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Laser–particle interactions in shaped beams: Beam power normalization

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ABSTRACT

We present a semi-analytic theory for calculating light–particle interactions in shaped laser beams even when the paraxial beam description is invalid. It requires weighting the expressions for the cross sections with a *beam normalization parameter*, $\varkappa$, associated with the incident power. An analytical formula for $\varkappa$ in terms of the beam shape coefficients [1–3] is derived. We show that approximate expressions for this beam normalization parameter based on either a Parseval or paraxial type approximation are inadequate for optics involving high numerical apertures.

1. Introduction

Shaped laser beams have become a routine tool in numerous light–particle applications like optical force experiments, particle size analyzers, and Doppler velocimetry. One of the most powerful theoretical methods for modeling shaped beam is to develop their wave function in terms of the vector partial waves (also known as vector spherical wave functions or multipolar fields). Such developments provide an efficient description of the beam throughout all space (both near and far fields), and when described in this framework, even complicated beam profiles are guaranteed to satisfy the Maxwell propagation equations. The coefficients in the vector partial waves (VPW) expansion can conveniently be formulated in terms of beam shape coefficients as has been studied extensively by Gouesbet, Grehan and Lock. (see Refs. [1–3] and references cited therein).

Quantitative theoretical predictions require establishing the relationship between the beam shape coefficients and the total beam power. This may appear trivial at first glance since the relationship between scattered field coefficients and scattered power is a simple and well-known analogue of the Parseval formula from signal analysis (cf. Eq. (8) below). In this work, we derive a convenient analytic formula between the incident field coefficients and the incident beam power and we will see that it is more complex than its scattered field analogue. Last, we show how this factor normalizes cross-sectional type formulas for shaped beams.

The outline of this work is as follows: our notation is introduced by reviewing VPW field developments and beam shape coefficients in Section 2 and recalling why the scattered power satisfies a Parseval type relation. We also explain why a Parseval type relation for incident beam power does *not* hold for the beam shape coefficients. We finally present an analytic formula that correctly relates beam power to the beam shape coefficients. This result is formulated in terms of beam normalization parameter, $\varkappa$. The utility of this formula for non-paraxial beams is tested on a generic case using the beam shape coefficients derived in the localized approximation for Davis beams. Finally, we derive formulas for calculating light particle cross sections in Section 3. Time harmonic fields with $\exp -i\omega t$ time dependence and SI units are used throughout.

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2. Electromagnetic partial wave expansions

The time harmonic Maxwell equations in an absorption free host medium takes the form of a second-order differential equation

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{r}) - k^2 \mathbf{E}(\mathbf{r}) = 0, \tag{1}$$

with $k = \sqrt{\varepsilon_b \mu_b}\sqrt{\epsilon_0 \mu_0}\,\omega = n_b \omega / c$, where (ϵ_0, μ_0) are the permittivity and permeability of the vacuum, and ε_b and μ_b are the relative permittivity and permeability of the "background" or "host" dielectric medium. The vector partial waves (VPWs), $\mathbf{M}_{n,m}$ and $\mathbf{N}_{n,m}$, are a set of spherical waves centered on a given origin and which form a complete basis for solutions to Eq. (1).

Any scattered field, $\mathbf{E}_s(\mathbf{r})$, in the homogeneous medium and outside of a circumscribing sphere surrounding the scattering system can be developed in terms of outgoing partial waves i.e.

$$\mathbf{E}_s(\mathbf{r}) = E \sum_{n,m} [\mathbf{M}^{(3)}_{n,m}(k\mathbf{r}) f_{h,n,m} + \mathbf{N}^{(3)}_{n,m}(k\mathbf{r}) f_{e,n,m}], \tag{2}$$

where $\mathbf{M}^{(3)}_{n,m}$, $\mathbf{N}^{(3)}_{n,m}$, are the outgoing VPWs which satisfy Eq. (1) with outgoing boundary conditions [4–6]. They can be analytically expressed in spherical coordinates as

$$\mathbf{M}^{(3)}_{n,m}(k\mathbf{r}) \equiv h_n(kr) \mathbf{X}_{n,m}(\theta,\phi)$$
$$\mathbf{N}^{(3)}_{n,m}(k\mathbf{r}) \equiv \sqrt{n(n+1)}\frac{h_n(kr)}{kr}\mathbf{Y}_{n,m}(\theta,\phi) + \frac{[krh_n(kr)]'}{kr}\mathbf{Z}_{n,m}(\theta,\phi), \tag{3}$$

where h_n are the spherical Hankel functions of the first kind and $[krh_n(kr)]'$ is the derivative of $krh_n(kr)$ with respect to kr. The three vector spherical harmonics, denoted as $\mathbf{X}$, $\mathbf{Y}$, and $\mathbf{Z}$, are given explicitly in Appendix A and are defined to be orthonormal under angular integration

$$\int_0^{\pi} \sin\theta \, d\theta \int_0^{2\pi} d\phi \, \mathbf{A}^*_{\nu,\mu}(\theta,\phi) \cdot \mathbf{B}_{n,m}(\theta,\phi) = \delta_{\nu,n}\delta_{\mu,m}\delta_{A,B}, \tag{4}$$

with $\mathbf{A} = \mathbf{X}$, $\mathbf{Y}$, or $\mathbf{Z}$ and $\mathbf{B} = \mathbf{X}$, $\mathbf{Y}$, or $\mathbf{Z}$.

In Eq. (2) and throughout the rest of this work, the summation $\sum_{n,m}$ is a shorthand for summing over all multipole orders i.e.

$$\sum_{n,m} \rightarrow \sum_{n=1}^{\infty} \sum_{m=-n}^{m=n}. \tag{5}$$

The $f_{h,n,m}$ and $f_{e,n,m}$ of Eq. (2) are the dimensionless outgoing field coefficients (for type TE and TM waves respectively). Since all other factors on the right hand side of Eq. (2) are dimensionless, the factor E has the dimension of electric field, and a modification of its value only changes the overall intensity of the field. The value of this factor is determined by the amplitude of the incident field for scattering problems.

