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Failure of the optical theorem for Gaussian-beam scattering by a spherical particle

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It is shown that when an electromagnetic wave with some degree of amplitude rolloff in the transverse direction is scattered by a spherical particle, the optical theorem is not valid. For such shaped beams the extinction cross section may be written as an infinite series in powers of the reciprocal of the beam width. The imaginary part of the forward-scattering amplitude is shown to be the first term in this series. Two approximations to the extinction cross section are presented for the special case of Gaussian-beam scattering. The first one is based on the dominance of diffraction in the forward direction for $w_0 \gtrsim a$, where w_0 is the beam half-width and a is the target particle radius. The second approximation, valid for $w_0 \lesssim a$, is based on transmission-compensating field interference.   1995 Optical Society of America

1. INTRODUCTION

A useful^{1,2} and long-celebrated³ result in the theory of wave scattering is the Bohr–Peierls–Placzek relation, otherwise known as the optical theorem. It states that the total cross section for elastic plus inelastic scattering by either a spherical or nonspherical particle is proportional to the imaginary part of the scattering amplitude evaluated in the forward direction. In this paper we show that the optical theorem is true only for incident plane waves or locally plane waves. It is not valid if the incident wave has some degree of amplitude rolloff in the transverse direction. We note, however, that scattering by a transversely localized beam is generally not important in quantum-mechanical scattering, since the wave function of a high-energy projectile incident on a small target is well modeled by a plane wave.⁴ Nevertheless, non-plane-wave incidence is important in light-scattering phenomena, since a laser beam can be focused down to a transverse focal waist that is only slightly larger than the wavelength.⁵ Consequently, when a target particle is located in the focal waist of such a beam, a proper description of the light scattering requires that the beam shape be taken into account.⁶

Since the failure of the optical theorem for shaped beams is of practical importance in light scattering, we carry out our analysis using the language of light scattering. Hereafter, the total cross section is called the extinction cross section. Furthermore, the scattering amplitude is proportional to the scattered electric field and is defined to be 90  out of phase with it in the complex

plane [see Eqs. (11)]. As a result of this phase difference, the optical theorem states that the extinction cross section is proportional to the real part of the light-scattering amplitude in the forward direction, $S(0)$, and is given by

$$\sigma_{\text{ext}} = \frac{4\pi}{k^2} \text{Re}[S(0)], \quad (1)$$

where the wave number is

$$k = \frac{2\pi}{\lambda}. \quad (2)$$

The body of this paper is organized as follows. In Section 2 we briefly sketch the derivation of the extinction cross section for the scattering of a transversely localized electromagnetic wave by a spherical particle and show that it is proportional to the real part of the forward light-scattering amplitude for only plane waves or locally plane waves. In Section 3 we specialize our discussion to the scattering by a sphere located along the axis of a focused Gaussian laser beam. For this geometry we carry out a series expansion of the extinction cross section in powers of the transverse beam confinement parameter s . We show that the familiar optical theorem expression is the first term of the series. We also find that the convergence rate of the series depends on the size of the spherical particle relative to the transverse beam width. In Section 4 we derive two approximations to the extinction cross section for Gaussian-beam scattering. The first proves to be accurate when the transverse width of the beam is larger than the target particle, and

the second is accurate when the transverse width of the beam is smaller than the particle. Last, in Section 5 we summarize our results.

2. EXTINCTION CROSS SECTION FOR SCATTERING OF A TRANSVERSELY LOCALIZED BEAM BY A SPHERICAL PARTICLE

Consider an electromagnetic wave, such as a laser beam, propagating along the z axis of a rectangular coordinate system and localized to a half-width w_0 centered on the origin. The light wave has wavelength λ , angular frequency ω , and wave number k . In the x - y plane its electric field is polarized in the x direction. Let the origin also be coincident with the center of a homogeneous spherical particle of radius a and complex refractive index $m = n + i\kappa$. For this geometry a beam propagating along the z axis is called an on-axis beam, since it strikes the target particle head on. A beam propagating parallel to but not along the z axis is known as an off-axis beam. The electric and magnetic fields of an on-axis beam may be written in terms of the TE and TM scalar radiation potentials as⁷

$$\begin{aligned}\mathbf{E}_{\text{beam}}(\mathbf{r}, t) &= -\mathbf{r} \times \nabla \psi^{\text{TE}} + \frac{ic}{\omega} \nabla \times (\mathbf{r} \times \nabla \psi^{\text{TM}}), \\ \mathbf{B}_{\text{beam}}(\mathbf{r}, t) &= \frac{i}{\omega} \nabla \times (\mathbf{r} \times \nabla \psi^{\text{TE}}) + \frac{1}{c} \mathbf{r} \times \nabla \psi^{\text{TM}}.\end{aligned}\quad (3)$$

The partial-wave decomposition of the radiation potentials is⁸

$$\begin{aligned}\left. \begin{aligned} \psi^{\text{TE}}(\mathbf{r}, t) \\ \psi^{\text{TM}}(\mathbf{r}, t) \end{aligned} \right\} &= E_0 \exp(-i\omega t) \sum_{l=1}^{\infty} \frac{i^l (2l+1)}{l(l+1)} g_l j_l(kr) P_l^1(\cos \theta) \\ &\quad \times \begin{cases} \sin \phi \\ \cos \phi \end{cases}.\end{aligned}\quad (4)$$

In Eqs. (3) and (4) c is the speed of light, E_0 is a measure of the peak electric-field amplitude, $j_l(kr)$ are spherical Bessel functions, and $P_l^1(\cos \theta)$ are associated Legendre polynomials. It should be noted that the authors of Ref. 8 employ a different sign convention for both the time dependence and the P_l^1 functions from that used here.

