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Note

On definition and measurement of extinction cross section

Michael I. Mishchenko [a,*], Matthew J. Berg [b], Christopher M. Sorensen [b], Cornelis V.M. van der Mee [c]

[a] NASA Goddard Institute for Space Studies, 2880 Broadway, New York, NY 10025, USA
[b] Department of Physics, Kansas State University, Manhattan, KS 66506-2601, USA
[c] Dipartimento di Matematica e Informatica, Università di Cagliari, Viale Merello 92, 09123 Cagliari, Italy

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ABSTRACT

Following the recent analyses of extinction by Berg et al. [J Opt Soc Am A 2008;25:1504–1513; J Opt Soc. Am A 2008;25:1514–1520], we show that although it is possible to define and measure the extinction cross section for a single particle using a detector of light facing the incident beam, this requires certain theoretical assumptions and experimental precautions.

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1. Introduction

There are two conventional ways to define the extinction cross section C_{ext} for a particle embedded in a non-absorbing host medium [1,2]. The operational way is used to define C_{ext} as a direct optical observable in the context of modeling the response of a detector of light facing the incident beam. The analytical way is used to define C_{ext} by integrating the Poynting vector of the total electromagnetic field over the surface of a large imaginary sphere centered at the particle and representing this integral as the difference between extinction and scattering components (see, e.g., Section 2.8 of [2]). Whereas the operational definition remains valid in the case of an absorbing host medium [3–6], the analytical definition becomes highly problematic if even applicable (see [7] and references therein).

In two recent publications, Berg et al. [8,9] revisited the operational definition of C_{ext} and concluded that the practical measurement of C_{ext} for a single particle may require the detector surface to subtend a very large solid angle around the direction of incidence, whereas extinction measurements for a random group of particles are free of this problem. The former conclusion appears to be paradoxical since the derivation of C_{ext} in [2] is based on the Saxon expansion of the incident plane wave into incoming and outgoing spherical waves containing solid-angle delta functions centered at the exact backscattering and forward-scattering directions, respectively. As such, it may seem to imply that the practical measurement of C_{ext} only requires the surface of the far-field detector to be larger than the particle projection.

In this note we give a simple explanation of this paradox and demonstrate that the classical operational definition of C_{ext} works well theoretically, except in singularly idealistic circumstances. Yet the practical use of the operational definition requires certain precautions. In a sense, our paper is intended to clarify and refine the discussion of the operational definition of the extinction cross section on p. 74 of Bohren and Huffman [10].

* Corresponding author. Tel.: +1 212 678 5590; fax: +1 212 678 5622.
E-mail address: mmishchenko@giss.nasa.gov (M.I. Mishchenko).

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2. Theoretical analysis

For simplicity, we will consider scattering of scalar time-harmonic waves and omit the common factor $\exp(-i\omega t)$, where $i = (-1)^{1/2}$ and ω is the angular frequency. The field illuminating a particle is given by $u_0 \exp(ik\mathbf{n}^{\rm inc} \cdot \mathbf{r})$, where k is the wave number, $\mathbf{r}$ is the position vector originating at a point P inside the particle, and $\mathbf{n}^{\rm inc}$ is the unit vector in the incidence direction (Fig. 1). The scattered field in the far zone is given by $u_1(\hat{\mathbf{r}}) \exp(ikr)/r$, where $r = |\mathbf{r}|$ and $\hat{\mathbf{r}} = \mathbf{r}/r = \hat{\mathbf{n}}^{\rm sca}$ is the unit vector in the scattering direction. Note that the dimension of u_1 is that of u_0 multipled by the dimension of length. The infinite homogeneous medium surrounding the scattering object is assumed to be nonabsorbing, and so k is real-valued.

Let us integrate the total intensity over a circular detector surface S perfectly centered at and exactly normal to the incidence direction (Fig. 1). The surface is perfectly flat and coincides with a $z = R$ plane, where the z axis originates at P and is directed along $\mathbf{n}^{\rm inc}$. Assuming that $D/2 \ll R$, where D is the diameter of the sensitive area, we have for a point O on the detector surface:

$$r \approx R + \frac{\rho^2}{2R}. \tag{1}$$

The total intensity at this point is then given by

$$\left| u_0 \exp(ikR) + \frac{u_1(\hat{\mathbf{r}}) \exp(ikr)}{r} \right|^2 \approx |u_0|^2 + \frac{2}{R} \mathrm{Re}[u_0^* u_1(\hat{\mathbf{r}}) \exp(ik\rho^2/2R)]. \tag{2}$$