In analogy with the scattered field, the incident field is developed in terms of *regular* VPWs with TE(TM) fields being respectively described by the coefficients $a_{h,n,m}(a_{e,n,m})$

$$\mathbf{E}_{\text{inc}}(\mathbf{r}) = E \sum_{n,m} [\mathbf{M}^{(1)}_{n,m}(k\mathbf{r}) a_{h,n,m} + \mathbf{N}^{(1)}_{n,m}(k\mathbf{r}) a_{e,n,m}], \tag{6}$$

where the 'regular' VPWs, $\mathbf{M}^{(1)}_{n,m}$, $\mathbf{N}^{(1)}_{n,m}$, have the same expression as in Eq. (3) except that one replaces the spherical Hankel functions, h_n, with spherical Bessel functions, j_n. The factor E can now be related to the incident power flux (i.e. irradiance) since for plane waves, $\mathbf{E}_{\text{inc}}(\mathbf{r}) = E\hat{\mathbf{e}}_{\text{inc}} \exp(i\mathbf{k}_{\text{inc}} \cdot \mathbf{r})$, the incident irradiance is given by

$$I_{\text{inc}} \equiv \mathbf{S}_{\text{inc}} \cdot \hat{\mathbf{k}}_{\text{inc}} \equiv \frac{1}{2}\text{Re}\{\mathbf{E}^*_{\text{inc}} \times \mathbf{H}_{\text{inc}}\} \cdot \hat{\mathbf{k}}_{\text{inc}} = \frac{E^2}{2}\sqrt{\frac{\varepsilon_b \epsilon_0}{\mu_b \mu_0}}, \tag{7}$$

where $\mathbf{S}_{\text{inc}}$ is the incident Poynting vector, and $\hat{\mathbf{k}}_{\text{inc}}$ and $\hat{\mathbf{e}}_{\text{inc}}$ are respectively the unit wavevector and polarization vectors. In Eq. (7), we invoked the fact that for a plane wave, the incident magnetic field is given by $\mathbf{H}_{\text{inc}}(\mathbf{r}) = \sqrt{\varepsilon_b \epsilon_0 / \mu_b \mu_0}\, \hat{\mathbf{k}}_{\text{inc}} \times \mathbf{E}_{\text{inc}}$.

2.1. Radiated power and cross sections

The most common use of partial wave developments has been to describe scattered fields, with the Mie theory of spherical scatterers being the most well-known example in electromagnetism. As long as the electromagnetic effects are linear, radiated power is proportional to the power of the incident plane wave, and the scattered electromagnetic field adopts a particularly simple and useful expression

$$P_{\text{scat}} = \frac{I_{\text{inc}}}{k^2}\sum_{n,m}[|f_{h,n,m}|^2 + |f_{e,n,m}|^2] = \frac{I_{\text{inc}}}{k^2}\sum_{q=h,e}\sum_{n,m}|f_{q,n,m}|^2, \tag{8}$$

where I_{inc} is the irradiance of the incident plane wave given in Eq. (7). This formula is analogous to Parseval's relation of signal analysis and it states that the total scattered power is simply the sum of the power in each multipole order.

One derives the result of Eq. (8) by first recalling that in the far field limit, $\mathbf{H}_{\text{scat}}(\mathbf{r}) \underset{r\to\infty}{=} \sqrt{\varepsilon_b \epsilon_0 / \mu_b \mu_0}\, \hat{\mathbf{r}} \times \mathbf{E}_{\text{scat}}$, and the total radiated (scattered) power is obtained by integrating over all directions in the far field i.e.

$$P_{\text{scat}} = \lim_{r\to\infty} \int r^2 \hat{\mathbf{r}} \cdot \mathbf{S}_{\text{scat}}(\mathbf{r})\, d\Omega$$
$$= \frac{1}{2}\sqrt{\frac{\varepsilon_b \epsilon_0}{\mu_b \mu_0}} \lim_{r\to\infty} \int r^2 \mathbf{E}^*_{\text{scat}}(\mathbf{r}) \cdot \mathbf{E}_{\text{scat}}(\mathbf{r})\, d\Omega. \tag{9}$$

One finishes the derivation of Eq. (8) by inserting the far-field expressions for $\mathbf{M}^{(3)}_{n,m}$ and $\mathbf{N}^{(3)}_{n,m}$

$$\lim_{r\to\infty} \mathbf{M}^{(3)}_{n,m}(k\mathbf{r}) \rightarrow i^{-n+1}\frac{\exp(ikr)}{kr}\mathbf{X}_{n,m}(\hat{\mathbf{r}}),$$
$$\lim_{r\to\infty} \mathbf{N}^{(3)}_{n,m}(k\mathbf{r}) \rightarrow i^{-n}\frac{\exp(ikr)}{kr}\mathbf{Z}_{n,m}(\hat{\mathbf{r}}) \tag{10}$$

into the scattered field development of Eq. (2). The final result of Eq. (8) is then obtained by appealing to the orthogonality of the VSHs over angular integration, cf. Eq. (4). Finally one uses Eq. (7) to fix the parameter, E, in terms to the incident irradiance, i.e.

$$E^2 = 2I_{\text{inc}}\sqrt{\frac{\mu_b \mu_0}{\varepsilon_b \epsilon_0}}. \tag{11}$$

An expression for the scattering cross section, σ_{scat}, naturally arises from Eq. (8)

$$P_{\text{scat}} = I_{\text{inc}} \sigma_{\text{scat}}, \tag{12}$$

which yields the well-known multipole expression for the scattering cross section

$$\sigma_{\text{scat}} = \frac{1}{k^2} \sum_{q=h,e} \sum_{n,m} \left| f_{q,n,m} \right|^2. \tag{13}$$

When the scatterers and the variations in beam intensity are both small with respect to the wavelength, one can approximate the light–matter interactions by interpreting Eq. (12) as a local relation, namely that the power scattered by a particle at a position $\mathbf{r}$, is approximately $P_{\text{scat}} \simeq I_{\text{inc}}(\mathbf{r})\sigma_{\text{scat}}$, where $I_{\text{inc}}(\mathbf{r})$ is the local irradiance of the shaped beam. However, this approximation is invalid in many situations involving high numerical aperture (NA) optics.

