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O-space analysis of scattering by particles: A review



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ABSTRACT

This review describes and demonstrates the Q-space analysis of light scattering by particles. This analysis involves plotting the scattered intensity versus the scattering wave vector $q = (4\pi/\lambda)\sin(\theta/2)$ on a double log plot. The analysis uncovers power law descriptions of the scattering with length scale dependent crossovers between the power laws. It also systematically describes the magnitude of the scattering and the interference ripple structure that often underlies the power laws. It applies to scattering from dielectric spheres of arbitrary size and refractive index (Mie scattering), fractal aggregates and irregularly shaped particles such as dusts. The benefits of Q-space analysis are that it provides a simple and comprehensive description of scattering in terms of power laws with quantifiable exponents; it can be used to differentiate scattering by particles of different shapes, and it yields a physical understanding of scattering based on diffraction. © 2013 Elsevier Ltd. All rights reserved.

1. Introduction

The scattering of light from particles is an important method for in situ, non-invasive, real time characterization of the scattering particles. Particle size, morphology, refractive index and concentration can be determined under the ideal situation in which the scattering magnitude and angular distribution are fully characterized and the inverse problem of using such data to determine these properties can be solved. However, whereas the task of calculating the scattering patterns from particles of known size, shape and refractive index has seen impressive advances, the inverse problem of going from the scattering back to the particle remains formidable.

Another very important application for light scattering is to understand the effects of particulate scattering and absorption in the Earth's atmosphere on the global environment. For this application the impressive advances for calculating scattering from a wide variety of particles mentioned above can be very useful. However, increasing

particle complexity requires increasingly complex calculations which hamper their facile application to the point where approximations are often applied. Moreover, these complex solutions yield little or no physical insight into the scattering process.

Thus it seems that the field of light scattering could use a new perspective that could quantitatively describe and differentiate the scatterings from different types of particles. It could also use a description that would yield a physical picture of the scattering process, a desire spurred both by the practical need to predict simply scattering as new types of particles are encountered, and the more general motive to understand fundamentally this aspect of nature.

In this paper I review a method which provides a new perspective on light scattering. The method is a simple change in the manner by which to view the angular scattering patterns. Instead of plotting the scattered intensity versus the scattering angle, the new perspective plots the scattered intensity versus the magnitude of the scattering wave vector, and the plots are made log-log. This method is not all together new. It has a long history of application to small angle X-ray and neutron scattering, however, it was not applied to light scattering until we

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first applied it to Mie scattering from spheres more than a decade ago [1]. When we did, we discovered patterns in the scattering that involved power laws that had never been described before. More work followed both from our lab [2–6] and others [7–12]. Recent application to random nonspherical particle geometries [13–15] indicates that the usefulness of the new perspective might be wide spread. We call this new perspective "Q-space analysis".

2. The scattering wave vector

As the name implies, the fundamental variable in the Q-space analysis is the scattering wave vector q. Thus it is very appropriate that our description of Q-space analysis starts with a description of the origin of q in the scattering theory. We follow the description given in [16]. Consider a scalar wave incident upon a point-like scattering element, or scatterer, at \overrightarrow{r} as drawn in Fig. 1. Since the scatterer is point-like, it scatters isotropically throughout space. The incident field at a position \overrightarrow{r} is

$$E(\overrightarrow{r}) = E_0 \exp(i \overrightarrow{k_i} \cdot \overrightarrow{r}) \tag{1}$$

where $i=\sqrt{-1}$ and \overrightarrow{k}_i is the incident wave vector, with magnitude $|\overrightarrow{k}_i|=2\pi/\lambda$. The wave scatters in the direction of \overrightarrow{k}_s toward the detector at $R\gg r$. Then the field at the detector is a plane wave described by

$$E(\overrightarrow{R}, \overrightarrow{r}) \sim E(\overrightarrow{r}) \exp(i \overrightarrow{k}_s \cdot (\overrightarrow{R} - \overrightarrow{r})),$$
 (2)

which with Eq. (1) yields

$$E(\overrightarrow{R},\overrightarrow{r}) \sim E_0 \exp(i\overrightarrow{k}_s \cdot \overrightarrow{R}) \exp(i(\overrightarrow{k}_i - \overrightarrow{k}_s) \cdot \overrightarrow{r})$$
 (3)

