter [5] as well. Both of these generalizations are important in the application of Q-space analysis to obtain a general description of light scattering by particles of any shape.

2. Q-space and the internal coupling parameter for spheres

Our need for a general formulation for the Rayleigh cross section arouse with our application of Q-space analysis to particles of arbitrary shape. Q-space analysis involves plotting the differential scattering cross section (or the scattered intensity) versus q or the dimensionless variable qR_{eq}, where R_{eq} is an equivalent radius such as the radius of a sphere R, the radius of gyration R_g , or a volume equivalent radius R_{veq}, and q is the magnitude of the scattering wave vector: $q = (4\pi/\lambda)\sin\left(\frac{\theta}{2}\right)$ with λ being the wavelength and θ is the scattering angle, on a log-log plot [6–8]. Q-space analysis reveals functionalities of the scattering with q that are not apparent with conventional plotting with the scattering angle θ. Often in Q-space analysis, the differential cross section is

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http://dx.doi.org/10.1016/j.jqsrt.2016.12.004
0022-4073/

normalized by the Rayleigh differential cross section of the particle [8,9] which for a sphere is given by

$$dC_{sca,\ Ray,\ sphere}/d\Omega = k^4R^6\left|\frac{m^2-1}{m^2-1}\right|^2. \tag{1}$$

In Eq. (1) $k = 2\pi/\lambda$, m is the relative index of refraction, and the term in the bars is the Lorentz-Lorenz factor. When Q-space analysis is applied to non-spherical particles, a method to determine the proper Rayleigh normalization is needed which is why this work is not only of general intellectual importance but will also play a key role in future Q-space studies.

When the Rayleigh normalized differential cross section of an arbitrary sphere is plotted vs qR, distinct regimes and limits in the scattering curves can be found that would not be apparent when plotting against the scattering angle θ. These regimes appear in the scattering as a function of a parameter that we have named the internal coupling parameter, ρ' [5] that provides a quasi-universal description of the scattering. The internal coupling parameter is derived by looking at the two limits of Mie scattering from spheres. In the $m \to 1$ limit, the Mie scattering from spheres gives the 3d Fraunhofer diffraction limit or the Rayleigh-Debye-Gans (RDG) limit [10]. Looking at the combined $m \to Large$ or $R \to Large$ limit, the scattering is in the 2d Fraunhofer circular aperture (or obstruction) diffraction limit. To define a parameter that describes both of these diffraction limits, we take the square root of the ratio of the differential cross section at zero scattering angle in each limit. For the RDG limit Eq. (1) is used, and for the 2d circular aperture limit the differential cross section is given by [11]

$$\frac{dC_{sca,circle}}{d\Omega}(0) = \frac{k^2R^4}{4}. \tag{2}$$

The square root of the ratio of Eqs. (1) and (2) results in the internal coupling parameter of a sphere given by

$$\rho'_{sphere} = 2kR\left|\frac{m^2-1}{m^2-1}\right|. \tag{3}$$

The internal coupling parameter of a sphere ρ'_{sphere} is related to the Lorentz-Lorenz factor, which is directly involved in the radiative coupling between the sub-volumes that comprise the particle [5]. When $\rho'_{sphere} < 1$, the coupling between sub-volumes is weak, i.e. the effects of internal multiple scattering are small, and thus the scattering is in the RDG limit which corresponds to diffraction from the volume of the particle. As ρ'_{sphere} increases, so does the coupling. As ρ'_{sphere} continues to increase, the scattering approaches the 2d diffraction limit [12].

One of the functionalities that has previously been found in the scattering from spheres is that as ρ'_{sphere} increases past unity, the Rayleigh normalized scattering in the forward direction begins to fall by a factor of $1/\left(\rho'_{sphere}\right)^2$ as shown in Fig. 1. Also, shown in Fig. 1 (right side) is the Rayleigh normalized differential cross section in the forward direction multiplied by $\left(\rho'_{sphere}\right)^2$which approaches 1 as ρ'_{sphere} goes to infinity.