Equations (3) and (4) are an exact solution of Maxwell's equations and describe in the greatest generality an on-axis, axisymmetric light beam. The partial-wave decomposition of an off-axis light beam is given in Ref. 9. The set of partial-wave coefficients g_l are known as beam-shape coefficients. The specification of these coefficients determines the specific functional form of the electric and magnetic fields of the on-axis beam. Alternatively, if the exact functional form of the fields (in particular, the radial components of the fields) is known, the beam-shape coefficients may be determined by¹⁰

$$g_l \frac{(-i)^{l-1}}{2} \frac{kr}{j_l(kr)} \frac{1}{l(l+1)} \int_0^\pi \sin^2 \theta d\theta f(kr, \theta) \times \exp(ikr \cos \theta) P_l^1(\cos \theta), \quad (5)$$

where for an on-axis beam the radial field components assume the form

$$\begin{aligned}E_{\text{beam}}^{\text{radial}} &= E_0 \exp(ikr \cos \theta) f(kr, \theta) \sin \theta \cos \phi, \\ B_{\text{beam}}^{\text{radial}} &= \frac{E_0}{c} \exp(ikr \cos \theta) f(kr, \theta) \sin \theta \sin \phi.\end{aligned}\quad (6)$$

For example, the set of beam-shape coefficients

$$g_l = 1 \quad (7)$$

for $1 \leq l \leq \infty$ exactly corresponds to a plane wave polarized in the x direction,

$$\begin{aligned}\mathbf{E}(\mathbf{r}, t) &= E_0 \exp[i(kz - \omega t)] \hat{u}_x, \\ \mathbf{B}(\mathbf{r}, t) &= \frac{E_0}{c} \exp[i(kz - \omega t)] \hat{u}_y.\end{aligned}\quad (8)$$

The set of beam-shape coefficients

$$g_l = \exp[-s^2(l+1/2)^2], \quad (9)$$

where the transverse beam confinement parameter s is given by

$$s = \frac{1}{kw_0}, \quad (10)$$

closely approximates a Gaussian laser beam focused to the half-width w_0 at the origin of coordinates and polarized in the x direction.^{11,12} For future reference, an analytical approximation to a Gaussian laser beam focused to the half-width w_0 at the origin of coordinates and polarized in the x direction is given by the Davis first-order beam model¹³

$$\begin{aligned}\mathbf{E}_{\text{beam}}^{\text{Davis}} &= \frac{E_0}{D} \exp[i(kz - \omega t)] \exp[-(x^2 + y^2)/w_0^2 D] \\ &\quad \times \left(\hat{u}_x - \frac{2isx}{w_0 D} \hat{u}_z \right), \\ \mathbf{B}_{\text{beam}}^{\text{Davis}} &= \frac{E_0}{cD} \exp[i(kz - \omega t)] \exp[-(x^2 + y^2)/w_0^2 D] \\ &\quad \times \left(\hat{u}_y - \frac{2isy}{w_0 D} \hat{u}_z \right),\end{aligned}\quad (11)$$

where

$$D = 1 + \frac{2isz}{w_0}. \quad (12)$$

Returning to the development of our formalism for a general axisymmetric beam, the shaped beam of Eqs. (3) and (4) is scattered by the spherical particle at the origin. In the far zone the scattered electric and magnetic fields are⁸

$$\begin{aligned}\mathbf{E}_{\text{scatt}}(\mathbf{r}, t) &= \frac{-iE_0}{kr} \exp[i(kr - \omega t)] [-S_2(\theta)(\cos \phi) \hat{u}_\theta \\ &\quad + S_1(\theta)(\sin \phi) \hat{u}_\phi], \\ \mathbf{B}_{\text{scatt}}(\mathbf{r}, t) &= \frac{-iE_0}{ckr} \exp[i(kr - \omega t)] [-S_1(\theta)(\sin \phi) \hat{u}_\theta \\ &\quad - S_2(\theta)(\cos \phi) \hat{u}_\phi],\end{aligned}\quad (13)$$

where the light-scattering amplitudes $S_1(\theta)$ and $S_2(\theta)$ are

$$S_1(\theta) = \sum_{l=1}^{\infty} \frac{2l+1}{l(l+1)} g_l [a_l \pi_l(\theta) + b_l \tau_l(\theta)],$$

$$S_2(\theta) = \sum_{l=1}^{\infty} \frac{2l+1}{l(l+1)} g_l [a_l \tau_l(\theta) + b_l \pi_l(\theta)]. \quad (14)$$