2.2. Partial wave developments and beam shape coefficients

Before the advent of lasers, the most common theoretical choice for incident fields in electromagnetic theory was a polarized homogeneous incident plane wave for which field coefficients can be determined analytically in terms of the VSHs [6,7]

$$p_{h,n,m} = 4\pi i^n \mathbf{X}^*_{n,m}(\hat{\mathbf{k}}_{\text{inc}}) \cdot \hat{\mathbf{e}}_{\text{inc}},$$
$$p_{e,n,m} = 4\pi i^{n-1} \mathbf{Z}^*_{n,m}(\hat{\mathbf{k}}_{\text{inc}}) \cdot \hat{\mathbf{e}}_{\text{inc}}, \tag{14}$$

where we replaced the arbitrary incident field coefficients, a, by the symbol, p, as a reminder that the $p_{h,n,m}$ and $p_{e,n,m}$ are the VPW coefficients of an incident *plane* wave.

Using the values of the plane wave coefficients given in Eq. (14), and defining the $\hat{\mathbf{z}}$ axis to lie along incident beam direction, the analytic expressions of the $|m|=1$ plane wave coefficients are

$$p_{h,n,1} \equiv 4\pi i^n \mathbf{X}^*_{n,m}(0,0) \cdot \hat{\mathbf{e}}_{\text{inc}} = i^n \sqrt{\pi(2n+1)}(i\hat{\mathbf{x}}+\hat{\mathbf{y}}) \cdot \hat{\mathbf{e}}_{\text{inc}},$$
$$p_{e,n,1} \equiv 4\pi i^{n-1} \mathbf{Z}^*_{n,m}(0,0) \cdot \hat{\mathbf{e}}_{\text{inc}} = i^n \sqrt{\pi(2n+1)}(i\hat{\mathbf{x}}+\hat{\mathbf{y}}) \cdot \hat{\mathbf{e}}_{\text{inc}},$$
$$p_{h,n,-1} = i^n \sqrt{\pi(2n+1)}(i\hat{\mathbf{x}}-\hat{\mathbf{y}}) \cdot \hat{\mathbf{e}}_{\text{inc}},$$
$$p_{e,n,-1} = i^n \sqrt{\pi(2n+1)}(-i\hat{\mathbf{x}}+\hat{\mathbf{y}}) \cdot \hat{\mathbf{e}}_{\text{inc}}, \tag{15}$$

with $p_{h,n,m} = p_{e,n,m} = 0$, when $|m| \neq 1$. Since we fixed the axial angle to be zero in Eq. (15), we made use of the simple relation between spherical and Cartesian unit vectors in this direction, namely $\hat{\boldsymbol{\theta}} = \hat{\mathbf{x}}$ and $\hat{\boldsymbol{\phi}} = \hat{\mathbf{y}}$.

The plane wave has an axisymmetric power distribution for arbitrary polarization vectors, $\hat{\mathbf{e}}_{\text{inc}}$. Given the axial symmetry of common optical elements, the power distribution of many shaped beams will also be axisymmetric (one should remark however, that when beam polarizers are present, incident field intensities, $\|\mathbf{E}_{\text{inc}}\|^2$, are *not* fully axisymmetric). These axisymmetric beams cover a wide variety of beams, like Gaussian, Bessel and top hat beams, but exclude more exotic beams like vortex and radially polarized beams (the treatment in this work can however be extended to include these cases).

It has been shown that axisymmetric beams can be described by the *beam shape coefficients*, g_n, which can be taken to be real, and depend on the orbital quantum number n, but *not* on the axial quantum number m or on the TE (TM) nature of the coefficients [3]

$$a_{h,n,m} = g_n p_{h,n,m}, \quad a_{e,n,m} = g_n p_{e,n,m}. \tag{16}$$

2.3. Beam power normalization

Given the close analogy between the partial wave developments of Eqs. (2) and (6), one might expect the incident power, P_{inc}, to satisfy a Parseval type relation analogous to that of Eq. (8). If this were true, the incident beam power would be proportional to the sum of the incident field coefficients such that

$$P_{\text{inc}} \overset{?}{\propto} \varkappa_{\text{parsv}} \equiv \frac{1}{4} \sum_{q=h,e} \sum_{n,m} \left| a_{q,n,m} \right|^2, \tag{17}$$

where we defined the dimensionless Parseval type beam normalization factor, $\varkappa_{\text{parsv}}$. The factor 1/4 in $\varkappa_{\text{parsv}}$ was introduced so that in the paraxial limit it agrees with the exact beam normalization parameter, $\varkappa$, given below in Eq. (23). Invoking Eqs. (15) and (16), one readily obtains an expression for $\varkappa_{\text{parsv}}$ in terms of the beam shape coefficients

$$\varkappa_{\text{parsv}} = \pi \sum_{n=1}^{\infty} (2n+1) g_n^2. \tag{18}$$

We will see in Fig. 1 that $\varkappa_{\text{parsv}}$ is only approximately proportional to the power of shaped beams.