Since it is the complex exponential factor on the right-hand side of this formula that ultimately leads to the optical theorem, we will simplify the analysis by assuming that $u_1(\hat{\mathbf{r}}) = \text{constant} = u_1$, which is usually referred to as the case of “isotropic scattering” by a “point-like particle”. Integrating the intensity (2) over the entire detector area, we find

$$\begin{aligned} &\frac{\pi D^2}{4} |u_0|^2 + \frac{2}{R} \mathrm{Re}\left\{ u_0^* u_1 \int_0^{2\pi} d\theta \int_0^{D/2} d\rho \rho \exp(ik\rho^2/2R) \right\} \\ &= \frac{\pi D^2}{4} |u_0|^2 - \frac{4\pi}{k} \mathrm{Im}\left\{ u_0^* u_1 \left[1 - \exp\left(\frac{ikD^2}{8R} \right) \right] \right\}. \end{aligned} \tag{3}$$

This formula is, in fact, quite remarkable and confirms one of the main results of [8]: the detector signal is a frequently and strongly oscillating function of the diameter of the detector surface (or, equivalently, of the acceptance solid angle subtended by the detector surface as viewed from the particle). Furthermore, the amplitude of the oscillations does not decrease with increasing D or R. This does appear to make the measurement of $C_{\rm ext}$ (according to its operational definition) highly problematic.

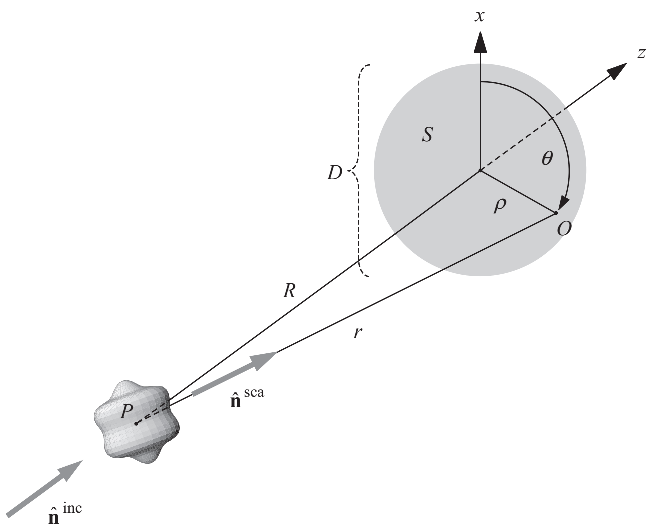

Fig. 1. Integration of the total intensity over a circular detector surface.

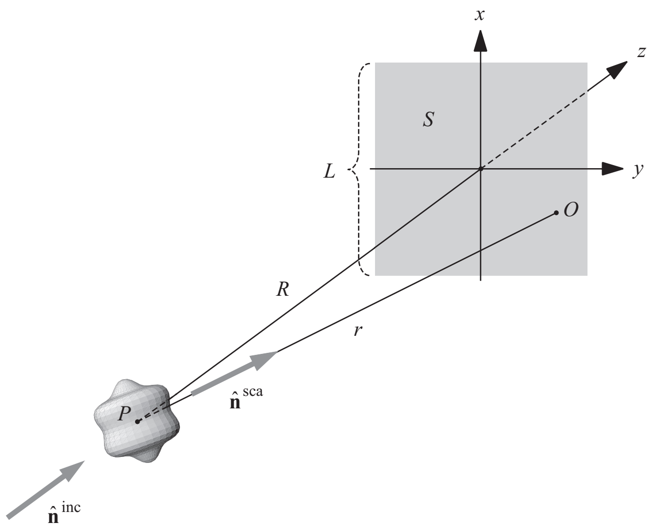

Fig. 2. Integration of the total intensity over a square detector surface.