The angular functions in Eqs. (14) are

$$\pi_l(\theta) = \frac{1}{\sin \theta} P_l^1(\cos \theta), \quad \tau_l(\theta) = \frac{d}{d\theta} P_l^1(\cos \theta), \quad (15)$$

and a_l and b_l are the partial-wave scattering amplitudes for plane-wave electromagnetic scattering. The partial-wave scattering amplitudes depend only on the partial-wave number, the particle size parameter

$$x = \frac{2\pi a}{\lambda}, \quad (16)$$

and the refractive index.¹⁴⁻¹⁶ The total electric and magnetic fields exterior to the target particle are

$$\mathbf{E}_{\text{total}} = \mathbf{E}_{\text{beam}} + \mathbf{E}_{\text{scatt}}, \quad \mathbf{B}_{\text{total}} = \mathbf{B}_{\text{beam}} + \mathbf{B}_{\text{scatt}}. \quad (17)$$

The absorption, scattering, and extinction cross sections are defined as^{17,18}

$$\sigma_{\text{abs}} = \frac{-cr^2}{E_0^2} \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi \operatorname{Re}(\mathbf{E}_{\text{total}}^* \times \mathbf{B}_{\text{total}}), \quad (18)$$

$$\sigma_{\text{scatt}} = \frac{cr^2}{E_0^2} \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi \operatorname{Re}(\mathbf{E}_{\text{scatt}}^* \times \mathbf{B}_{\text{scatt}}), \quad (19)$$

$$\sigma_{\text{ext}} = \frac{-cr^2}{E_0^2} \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi \operatorname{Re}(\mathbf{E}_{\text{beam}}^* \times \mathbf{B}_{\text{scatt}} + \mathbf{E}_{\text{scatt}}^* \times \mathbf{B}_{\text{beam}}), \quad (20)$$

respectively, and are related to each other by the energy conservation condition

$$\sigma_{\text{ext}} = \sigma_{\text{scatt}} + \sigma_{\text{abs}}. \quad (21)$$

Substitution of Eqs. (3), (4), (13), (14), and (17) into Eqs. (18)–(20) gives the general formulas for the scattering and extinction cross sections¹⁹:

$$\sigma_{\text{scatt}} = \frac{4\pi}{k^2} \sum_{l=1}^{\infty} (l+1/2) |g_l|^2 (|a_l|^2 + |b_l|^2), \quad (22)$$

$$\sigma_{\text{ext}} = \frac{4\pi}{k^2} \sum_{l=1}^{\infty} (l+1/2) |g_l|^2 \operatorname{Re}(a_l + b_l). \quad (23)$$

The general formulas for an off-axis light beam are given in Ref. 9.

We now assess the validity of the optical theorem for scattering of a general on-axis beam by a spherical particle. The angular functions of Eqs. (15) evaluated at $\theta = 0^\circ$ are

$$\pi_l(0) = \tau_l(0) = \frac{l(l+1)}{2}. \quad (24)$$

The forward-scattering amplitude is then

$$S(0) = S_1(0) = S_2(0) = \sum_{l=1}^{\infty} (l+1/2) g_l (a_l + b_l). \quad (25)$$

A comparison of Eqs. (23) and (25) reveals that since σ_{ext} contains $|g_l|^2$ within the sum over partial waves and $S(0)$ contains g_l within the sum, the familiar optical theorem expression of Eq. (1) is strictly valid for an on-axis beam when each of the nonzero beam-shape coefficients has $g_l = 1$. The most notable example of such a beam is the plane wave of Eqs. (7) and (8). Another example is provided by the so-called top hat beam of Ref. 20 for which $g_l = 1$ for $1 \leq l \leq l_{\text{max}}$ and $g_l = 0$ for $l > l_{\text{max}}$. This beam, though somewhat localized in the transverse direction, strongly resembles a plane wave in both amplitude and phase in its plateau region. It may be thought of as being a locally plane wave, since a particle smaller than the width of the plateau region and placed at the beam waist experiences only the $g_l = 1$ partial waves of the beam. A similar argument concerning the validity of Eq. (1) can be made for scattering by an off-axis beam.

3. SERIES EXPANSION OF THE EXTINCTION CROSS SECTION FOR SCATTERING OF A GAUSSIAN BEAM BY A SPHERICAL PARTICLE

For the remainder of this paper we restrict our discussion to on-axis Gaussian-beam scattering, where g_l is given by Eq. (9). The forward-scattering amplitude of Eq. (25) may be interpreted as being a first moment of the partial waves. The weighting factor $g_l(a_l + b_l)$ takes into account both the details of the incident beam (through g_l) and the details of the target particle (through $a_l + b_l$). Using this interpretation, we define the higher moments of the partial waves as

$$S^{(j)}(0) = \sum_{l=1}^{\infty} (l+1/2)^j g_l (a_l + b_l). \quad (26)$$

When Eq. (9) is substituted into Eq. (23), we can replace $|g_l|^2$ by g_l^2 since the beam-shape coefficients are real for the on-axis Gaussian beam. If we then Taylor-series expand one of the g_l factors in powers of s , we obtain

$$\sigma_{\text{ext}} = \frac{4\pi}{k^2} \sum_{j=0}^{\infty} \frac{(-1)^j}{j!} s^{2j} \operatorname{Re}[S^{2j+1}(0)]. \quad (27)$$

The infinite series in Eq. (27) is exactly equal to the extinction cross section of Eqs. (20) and (23) for the Gaussian beam of Eq. (9) and may be considered as a generalization of the optical theorem to Gaussian-beam scattering. The familiar optical theorem expression given in Eq. (1) is the $j = 0$ term of the series. This particular expression was motivated by the desire to relate σ_{ext} to the forward-scattering amplitude or to something as close to it as possible. But as we will presently see, Eq. (27) turns out to be rather unwieldy to use in certain practical situations.