One way to see why the Parseval expression, $\varkappa_{\text{parsv}}$, is not proportional to the incident beam power is to remark that the scattered power Parseval relation of Eq. (8) relied on the orthonormality of the vector spherical harmonics for a 4π solid angular integration around a field source. Regular partial waves, on the other hand, can be viewed as fields whose sources have been sent to infinity, and they propagate into any closed surface from infinity and then proceed to propagate outside of this volume. The power integral of the incident field over any closed surface is null as is routinely invoked in scattering theory [4]. Although the incident beam power could be obtained by integrating the incident irradiance over a $z<0$ or $z>0$ hemisphere whose radius is sent to infinity, the vector spherical harmonics are no longer orthogonal under a hemispherical angular integration, which prevents the occurrence of a Parseval type expression. Another way to proceed, used here, is to obtain the incident beam power by integrating irradiance over an infinite $z=$ constant plane, which is most readily performed in the $z=0$ plane as outlined in Appendix B.

The incident magnetic field is determined from Faraday's law

$$\mathbf{H}_{\text{inc}}(\mathbf{r}) = \frac{\mathbf{B}_{\text{inc}}}{\mu_b \mu_0} = \frac{1}{i\omega\mu_b\mu_0} \nabla \times \mathbf{E}_{\text{inc}}(\mathbf{r})$$
$$= E\sqrt{\frac{\varepsilon_b \epsilon_0}{\mu_b \mu_0}} \sum_{n,m} [\mathbf{N}^{(1)}_{n,m}(k\mathbf{r}) a_{e,n,m} + \mathbf{M}^{(1)}_{n,m}(k\mathbf{r}) a_{e,n,m}], \tag{19}$$

and the convenient curl properties of the VPWs, $\nabla \times \mathbf{M} = k\mathbf{N}$ and $\nabla \times \mathbf{N} = k\mathbf{M}$. Defining the z direction to lie along the beam axis, the total incident beam power, P_{inc}, is obtained as an integral of the irradiance in any

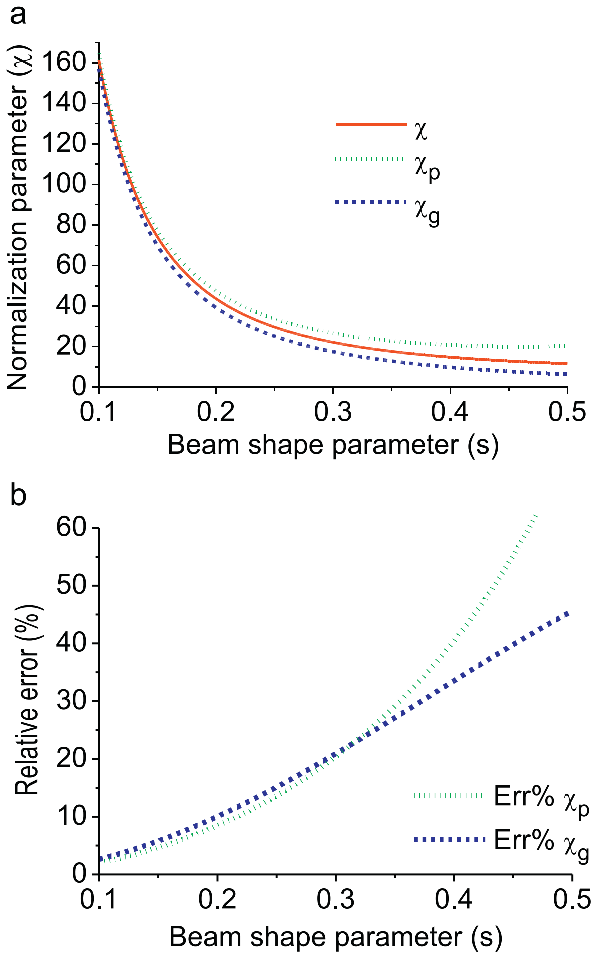

Fig. 1. (a) The red solid line represents analytic results for the beam normalization parameter, $\varkappa$, plotted as a function of the beam shape parameter, s, when the beam shape coefficients of a localized beam are given by Eq. (31). The dashed blue line represents the Gaussian approximation, $\varkappa_g = \pi/2s^2$, and the dotted Green curve is the Parseval normalization parameter, $\varkappa_p$, of Eq. (18). In (b), the relative errors with respect to $\varkappa$ are plotted for $\varkappa_g$ (dashed blue curve) and $\varkappa_p$ (dotted green curve). (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

$z=$ constant plane

$$P_{\rm inc} = \frac{2\pi}{k^2}\int_0^\infty I_{\rm inc}(\mathbf{r}) k\rho (k\,d\rho)\Big|_{z={\rm cst}}, \tag{20}$$

where ρ is the distance from the beam axis in cylindrical coordinates, and $I_{\rm inc}(\mathbf{r})$ is the incident field irradiance in the $\hat{\mathbf{z}}$ direction

$$I_{\rm inc}(\mathbf{r}) = \tfrac{1}{2}{\rm Re}\{\mathbf{E}^*_{\rm inc}(\mathbf{r}) \times \mathbf{H}_{\rm inc}(\mathbf{r})\} \cdot \hat{\mathbf{z}}. \tag{21}$$

From dimensional arguments, it is convenient to define a dimensionless beam normalization parameter, $\varkappa$, that is proportional to the incident power

$$P_{\rm inc} \equiv \varkappa \frac{E^2}{2k^2}\sqrt{\frac{\varepsilon_b \epsilon_0}{\mu_b \mu_0}}. \tag{22}$$

Combining Eq. (20) with Eq. (22), the dimensionless beam normalization parameter, $\varkappa$, is expressed as

$$\varkappa = \sqrt{\frac{\mu_b\mu_0}{\varepsilon_b\epsilon_0}}\frac{4\pi}{E^2}\int_0^\infty I_{\rm inc}(\mathbf{r}) k\rho (k\,d\rho)\Big|_{z={\rm cst}}. \tag{23}$$