Let us now consider a square detector surface (Fig. 2). Now the surface integral can be computed using rectangular Cartesian coordinates. We then have

$$L^2|u_0|^2 + \frac{2}{R}\mathrm{Re}\left\{u_0^* u_1 \int_{-L/2}^{+L/2} \mathrm{d}x \int_{-L/2}^{+L/2} \mathrm{d}y \exp[\mathrm{i}k(x^2+y^2)/2R]\right\}$$
$$= L^2|u_0|^2 + \frac{8\pi}{k}\mathrm{Re}\left\{u_0^* u_1 \left[C\left(\frac{L}{2}\sqrt{\frac{k}{\pi R}}\right) + \mathrm{i}S\left(\frac{L}{2}\sqrt{\frac{k}{\pi R}}\right)\right]^2\right\}, \tag{4}$$

where

$$C(\alpha) = \int_0^{\alpha} \mathrm{d}x \cos\left(\frac{\pi x^2}{2}\right) \tag{5}$$

and

$$S(\alpha) = \int_0^{\alpha} \mathrm{d}x \sin\left(\frac{\pi x^2}{2}\right) \tag{6}$$

are Fresnel integrals. Using the rational approximations [11]

$$C(\alpha) = \frac{1}{2} + f(\alpha)\sin\left(\frac{\pi}{2}\alpha^2\right) - g(\alpha)\cos\left(\frac{\pi}{2}\alpha^2\right), \tag{7}$$

$$S(\alpha) = \frac{1}{2} - f(\alpha)\cos\left(\frac{\pi}{2}\alpha^2\right) - g(\alpha)\sin\left(\frac{\pi}{2}\alpha^2\right), \tag{8}$$

$$f(\alpha) \approx \frac{1 + 0.926\alpha}{2 + 1.792\alpha + 3.104\alpha^2}, \tag{9}$$

$$g(\alpha) \approx \frac{1}{2 + 4.142\alpha + 3.492\alpha^2 + 6.670\alpha^3}, \tag{10}$$

we can conclude that although the second term on the right-hand side of Eq. (4) is an oscillating function of L, the amplitude of the oscillations decreases with increasing L, and the integral over the detector surface approaches the well-known limit [1]

$$L^2|u_0|^2 - \frac{4\pi}{k}\mathrm{Im}\{u_0^* u_1\}. \tag{11}$$

To help illustrate the significance of Eqs. (3) and (4), the main functional form of these equations is plotted in Fig. 3 as a function of the “detector size parameter” kL. For simplicity, the amplitude of the incident wave u_0 is taken to be unity and the amplitude of the forward scattered wave is taken as $u_1 = \exp(\mathrm{i}\pi/4)$. One can see the asymptotic damping of Eq. (4) as roughly $1/kL$ and the lack of damping for Eq. (3). Notice that both curves oscillate about the value $-\mathrm{Im}\,u_1 = -\sin(\pi/4)$, thereby showing that C_{ext} is ultimately determined by the phase and magnitude of the scattered wave in the forward