When a tightly focused beam is incident on a large particle, so that $w_0 \ll a$, Eq. (27) has poor convergence properties. This can be seen in the following numerical example, where a focused Gaussian beam with $\lambda = 0.6328 \mu\text{m}$ and variable w_0 is incident on a spherical water droplet with $a = 50 \mu\text{m}$ and $n = 1.333$. In this example the particle radius is sufficiently large that even when $w_0 \ll a$, we still have $w_0 \gg \lambda$, so that both the local-

Table 1. Number of Terms j_{\max} in Eq. (27) for 1 Part in 10^6 Agreement with Eq. (23) for $\lambda = 0.6328 \mu\text{m}$, $a = 50 \mu\text{m}$, and $n = 1.333$

w_0 (μm)	j_{\max}
100,000	0
10,000	1
1,000	2
500	2
100	5
50	12
10	147

ized approximation^{21,22} of Eq. (9) and the Davis first-order beam model²³ of Eqs. (11) and (12) closely approximate a focused Gaussian beam. For this situation the extinction cross section was computed with Eqs. (9) and (23). The number of terms j_{\max} in Eq. (27) required for 1 part in 10^6 agreement with Eq. (23) was determined, and the results are shown in Table 1. For $w_0 \geq 10a$ the Gaussian beam does not differ much from a plane wave in the vicinity of the target particle. As a result, only a few terms in Eq. (27) are required for convergence of the series. Conversely, for $w_0 < a$, a large number of terms is required for convergence, and a large number of significant digits is required for each term for the prevention of roundoff error, i.e., 10 significant digits are required for $w_0 = a$, and 29 significant digits are required for $w_0 = 0.2a$. Efficient methods for approximating σ_{ext} for both weakly focused and tightly focused Gaussian beams are pursued in Section 4.

4. TWO APPROXIMATIONS TO THE EXTINCTION CROSS SECTION FOR GAUSSIAN-BEAM SCATTERING

In this section we derive two simple approximations for σ_{ext} , one for $w_0 \geq a$ and the other for $w_0 \leq a$. Our first approximation, which we call the wide-beam approximation (WBA), is motivated theoretically by the desire to relate σ_{ext} solely to $S(0)$ rather than to both $S(0)$ and the higher moments of the partial waves defined in Eq. (26). It is motivated experimentally by the following observations. A strong correspondence between light scattering and the total intensity in the forward direction is easily illustrated for an on-axis laser beam striking a spherical particle. For beam and droplet radii of comparable magnitude the far-field total intensity in and about the forward direction is reduced substantially compared with the forward intensity occurring in the absence of a particle. This phenomenon is unlike the case of plane-wave scattering, for which the effect of a microscopic particle on the far-field intensity is imperceptible to the eye. Such experiments are described in Ref. 24 and provided the impetus to seek a connection between the forward intensity and the total extinction cross section.

The derivation of the WBA begins by an examination of the intensity in the forward direction corresponding to the total fields of Eqs. (17). When we substitute Eqs. (13) and the spherical coordinate form of Eqs. (11) into Eqs. (17) and use the Poynting theorem, the far-zone forward total intensity is

$$I_{\text{total}}(0) = \text{Re} \left(\frac{E_{\text{total}}^{\theta*} B_{\text{total}}^{\phi} - E_{\text{total}}^{\phi*} B_{\text{total}}^{\theta}}{2\mu_0} \right) \\ = \frac{E_0^2}{2\mu_0 c} \frac{1}{k^2 r^2} \left[\frac{k^4 w_0^4}{4} - k^2 w_0^2 \text{Re}[S(0)] + |S(0)|^2 \right]. \quad (28)$$

The first term on the right-hand side of Eq. (28) is the incident beam intensity in the forward direction. The second term is the intensity corresponding to the interference between the incident beam and the scattered wave. The third term is the scattered intensity in the forward direction.

At this point two assumptions must be made. These are that (1) diffraction dominates all other scattering processes in the forward direction, and (2) the extinction efficiency is roughly 2. Consider first the role of diffraction. The contribution of diffraction by the spherical obstacle to the intensity is obtained by a Debye-series decomposition of the partial-wave scattering amplitudes.^{25,26} When the result

$$a_l^{\text{diffraction}} = b_l^{\text{diffraction}} = 1/2 \quad (29)$$

is inserted into Eqs. (14) and the partial-wave series is summed between $l = ka$ and $l = \infty$, the forward-diffracted intensity for Gaussian-beam scattering is^{24,27}

$$I_{\text{diffracted}}(0) = \frac{E_0^2}{2\mu_0 c k^2 r^2} \left(\frac{k^4 w_0^4}{4} \right) \exp(-2a^2/w_0^2). \quad (30)$$

Consider next the extinction efficiency ϵ_{ext} , which is the extinction cross section divided by the cross section for the beam striking the target particle

$$\epsilon_{\text{ext}} = \frac{\sigma_{\text{ext}}}{\sigma_{\text{inc}}}. \quad (31)$$