Making the convenient choice of $z=0$, one obtains an analytic expression for $\varkappa$ in terms of the shape coefficients, g_n, as outlined Appendix B, yielding

$$\varkappa = \left(\pi \sum_{p,q=0}^{\infty} g_{2p+1} g_{2q+1}(4p+3)(4q+3) \frac{(2p-1)!!}{(2p+2)!!}\frac{(2q-1)!!}{(2q+2)!!}(-1)^{p-q} + \pi \sum_{p=1}^{\infty}\sum_{q=0}^{\infty} g_{2p} g_{2q+1} \frac{(2q+1)!!}{(2q)!!}\frac{(2p-1)!!}{(2p)!!}\frac{(4p+1)(4q+3)}{p(2p+1)-(2q+1)(q+1)}(-1)^{p-q+1}\right), \tag{24}$$

where even double factorials are taken to stop at 2 (ex. $6!! = 6\times 4\times 2$). The interest of Eq. (24) is that it holds for arbitrary beam profiles, but it should be remarked that this problem has previously been addressed in the context of some specific beam profiles [8,9].

This formula will be compared with approximate expressions in Fig. 1 after a brief discussion of the Gaussian (paraxial) beam approximation in the next section.

2.4. *Gaussian (paraxial) approximation*

The most common description of laser beams is to invoke the paraxial approximation of the TEM_{00} mode in which the beam irradiance has an approximately Gaussian profile. In the standard paraxial approximation, the tightness of the beam focusing can be parameterized via the dimensionless beam shape parameter, s, which is defined

$$s \equiv \frac{1}{kw_0} \equiv \frac{w_0}{2z_R} \simeq \frac{\tan\theta_d}{2}, \tag{25}$$

where w_0 is the minimal beam radius or 'waist', z_R is the Rayleigh diffraction length, and $\theta_{\rm d}$ is the angle of beam divergence. The first equality in Eq. (25) gives us a physically transparent expression of the s parameter as the wavelength divided by the beam circumference at the minimal focus or 'spot'. This s factor in most familiar laser applications is extremely small due to the low divergence of most laser beams. However, this factor is no longer minuscule for laser beams that have traveled through high NA optics, where it can be on the order of $\sim 1/4$ or more.

Defining the z-axis to lie along the beam axis, the Gaussian approximation for *irradiance* in the paraxial approximation is expressed as

$$I_{\rm gauss}(\mathbf{r}) = I_{\rm gauss}(\mathbf{0})\left(\frac{w_0}{w(z)}\right)^2 \exp\left(-\frac{2\rho^2}{w^2(z)}\right) \quad \text{with} \quad w(z) = w_0\sqrt{1+\left(\frac{z}{z_R}\right)^2}, \tag{26}$$

where $I_{\rm gauss}(\mathbf{0})$ is the irradiance at the focal point. The power integral of Eq. (20) for a Gaussian irradiance readily yields

$$P_{\text{gauss}} = \frac{\pi}{2} w_0^2 I_{\text{gauss}}(\mathbf{0}) = \frac{\pi}{2} \frac{1}{k^2 s^2} I_{\text{gauss}}(\mathbf{0}). \tag{27}$$

A direct calculation of the incident irradiance, $I_{\text{inc}}(\mathbf{0})$, at the center of the VPW coordinate system is presented in Eq. (C.4) of Appendix C and results in

$$I_{\text{inc}}(\mathbf{0}) = \frac{1}{2} E^2 g_1^2 \sqrt{\frac{\varepsilon_b \epsilon_0}{\mu_b \mu_0}}. \tag{28}$$

Finally, inserting this result into $I_{\text{gauss}}(\mathbf{0})$ of Eq. (27), gives:

$$P_{\text{gauss}} = \frac{\pi}{4} \frac{E^2}{k^2 s^2} g_1^2 \sqrt{\frac{\varepsilon_b \epsilon_0}{\mu_b \mu_0}} = \varkappa_{\text{gauss}} \frac{E^2}{2k^2} \sqrt{\frac{\varepsilon_b \epsilon_0}{\mu_b \mu_0}}, \tag{29}$$

where the second equality invokes the definition of beam normalization parameter in Eq. (22), thus fixing the beam normalization parameter, $\varkappa_{\text{gauss}}$, in the Gaussian beam approximation

$$\varkappa_{\text{gauss}} = \frac{\pi}{2s^2} g_1^2. \tag{30}$$

Consequently, as long as g_1 is non-zero, which is the case for Gaussian type beams, we are free to arbitrarily fix $g_1 = 1$, which simplifies the Gaussian approximation to the beam normalization parameter to $\varkappa_{\text{gauss}} = \pi/2s^2$.

There are, however, well established inadequacies of the paraxial beam description. Notably, the paraxial approximation is invalid for beams produced by high NA optics which results in the Gaussian irradiance profile of Eq. (26) being incompatible with the Maxwell equations. Non-paraxial beam corrections can be treated in the Davis prescription and take the form of a perturbation expansion in terms of the s^2 parameter [10]. Gouesbet, Grehan and Lock et al. have shown that in the localized approximation, one can obtain simple analytic expressions for the beam coefficients of a localized beam [1,3]. The details can be found in their references, but are not essential for our purpose here. Suffice it to say that one can find an analytic expression for the beam shape coefficients that can be pushed beyond paraxial approximation

$$g_n = \exp\{-s^2(n-1)(n+2)\}. \tag{31}$$

At this point, we have derived an exact expression for the beam normalization parameter, $\varkappa$, and two approximate formulas, $\varkappa_{\text{gauss}}$ and $\varkappa_{\text{parsv}}$. The values of $\varkappa$, $\varkappa_{\text{gauss}}$, and $\varkappa_{\text{parsv}}$ are all three plotted in Fig. 1(a). The relative errors of $\varkappa_{\text{gauss}}$, and $\varkappa_{\text{parsv}}$ with respect to the exact value of $\varkappa$ are plotted in Fig. 1(b). It is interesting to remark that the Gaussian beam approximation underestimates the value of $\varkappa$, while the Parseval relation overestimates it. All three results agree in the paraxial limit of $s \to 0$, but the relative errors are on the order of 10–20% for beam shape parameters, s, on the order of ~ 0.25 which is characteristic of the values in high NA beams. For the purposes of numerical comparison, when $s = 0.25$ one finds: $\varkappa = 29.616$, $\varkappa_{\text{gauss}} = 25.133$, and $\varkappa_{\text{parsv}} = 33.65$. It is worth remarking from Fig. 1(b), that even for beam shape parameters of $s \sim 0.1$, that the errors incurred by the approximate formulas of $\varkappa_{\text{parsv}}$ and $\varkappa_{\text{gauss}}$ are on the order of a few percent.