3. Rayleigh scattering for arbitrary shapes

As stated above, descriptions of the Rayleigh differential cross section for spheres can be found in numerous locations [1–4]. It should not be surprising that the Rayleigh differential cross section for a sphere is just a special case of the Rayleigh differential cross section of ellipsoids[2,4]. For randomly oriented ellipsoids the Rayleigh differential cross section is given by [2,4]

$$\frac{dC_{sca,\ Ray,\ ellipsoids}}{d\Omega} = \frac{k^4a^2b^2c^2}{3}\left[\left|\frac{\left(m^2-1\right)}{\left(3+3L_1\left(m^2-1\right)\right)}\right|^2 + \left|\frac{\left(m^2-1\right)}{\left(3+3L_2\left(m^2-1\right)\right)}\right|^2 + \left|\frac{\left(m^2-1\right)}{\left(3+3L_3\left(m^2-1\right)\right)}\right|^2\right] \tag{4}$$

where a, b, and c are the semi-principle axes, and L_1, L_2,*and* L_3 are geometric parameters given by the integrals

$$L_x = \frac{abc}{2}\int_0^\infty \frac{dq}{\left(q+x^2\right)\sqrt{\left(q+a^2\right)\left(q+b^2\right)\left(q+c^2\right)}} \tag{5}$$

with x being equal to a, b, or c for L_1, L_2,*and* L_3, respectively. There are no known analytical results for more complex shapes and finding analytical solutions for Rayleigh scattering by such shapes appears to be extremely difficult, if not impossible. So how can we find the Rayleigh differential cross section for an arbitrary shape?

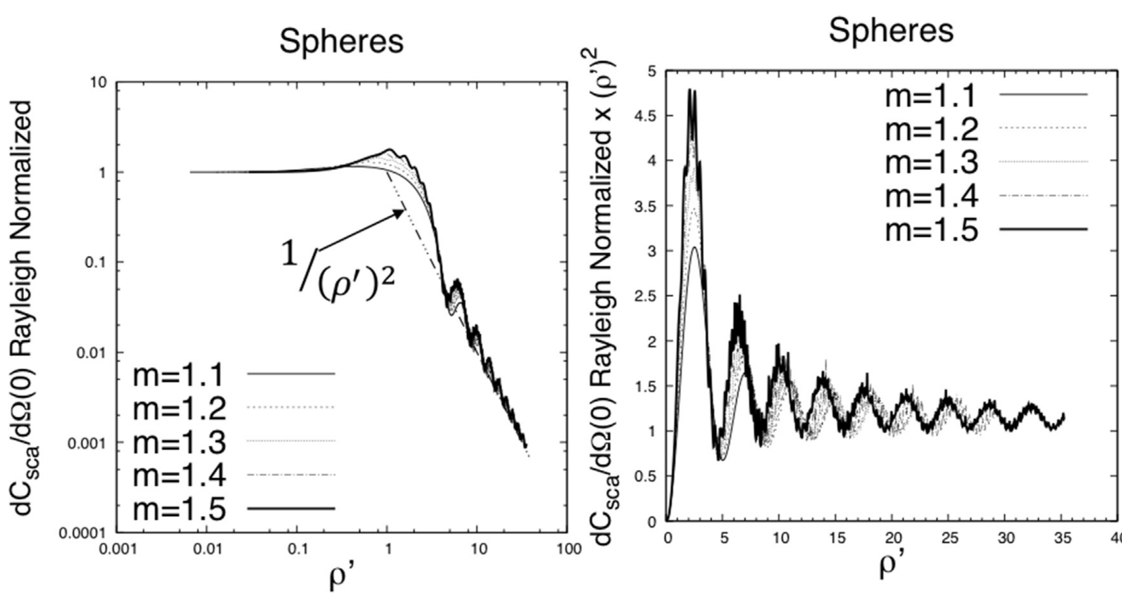

Fig. 1. Left: Forward scattered (θ and q = 0) Rayleigh normalized differential cross section of spheres vs ρ'_{sphere}. Right: Rayleigh normalized differential cross section x $\left(\rho'_{sphere}\right)^2$ of spheres vs ρ'_{sphere}.