For a plane wave incident on a spherical particle of radius a the incident beam cross section is

$$\sigma_{\text{inc}} = \pi a^2, \quad (32)$$

and, for Gaussian-beam incidence and with the use of Eqs. (11), it is approximately

$$\sigma_{\text{inc}} \approx \int_0^a \rho d\rho \int_0^{2\pi} d\xi \exp(-2\rho^2/w_0^2) \\ = \frac{\pi w_0^2}{2} [1 - \exp(-2a^2/w_0^2)]. \quad (33)$$

The extinction efficiency is roughly 2 when the target particle is large ($a \gg \lambda$) and when the incident beam is wide ($w_0 > a$). A consequence of this assumption is that when Eqs. (30) and (31) and relation (32) are combined with

$$\epsilon_{\text{ext}} \approx 2, \quad (34)$$

the extinction cross section is approximately²⁴

$$\sigma_{\text{ext}} \approx \pi w_0^2 [1 - \exp(-2a^2/w_0^2)] \\ = \pi w_0^2 \left[1 - \frac{2\mu_0 c k^2 r^2}{E_0^2} \left(\frac{4}{k^4 w_0^4} \right) I_{\text{diffraction}}(0) \right]. \quad (35)$$

Since the largest contribution to the forward total intensity is given by the diffracted intensity of Eq. (30), we take

$$I_{\text{total}}(0) \approx I_{\text{diffraction}}(0). \quad (36)$$

This is again valid for $a \gg \lambda$ and $w_0 \gtrsim a$. As a result, we may substitute Eq. (28) into relation (35) in place of $I_{\text{diffraction}}(0)$ and obtain

$$\sigma_{\text{ext}} \approx \frac{4\pi}{k^2} \text{Re}[S(0)] \left\{ 1 - \frac{s^2 |S(0)|^2}{\text{Re}[S(0)]} \right\} \quad (37)$$

as our first approximation (i.e., WBA) to the extinction cross section for either a dielectric or absorbing spherical particle.²⁸ Since the WBA was derived under the assumption that $w_0 > a$, we will find shortly that it works well for $w_0 \gtrsim a$ but not for $w_0 \lesssim a$ for a dielectric particle. For $w_0 \rightarrow \infty$ or $s = 0$ it reduces to Eq. (1).

The $w_0 \lesssim a$ regime will be handled by our second approximation, which we call the narrow-beam approximation (NBA). In the NBA σ_{ext} is not related to $S(0)$. Rather it is related to the physical processes that contribute most importantly to scattering. As an introduction to this physically based point of view, we briefly review how it has been applied previously to plane-wave scattering by a nonabsorbing spherical particle. For plane-wave incidence, forward scattering by a dielectric spherical particle is dominated by diffraction, the specular reflection forward glory,^{29,30} and transmission through the particle. In this case, for $a \gg \lambda$, the forward-scattering amplitude is approximately³¹

$$S(0) \approx \frac{x^2}{2} + 0.49805(1 + \sqrt{3}i)x^{4/3} + \frac{2xn^2}{(n+1)(n+1)^2} \times \exp[2ix(n-1) - 3\pi i/2]. \quad (38)$$

The first term in relation (38) is due to Fraunhofer diffraction by the complementary circular aperture, the second term is due to reflection, and the third term is due to transmission and is evaluated with the use of ray optics. When we use the optical theorem of Eq. (1) for plane-wave incidence, the resulting scattering efficiency is

$$\epsilon_{\text{scatt}} \approx 2 + 1.9922x^{-2/3} - \frac{8}{x} \frac{n^2}{(n-1)(n+1)^2} \times \sin[2(n-1)x]. \quad (39)$$

This approximates well the numerical evaluation of Eqs. (22) and (23) for plane-wave incidence³² with $g_l = 1$, since for a nonabsorbing particle the extinction and scattering efficiencies are equal.

We now apply this physically based line of reasoning to scattering by an on-axis Gaussian beam. Numerical computations of Gaussian-beam scattering²¹ show that for a nonabsorbing particle with $a \gg \lambda$ more light is scattered in the near-forward direction than in any other direction. Thus the integrated near-forward intensity provides the bulk of the scattered power. For a tightly focused beam incident on a large particle, such that $w_0 \ll a$, diffraction in the near-forward direction is not important, since only the dying tail of the beam in the transverse direction grazes the edge of the target particle.²⁷ For the same reason near-forward specular reflection is also

not important. On the other hand, transmission that we model as

$$S_{\text{transmission}}(\theta) = \frac{2n^2x}{(n-1)(n+1)^2} \exp[2ix(n-1) - 3i\pi/2] \times \exp\left[ix\frac{\theta^2}{4}\left(\frac{n}{n-1}\right)\right] G(\theta), \quad (40)$$

where

$$G(\theta) = \exp(-\gamma\theta^2) \quad (41)$$

is expected to be important for small θ . All the factors in Eq. (40) with the exception of $G(\theta)$ are calculated with the use of ray optics with plane-wave incidence.²⁵ The $G(\theta)$ factor qualitatively models the effect of the Gaussian profile of the incident beam on the amplitude of the transmitted rays. In order to evaluate γ , we assume that both the reflected power and the power transmitted following one or more internal reflections are negligible. In this case and for a nonabsorbing particle the integrated transmitted power is set equal to the power incident on the particle, which is given by relation (33) with $a \ll w_0$. This gives