3. Power normalized cross section in shaped beams

For plane waves, the total incident power is infinite, and one calculates scattered power in terms of incident irradiance (dimensions of power per unit surface). This irradiance formulation is no longer practical for shaped beams, and it is consequently preferable to formulate scattered power in terms of the (finite) incident power which requires normalizing the cross sections with the beam normalization parameter derived in Eq. (24). One way to do this is to invoke some of the translation–addition theorem tools that are familiar from multiple scattering theory [4,5].

In scattering theory, the transition matrix (or simply T-matrix) of a scatterer characterizes the electromagnetic response subject to all possible incident fields. In the VPW basis, the T-matrix is formulated in a coordinate system chosen to favor the particle's position and symmetry [11]. For the beam description in Section 2 on the other hand, we adopted a coordinate system adapted to the beam geometry (z-axis lying along the beam axis, and the origin of the coordinate system preferentially positioned at the beam focal point).

The translation–addition theorem for VPWs allows one to express the incident field at the particle position, $a_{q,n,m}(\mathbf{r})$, in terms of the incident field coefficients of the beam coordinate system, $a_{q',\nu,\mu}(\mathbf{0})$, via the regular translation–addition matrix, $J(k\mathbf{r})$ [4,5,12–14]

$$a_{q,n,m}(\mathbf{r}) = \sum_{q'=(h,e)} \sum_{\nu,\mu} [J(k\mathbf{r})]_{q,n,m;q',\nu,\mu} a_{q',\nu,\mu}(\mathbf{0}). \tag{32}$$

The scattering coefficients, $f_{q,n,m}(\mathbf{r})$ for a particle located at the position $\mathbf{r}$ can then be obtained from the incident field coefficients at this point, $a_{q,n,m}(\mathbf{r})$, by using the T-matrix, T, of the particle [5,11,4]

$$f_{q,n,m}(\mathbf{r}) = \sum_{q'=(h,e)} \sum_{\nu,\mu} T_{q,n,m;q',\nu,\mu} a_{q',\nu,\mu}(\mathbf{r}). \tag{33}$$

The scattered power, P_{scat}, can now be related to the incident beam power, P_{inc}, via a power normalized cross section, $\tilde{\sigma}_{\text{scat}}$ i.e.

$$P_{\text{scat}}(\mathbf{r}) \equiv k^2 \tilde{\sigma}_{\text{scat}}(\mathbf{r}) P_{\text{inc}}, \tag{34}$$

where the position dependent scattering cross section $\tilde{\sigma}_{\text{scat}}(\mathbf{r})$ is given by

$$\tilde{\sigma}_{\text{scat}}(\mathbf{r}) = \frac{1}{k^2 \varkappa} \sum_{q=(h,e)} \sum_{n,m} \left| f_{q,n,m}(\mathbf{r}) \right|^2. \tag{35}$$

It should be remarked that when defined in this way, the $\tilde{\sigma}_{\text{scat}}$ are independent of the overall normalization of the beam shape coefficients and that they only differ from the ordinary cross sections of Eq. (12) by the presence of the beam normalization parameter, $\varkappa$ in the denominator. Another interesting observation is that $k^2 \tilde{\sigma}_{\text{scat}}$ can be regarded as a scattering *efficiency* in the sense that it is constrained by energy conservation to always be less than or equal to 1.

A power normalized extinction cross section can also be derived in analogy with plane-wave cross sections

$$\tilde{\sigma}_{\rm ext}(\mathbf{r}) = \frac{1}{k^2\varkappa}\sum_{q=(h,e)}\sum_{n,m}{\rm Re}[a^*_{q,n,m}(\mathbf{r})f_{q,n,m}\mathbf{r})]. \quad (36)$$

It is important to remark that the extinction cross section defined in Eq. (36) is the correct expression for shaped beams in that it avoids an erroneous application of the optical theorem (see Refs. [15–17] for detailed discussions on this topic).

Finally, one defines a power normalized absorption cross section in the usual manner

$$\tilde{\sigma}_{\rm abs}(\mathbf{r}) = \tilde{\sigma}_{\rm ext}(\mathbf{r}) - \tilde{\sigma}_{\rm scat}(\mathbf{r}). \quad (37)$$

4. Conclusions

The beam normalization parameter derived in this work allows cross sections in shaped beams to be formulated in a fully analytic manner in terms of the particle's T matrix; something which was previously possible only for incident plane waves. We demonstrated that if one does not calculate this parameter exactly, but instead adopts a Parseval type expression or a Gaussian approximation then the errors can be of the order of 10–20%. Such errors are consequential given the precision one usually strives for in the calculation of the particle's T-matrix.

Although the translation–addition matrix formulation of Section 3 is a relatively simple and flexible means of solving the problem of the particle's position in a shaped beam, it is not the only way to solve this problem. The beam normalization parameter on the other hand does seem to be an essential element of treating the problem of beams formed with high NA optics (in the context of a partial wave framework at least). Optical tweezers and confocal microscopy are two important applications where this formulation should prove useful.