We have dropped the equality for the proportionality because we do not know and do not need to know the strength of the scattering element at \overrightarrow{r} . The second term of Eq. (3) shows that the phase at the detector is a function of the position of the scattering element and the vector

$$\overrightarrow{q} = \overrightarrow{k_i} - \overrightarrow{k_s} \tag{4}$$

Eq. (4) defines the *scattering wave* vector \overrightarrow{q} . Its direction is in the scattering plane from \overrightarrow{k}_s to \overrightarrow{k}_i , and if the

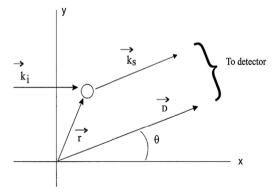


Fig. 1. Diagram of light with an incident wave vector \vec{k}_{\perp} scattering from a point scatterer at \vec{r} into the scattering wave vector \vec{k}_{s} at an angle θ directed to a distant detector.

scattering is elastic, i.e. $|\overrightarrow{k_i}| = |\overrightarrow{k_s}|$, the magnitude of q is $q = 2k\sin(\theta/2)$ (5a)

$$= (4\pi/\lambda)\sin(\theta/2) \tag{5b}$$

where θ is the scattering angle. Finally, we strip Eq. (3) to is essentials and write for the amplitude of the scattered wave

$$E_{\text{sca}}(\overrightarrow{q}, \overrightarrow{r}) \sim E_0 \exp(i\overrightarrow{q} \cdot \overrightarrow{r})$$
 (6)

The importance of \overrightarrow{q} is that it describes how the phase at the detector depends on the position of the scatterer and the scattering angle. Any finite size object can be thought of as composed of a great many sub-volumes that act as point-like scatterers at various \overrightarrow{r} , a system of scatterers [16,17]. Hence the total scattered wave is the sum of all the waves from the scatterers that make up the object. In taking this sum a baseline and very useful approximation can be made that the scattering from each individual scatterer of the object is so weak that it does not affect the other scatterers. Then each scatterer only sees the incident field and the interior of the scattering object is uniformly illuminated. This is the so-called Rayleigh-Gans or Rayleigh-Debye-Gans (RDG) [18-21] approximation which leads to the total scattered field at the detector to be

$$E_{sca}(\overrightarrow{q}) \sim E_0 \sum \exp(i\overrightarrow{q} \cdot \overrightarrow{r_i}).$$
 (7)

To convert the sum in Eq. (7) to an integral write the density function of the system of scatterers as

$$n(\overrightarrow{r}) = \sum \delta(\overrightarrow{r} - \overrightarrow{r_i}) \tag{8}$$

where $\delta(\vec{r})$ is the Dirac delta function. Then

$$\sum \exp(i\overrightarrow{q}\cdot\overrightarrow{r}) = \int \exp(i\overrightarrow{q}\cdot\overrightarrow{r})n(\overrightarrow{r})d\overrightarrow{r}$$
 (9)

Thu

$$E_{\text{sca}}(q) \sim E_0 \int \exp(i \overrightarrow{q} \cdot \overrightarrow{r}) n(\overrightarrow{r}) d\overrightarrow{r}$$
 (10)

In Eq. (10) we have anticipated the experimental situation where scattering will take place from an ensemble of particles of random orientations; thus the vector nature of q is eliminated. Eq. (10) brings the realization that the functionality of the scattered wave under the RDG approximation is the Fourier transform of the real space structure of the scattering object. Given the reciprocity of the Fourier transform, it also implies that the Fourier transform of the wave scattered from the object is the real space structure functionality of the object. Indeed, the real space (r-space) and q-space (r-ciprocal space) descriptions of the object carry the same information only in different units.

One may also recognize that Eq. (10) describes diffraction from the scattering object, so it also brings the important realization that scattering under the RDG approximation is simply diffraction [22]. In this context it depends neither on the electromagnetic character of the light wave nor the electric properties of the scattering object as specified by its complex index of refraction.

The intensity of the scattered wave is the square of the complex scattering amplitude; hence the q-space

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