$$\gamma = \frac{4a^2}{w_0^2} \frac{n^4}{(n-1)^2(n+1)^4}. \quad (42)$$

The only other physical process important for small θ when $a \ll w_0$ is the effect of the compensating field.^{33,34} The compensating field is a result of our decomposition of the total fields into the sum of a beam part and a scattered part as in Eqs. (17) for $w_0 < a$. When a narrow beam is incident on a wide particle, the particle stops the unimpeded propagation of the beam. As a result, the beam is absent behind the particle, and the only fields there are due to diffraction, reflection, transmission, etc. Despite this, \mathbf{E}_{beam} and \mathbf{B}_{beam} appear in Eqs. (17). Thus behind the particle there must be a contribution to $\mathbf{E}_{\text{scatt}}$ and $\mathbf{B}_{\text{scatt}}$ that cancels \mathbf{E}_{beam} and \mathbf{B}_{beam} , mathematically removing them from the equation. This contribution is known as the compensating field^{33,34} and is given by

$$S_{\text{compensating}}(\theta) \approx \frac{-k^2w_0^2}{2} \exp(-\theta^2/4s^2). \quad (43)$$

We now compute the scattered power for $w_0 < a$ by integrating over the magnitude squared of the scattered electric field given by

$$\mathbf{E}_{\text{scatt}} = \mathbf{E}_{\text{transmission}} + \mathbf{E}_{\text{compensating}}, \quad (44)$$

where $S_{\text{transmission}}$ and $S_{\text{compensating}}$ are given by Eqs. (40)–(42) and relation (43). We obtain

$$\epsilon_{\text{scatt}} = 2.0 - \frac{4xn^2}{(n-1)(n+1)^2} \left[\left(\frac{1}{4s^2} + \gamma \right)^2 + \frac{x^2n^2}{16(n-1)^2} \right]^{-1/2} \sin[2x(n-1) + \eta], \quad (45)$$

where

$$\tan \eta = \frac{xn}{4(n-1)} \left(\frac{1}{4s^2} + \gamma \right)^{-1}. \quad (46)$$

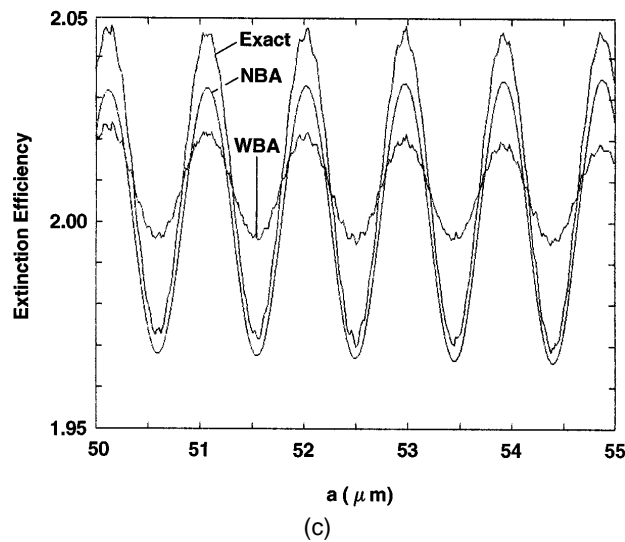
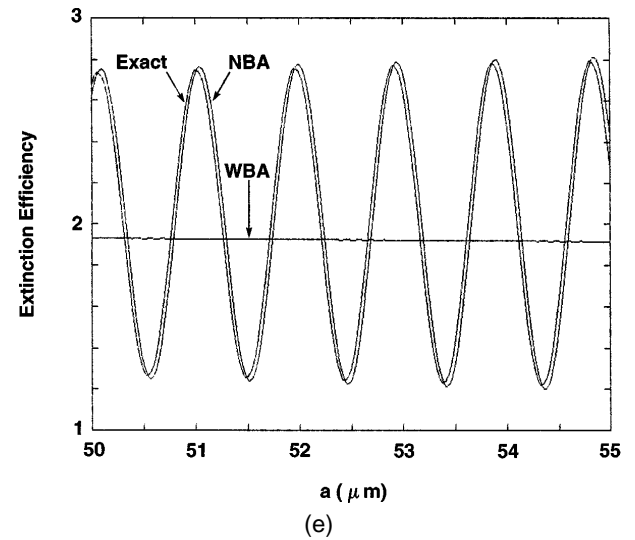
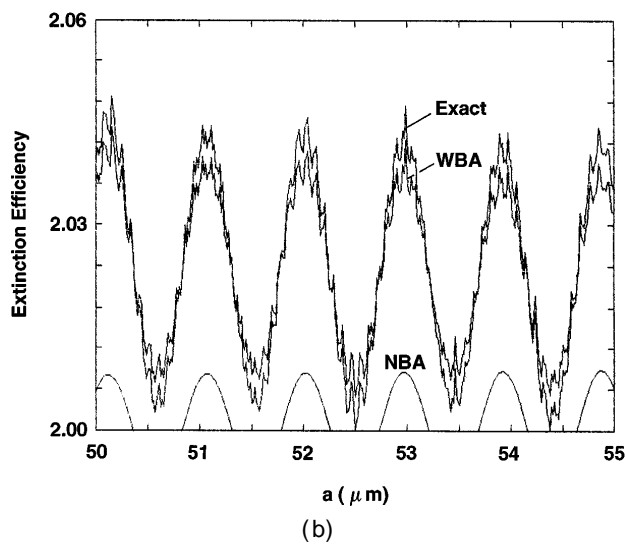
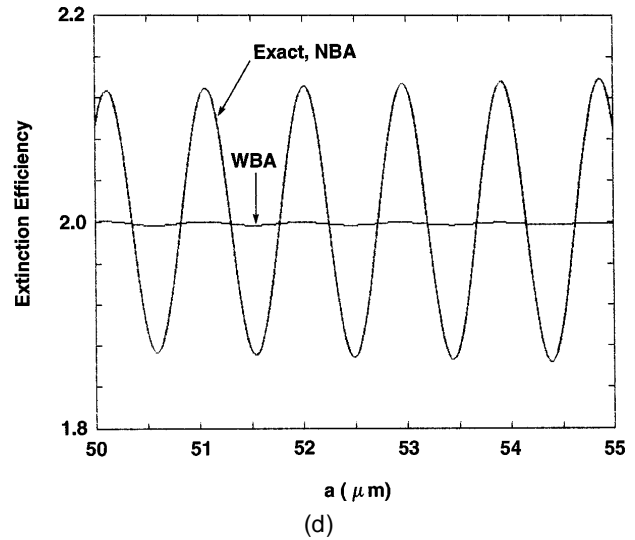
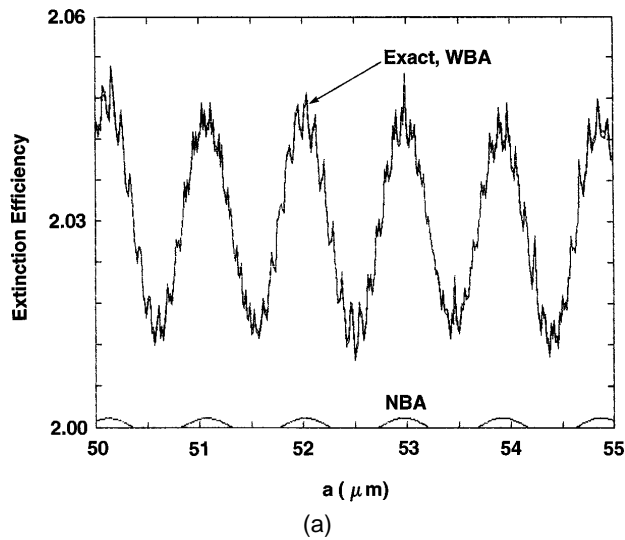