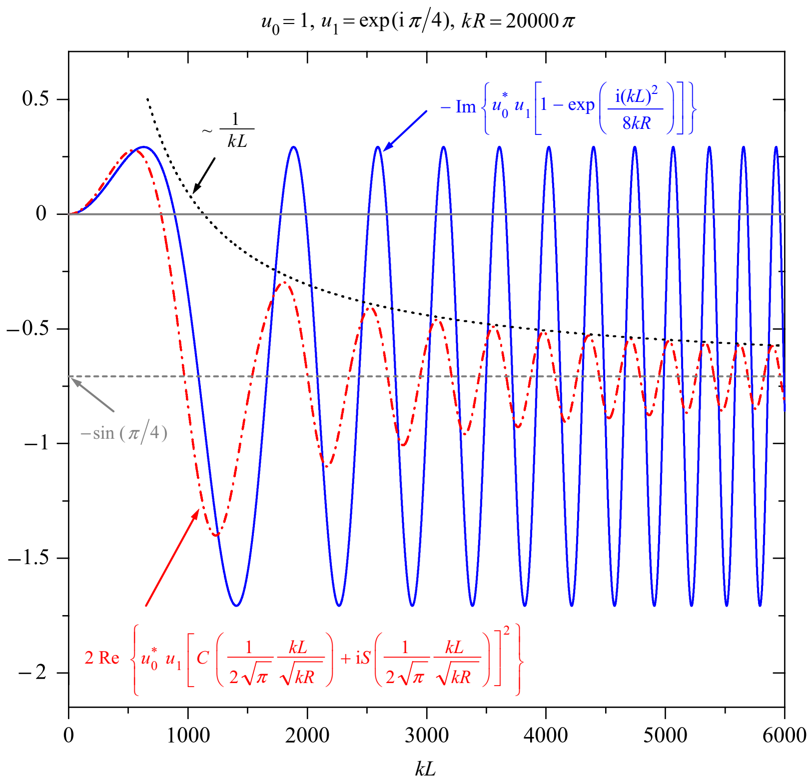

Fig. 3. Examples of the behavior of the integrals in Eqs. (3) and (4) as a function of the "detector size parameter" kL. The main functional form of the integral in Eq. (3) is shown in blue and its curve is the solid blue line. Likewise, Eq. (4) is shown in red and its curve is the dashed red line. The dotted black line indicates a $1/kL$ functionality, and one can see its similarity to the large-argument behavior of Eq. (4). Both curves oscillate about a value of $-\mathrm{Im}\,u_1 = -\sin(\pi/4)$, as shown by the gray straight dashed line assuming the values of u_0, u_1 and kR indicated. Note that the substitution $D = L$ has been made, recall Figs. 1 and 2. Also note that the restriction of Eq. (12) is not satisfied here. The values of kR and kL selected are such that only the general behavior of Eqs. (3) and (4) is shown.

direction. This is, of course, expected from the optical theorem, see Eq. (34) in [8]. This result shows that the operational definition of C_{ext} can work in the case of a square detector surface for large enough kL. Furthermore, one can easily derive a formula for the angular diameter of the detector (as viewed from the particle) that ensures better than 1% accuracy of the measurement of C_{ext}:

$$\frac{L}{R} > 200\sqrt{\frac{\pi}{kR}} = 200\sqrt{\frac{\lambda}{2R}}, \tag{12}$$

where λ is the wavelength in the surrounding medium. Obviously, the requisite angular size decreases rather slowly with R. However, the actual angular variability of $u_1(\hat{\mathbf{r}})$ for wavelength-sized and larger particles, especially those lacking spherical symmetry, is likely to result in a significantly less demanding condition than Eq. (12).

Eq. (12) refines the generic requirement $kL^2/4R \gg 4\pi$ quoted on [10, p. 74] below Eq. (3.32).

3. Discussion

The above analysis can be used to explain the somewhat paradoxical results of [8,9]. Indeed, it shows that the operational definition of C_{ext} fails only if one considers the highly idealistic case of a perfectly circular detector surface perfectly centered at and exactly normal to the line drawn through the particle origin in the incidence direction. This conclusion is consistent with the numerically exact Lorenz–Mie results reported in [8] as well as with the requirement to exclude a circular detector boundary in the derivation of Eq. (3.32) on [10, p. 74]. Any deviation from this perfect geometry mitigates the problem. For example, imperfect centering of the circular detector surface, essentially any other shape of the detector surface, or random movements of the particle(s) during the measurement can restore the validity of the operational definition of C_{ext} under conditions similar to and perhaps even weaker than Eq. (12). This happens because the high-frequency oscillations caused by the complex exponential $\exp(\mathrm{i}kD^2/8R)$ in Eq. (3) get effectively averaged out. In fact, this is exactly what the results of [9] for a finite group of arbitrarily positioned particles imply. Obviously, the measurement of extinction for a group of randomly moving particles should be long enough to ensure ergodicity and average out dynamic-scattering effects [12,13].

The reason that the circular detector case appears to be special is because the surfaces of constant phase of the far-field scattered wave intercept the detector in circular contours that are exactly centered on and degenerate in shape with the detector. Consequently, when the detector radius $D/2$ increases, the phase of the scattered wave on the detector's edge advances uniformly over the entire detector-edge circumference. To compare this to the square detector case, one can think of the square as being separated into a circular surface of radius $L/2$ and four ''corner pieces''. The phase of the far-field scattered wave varies over the circular portion as L is increased exactly as is it does for the circular detector. However, the corner pieces experience a different functionality of scattered-wave phase advance with increasing L. This adds extra oscillations to the energy flow that are not in ''harmony'' with the circular part, evidently resulting in a damping of the integral.

The importance of our analysis is at least three-fold. First, it confirms the classical operational definition of the extinction cross section [1,2]. Second, it reinforces the validity of the analyses of extinction in the case of an absorbing host medium in [3–7]. Third, it facilitates the practical measurement of C_{ext} for a single particle.

Still, the criterion (12) appears to be quite damaging to the operational definition and measurement of the extinction cross section. For example, evaluating Eq. (12) for $R = 1$ m and $\lambda = 532$ nm implies $L > 10$ cm, although, as we have already mentioned, the situation can be expected to improve for wavelength-sized and larger particles, especially those lacking perfect spherical shape. All in all, Eq. (12) implies that although the use of the Saxon expansion in the operational definition of the extinction cross section allows the angular size of the detector surface to become infinitesimal as R tends to infinity, the geometrical size of the detector surface must still grow as the square root of R.

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