Appendix A. Vector spherical harmonics

There is no universally accepted notation for the vector spherical harmonics (VSH). Our notation for their *normalized* forms (cf. Eq. (4)) is $\mathbf{X}_{n,m}$, $\mathbf{Y}_{n,m}$, and $\mathbf{Z}_{n,m}$

$$\mathbf{X}_{n,m}(\theta,\phi) \equiv \mathbf{Z}_{n,m}(\theta,\phi)\times\hat{\mathbf{r}},$$
$$\mathbf{Y}_{n,m}(\theta,\phi) \equiv \hat{\mathbf{r}}Y_{n,m}(\theta,\phi),$$
$$\mathbf{Z}_{n,m}(\theta,\phi) \equiv \frac{r\nabla Y_{n,m}(\theta,\phi)}{\sqrt{n(n+1)}} = \hat{\mathbf{r}}\times\mathbf{X}_{n,m}(\theta,\phi), \quad (A.1)$$

where $Y_{n,m}(\theta,\phi)$ are the scalar spherical harmonics and the normalization coefficients, $\gamma_{n,m}$, are defined

$$\gamma_{n,m} \equiv \sqrt{\frac{(2n+1)(n-m)!}{4\pi n(n+1)(n+m)!}}. \quad (A.2)$$

It is also convenient to introduce the normalized functions $\overline{u}_n^m$ and $\overline{s}_n^m$ defined in terms of the associated Legendre functions P_n^m

$$\overline{u}_n^m(\cos\theta) \equiv \frac{1}{\sqrt{n(n+1)}}\gamma_{n,m}\frac{m}{\sin\theta}P_n^m(\cos\theta), \quad (A.3)$$

$$\overline{s}_n^m(\cos\theta) \equiv \frac{1}{\sqrt{n(n+1)}}\gamma_{n,m}\frac{d}{d\theta}P_n^m(\cos\theta), \quad (A.4)$$

which allow us to conveniently express the transverse VSHs as

$$\mathbf{X}_{n,m}(\theta,\phi) = [i\overline{u}_n^m(\cos\theta)\hat{\theta} - \overline{s}_n^m(\cos\theta)\hat{\boldsymbol{\phi}}]\exp(im\phi),$$
$$\mathbf{Z}_{n,m}(\theta,\phi) = [\overline{s}_n^m(\cos\theta)\hat{\boldsymbol{\theta}} + i\overline{u}_n^m(\cos\theta)\hat{\boldsymbol{\phi}}]\exp(im\phi). \quad (A.5)$$

Appendix B. Shaped beam power

The power of an incident beam is calculated by integrating the normal component of the time averaged incident Poynting vector, $\mathbf{S}_{\rm inc}$, over any infinite open surface that the beam passes through. Since we are working with spherical coordinates, it is convenient to perform our analytic integrations in the $z=0$ plane. Using the field VSWF field developments of Eqs. (6) and (9), the irradiance for time harmonic fields is explicitly

$$\begin{aligned} I_{\rm inc}(\mathbf{r}) &= \frac{1}{2}{\rm Re}\{\mathbf{E}^*_{\rm inc}\times\mathbf{H}_{\rm inc}\}\cdot\hat{\mathbf{z}} \\ &= -\frac{1}{2}\sqrt{\frac{\varepsilon_b\epsilon_0}{\mu_b\mu_0}}E^2\sum_{n,m;\nu\mu}{\rm Re}\{-i[a^*_{h,n,m}\mathbf{M}^{(1),*}_{n,m}(k\mathbf{r}) \\ &\quad + a^*_{e,n,m}\mathbf{N}^{(1),*}_{n,m}(k\mathbf{r})]\times[a_{h,\nu\mu}\mathbf{N}^{(1)}_{\nu,\mu}(k\mathbf{r}) + a_{e,\nu,\mu}\mathbf{M}^{(1)}_{\nu,\mu}(k\mathbf{r})]\cdot\hat{\mathbf{z}}\}. \end{aligned} \quad (B.1)$$

The irradiance integral in the $z=0$ plane then corresponds to taking $\theta=\pi/2$, and integrating over $\phi=[0,2\pi]$ and $r=[0,\infty]$.

An inspection of Eq. (B.1) shows that an analytic calculation of the beam power, Eq. (20), will involve four integrals involving vector products of the VSWFs. The contribution to the total beam power involving the coefficient product $a^*_{h,n,m}a_{e,\nu\mu}$ (denoted $\delta P^{(h,e)}$) is zero since $\mathbf{M}^{(1),*}_{nm}\times\mathbf{M}^{(1)}_{\nu\mu}\cdot\hat{\mathbf{z}}=0$ in the $z=0$ plane. The vector product involving $a^*_{e,n,m}a_{h,\nu,\mu}$ (denoted $\delta P^{(e,h)}$) does however have a non-zero contribution to the power integral of Eq. (20), namely

$$\begin{aligned} \delta P^{(e,h)} &= \int_0^\infty r\,dr\int_0^{2\pi}d\phi\,{\rm Re}\{-i[a^*_{e,n,m}a_{h,\nu,\mu}\mathbf{N}^{(1),*}_{n,m}(k\mathbf{r})\times\mathbf{N}^{(1)}_{\nu,\mu}(k\mathbf{r})]\}\cdot\hat{\mathbf{z}}\Big|_{\theta=\pi/2} \\ &= -E^2\frac{\pi}{k^2}\sqrt{\frac{\varepsilon_b\epsilon_0}{\mu_b\mu_0}}\sum_{n,\nu,m=\pm1}{\rm Re}[a^*_{e,n,m}a_{h,\nu,m}]\frac{\overline{u}_n^m(0)\overline{u}_\nu^m(0)}{m} \\ &\quad\times\left\{n(n+1)\int_0^\infty\frac{j_n(x)}{x}[xj_\nu(x)]'\,dx + \nu(\nu+1)\int_0^\infty[xj_n(x)]'\frac{j_\nu(x)}{x}\,dx\right\}, \end{aligned} \quad (B.2)$$

where the $\overline{u}_n^m(\cos\theta)$ are defined in Eq. (A.5). One finds that $\overline{u}_n^m(0)\overline{u}_\nu^m(0)$ with $|m|=1$ is non-zero only if both n and ν are odd. The analytic expression for $\overline{u}_n^m(0)\overline{u}_\nu^m(0)$ with both n and ν odd is

$$\overline{u}_n^m(0)\overline{u}_\nu^m(0) = \frac{(-1)^{(n-\nu)/2}}{4\pi}\sqrt{(2n+1)(2\nu+1)}\;\frac{(n-2)!!}{(n+1)!!}\frac{(\nu-2)!!}{(\nu+1)!!}. \quad (B.3)$$