Fig. 1. Extinction efficiency as a function of the nonabsorbing target particle radius for $50 \mu\text{m} \leq a \leq 55 \mu\text{m}$, $n = 1.333 + 0i$, and $\lambda = 0.6328$ and for (a) $w_0 = 250 \mu\text{m}$, (b) $w_0 = 100 \mu\text{m}$, (c) $w_0 = 50 \mu\text{m}$, (d) $w_0 = 25 \mu\text{m}$, and (e) $w_0 = 10 \mu\text{m}$. The exact extinction cross section is given by Eq. (23). The WBA is given by relation (37), and the NBA is given by Eqs. (45) and (46). The WBA accurately approximates ϵ_{ext} for $w_0/a \gtrsim 1.5$, and the NBA accurately represents ϵ_{ext} for $w_0/a \lesssim 1.0$.

Again, for a nonabsorbing particle, the scattering and extinction efficiencies are equal. The factor of 2.0 in Eq. (45) is due to the combined effects of transmission (i.e., all the light striking the target particle is transmitted) and the compensating field (i.e., all of

the incident beam is blocked by the particle). The oscillations in Eq. (45) are produced by the transmission-compensating field interference, in analogy to the oscillations in relation (39) for plane-wave incidence produced by transmission-diffraction interference.^{35,36}

In order to assess the accuracy of the WBA [relation (37)] and the NBA [Eqs. (45) and (46)] for a nonabsorbing particle, we calculated the extinction efficiency for $\lambda = 0.6328 \mu\text{m}$, $n = 1.333 + 0i$, $50 \mu\text{m} \leq a \leq 55 \mu\text{m}$, and $10 \mu\text{m} \leq w_0 \leq 1000 \mu\text{m}$. Our results are summarized in Figs. 1(a), 1(b), 1(c), 1(d), and 1(e), corresponding to $w_0 = 250 \mu\text{m}$, $100 \mu\text{m}$, $50 \mu\text{m}$, $25 \mu\text{m}$, and $10 \mu\text{m}$, respectively. For every value of s , a , and w_0/a examined, the WBA differed from the exact extinction cross section of Eq. (23) by a smaller amount than did the familiar optical theorem of Eq. (1). The amount was often smaller by orders of magnitude. Similarly, even though the WBA was derived under the condition $\epsilon_{\text{ext}} \approx 2$, it was found to be accurate for small particles with $x \approx 1$, where $\epsilon_{\text{ext}} < 2$. For $w_0 \geq 400 \mu\text{m}$ the WBA is virtually identical to the results of Eq. (27) with $j_{\text{max}} = 1$. But for $w_0 < 400 \mu\text{m}$ the WBA differs from the extinction cross section by at most 0.3% for $w_0/a = 2.0$ and by at most 1.2% for $w_0/a = 1.0$, while the series expansion of Eq. (27) with $j_{\text{max}} = 1$ differs from the extinction cross section by 2.5% and 20% in the two cases, respectively. For $w_0/a \lesssim 1.5$ the oscillations in the WBA decrease rapidly as w_0 decreases while the oscillations in the extinction cross section increase, limiting the utility of WBA for nonabsorbing particles to $w_0/a \gtrsim 1.5$.

On the other hand, the oscillations in the NBA are too small for $w_0/a \gtrsim 1.5$, which makes it a poor approximation to the extinction cross section for wide beams. By the time w_0 has decreased to $w_0 \approx a$, however, the transmission-compensating field oscillations in the NBA have grown so as to match the extinction cross section well. In Figs. 1(c)–1(e) the NBA is seen to be accurate for $0.2 \leq w_0/a \leq 1.0$. For $w_0/a = 0.1$ the oscillations in the NBA grow to such an extent that the NBA becomes negative at the low points of the oscillations, which limits the utility of the NBA approximation to $0.2 \leq w_0/a \leq 1.0$.

Concerning scattering by absorbing particles with $\kappa \approx 0.1$, the WBA was found to be accurate both for $w_0 > a$ and for $w_0 < a$. The good agreement for $w_0 < a$ is due to the fact that absorption damps the oscillations in σ_{ext} , matching the near constancy of the WBA for $w_0 < a$. The damping of the oscillations in σ_{ext} is also evident in the NBA. For an absorbing particle Eq. (40) and the second term in Eq. (45) should contain an additional $\exp(-2x\kappa)$ factor that describes the attenuation of the forward-transmitted ray through the particle. This factor is the source of the damping of the transmission-compensating field interference in σ_{ext} .

A final comment should be made concerning both the WBA and the NBA. With regard to the WBA, the form of relation (37), containing a term of order s^0 plus another term of order s^2 , might suggest that these are the first two terms of another series expansion of σ_{ext} in powers of s with coefficients that contain powers of $\text{Re}[S(0)]$ and $|S(0)|^2$. Attempts were made to construct the higher-order terms of such a series. The series obtained, however, were in general no closer an approximation to the extinction cross section than was relation (37). Perhaps this is not surprising in light of our derivation of relation (37). In particular, Eq. (28) which contains the $\text{Re}[S(0)]$ term describing incident beam-scattering interference and the $s^2|S(0)|^2$ term describing the scattered intensity, is an exact evaluation of the forward-direction

total intensity. It is not the first two terms in a series expansion of the total forward intensity. So trying to construct higher-order terms in s^2 for Eq. (28) is equivalent to attempting to impose additional contributions to the total forward intensity that in fact do not exist.

With regard to the NBA, the extinction efficiency itself suffers from a difficulty in interpretation for $w_0 \ll a$. This is because the compensating field, which plays such a major role in Eqs. (45) and (46) is not observable in experiments. Rather, it is the intensity corresponding to the total fields given by Eqs. (17) that is observed in near-forward-direction scattering experiments. When the scattered field is combined with the beam field in Eqs. (17), the compensating field and the beam field cancel for small θ . This cancellation precludes the observability of them individually or of any quantity such as ϵ_{ext} of Figs. 1(d) and 1(e) whose central feature is based on transmission-compensating field interference. A more physically meaningful cross section for $w_0 \ll a$ that is free of these nonobservable oscillations is described in detail elsewhere.³⁴

5. CONCLUSION

In summary, the main point of this study is that the familiar optical theorem expression given in Eq. (1) is not a general result independent of the form of the incident field. In particular, it is limited to the case of plane-wave or locally plane-wave incidence. As a practical matter, for the special case of scattering of a Gaussian beam by a spherical particle, $(4\pi/k^2)\text{Re}[S(0)]$ is a good approximation to σ_{ext} when the transverse size of the beam is much larger than the target particle (i.e., $w_0/a \gtrsim 50$). But, already for $w_0/a \approx 10$, the familiar optical theorem expression yields a cross section that is in error by approximately 0.5% of the exact result. This may not seem like a large error. But at $w_0/a \approx 10$ the WBA of relation (36) is in error by only approximately 0.006% of the exact result, which clearly illustrates its superiority over Eq. (1) for shaped-beam scattering. We have given two approximations for σ_{ext} for Gaussian beams. As seen in Figs. 1(a) and 1(b), the WBA is accurate for $w_0/a \gtrsim 1.5$, and, as seen in Figs. 1(c)–1(e), the NBA is accurate for $0.2 \leq w_0/a \leq 1.0$. In practice, one achieves plane-wave-like illumination on a small particle by using a wide Gaussian laser beam. Consequently, under these common circumstances, the calculations of Section 4 suggest that it is more accurate to approximate the extinction cross section by means of the WBA of relation (37) instead of the familiar optical theorem expression of Eq. (1).

The WBA and the NBA were derived under the assumption that the target particle was spherical in shape. The greatest practical utility of the optical theorem, however, is in the estimation of the extinction cross section for nonspherical particles with the anomalous diffraction method.^{37,38} In light of this, it would be of great interest to extend the two approximations presented here to scattering of shaped beams by nonspherical particles.

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