The Bessel function integral gives a particularly simple result

$$n(n+1)\int_0^\infty\frac{j_n(x)}{x}[xj_\nu(x)]'\,dx + \nu(\nu+1)\int_0^\infty[xj_n(x)]'\frac{j_\nu(x)}{x}\,dx = (-1)^{(n-\nu)/2}, \quad (B.4)$$

to yield finally

$$\delta P^{(e,h)} = -\frac{I_{\text{inc}}(\mathbf{0})}{2k^2}\sum_{p,q=0}^{\infty}\sum_{m=\pm 1}\frac{\text{Re}[a^*_{e,2p+1,m}a_{h,2q+1,m}]}{m} \times\sqrt{(4p+3)(2q+3)}\frac{(2p-1)!!}{(2p+2)!!} \times\frac{(2q-1)!!}{(2q+2)!!}. \tag{B.5}$$

Finally, using the defining property of the beam shape coefficients, g_n, of Eq. (16), and the expressions for the $p_{e,n,m}$ and $p_{h,n,m}$ of Eq. (15), we can write this sum directly in terms of the g_n.

$$\delta P^{(e,h)} = I_{\text{inc}}(\mathbf{0})\frac{\pi}{k^2}\sum_{p,q=0}^{\infty} g_{2p+1}g_{2q+1}(4p+3)(4q+3) \frac{(2p-1)!!}{(2p+2)!!}\frac{(2q-1)!!}{(2q+2)!!}(-1)^{p-q}. \tag{B.6}$$

Evaluating the remaining $\delta P^{(h,h)}$ and $\delta P^{(e,e)}$ contributions to the total beam power in a similar manner, and appealing to the defining relation, Eq. (16) for the beam normalization parameter, $\varkappa$, yields the analytic expression for $\varkappa$ found in Eq. (24).

Appendix C. Incident irradiance at the beam focus

The irradiance at the beam focus (fixed as the coordinate system origin) can be calculated by remarking that as $\mathbf{r}\to\mathbf{0}$, only the $\mathbf{N}^{(1)}_{1,m}(k\mathbf{r})$ VSWFs are non-zero, and that

$$\begin{aligned}\mathbf{N}^{(1),*}_{1,m}(k\mathbf{r}) \times \mathbf{N}^{(1)}_{1,\mu}(k\mathbf{r})\cdot\hat{\mathbf{z}} &= \frac{\sqrt{2}j_1(kr)[krj_1(kr)]' Y^*_{1,m}(\hat{\mathbf{r}})\mathbf{X}_{1,\mu}(\hat{\mathbf{r}})}{k^2r^2}\cdot\hat{\mathbf{z}} \\ &\quad - \frac{\sqrt{2}[krj_1(kr)]' j_1(kr)Y_{1,\mu}(\hat{\mathbf{r}})\mathbf{X}^*_{1,m}(\hat{\mathbf{r}})}{k^2r^2}\cdot\hat{\mathbf{z}} \\ &\quad - \frac{[(krj_v(kr))']^2\mathbf{Z}^*_{n,m}(\theta,\phi)\cdot\mathbf{X}_{v,\mu}(\theta,\phi)\hat{\mathbf{r}}}{k^2r^2}\cdot\hat{\mathbf{z}}.\end{aligned} \tag{C.1}$$

Using the limits

$$\lim_{x\to 0} j_1(x) \approx \frac{x}{3} \quad \lim_{x\to 0}[xj_1(x)]' \approx \frac{2x}{3}, \tag{C.2}$$

we obtain

$$\begin{aligned}\frac{1}{2\pi}\int_0^{2\pi} d\phi \sum_{m,\mu=-1}^{1} a^*_{e,1,m}a_{h,1,\mu}\mathbf{N}^{(1),*}_{1,m}(\mathbf{0})\times\mathbf{N}^{(1)}_{1,\mu}(\mathbf{0})\cdot\hat{\mathbf{z}}\Big|_{\theta=\pi/2} &= -i\frac{8}{9}\sum_{m=\pm 1} m\, a^*_{e,1,m}a_{h,1,m}\overline{u}^m_1(0)\overline{u}^m_1(0) \\ &= \frac{i}{6\pi}\{a^*_{e,1,-1}a_{h,1,-1}-a^*_{e,1,1}a_{h,1,1}\},\end{aligned} \tag{C.3}$$

where we used $\overline{u}^m_1(0) = -\frac{1}{4}\sqrt{3/\pi}$. Putting this result into Eq. (B.1), the irradiance at the origin takes the form

$$\begin{aligned}I_{\text{inc}}(\mathbf{0}) &= \frac{1}{2}\sqrt{\frac{\varepsilon_b\epsilon_0}{\mu_b\mu_0}}E^2\frac{1}{6\pi}\text{Re}\{a^*_{e,1,-1}a_{h,1,-1}-a^*_{e,1,1}a_{h,1,1}\} \\ &= \frac{1}{2}E^2g_1^2\sqrt{\frac{\varepsilon_b\epsilon_0}{\mu_b\mu_0}},\end{aligned} \tag{C.4}$$

where in the last line, we used Eqs. (16) and (15) to put this result in terms of the beam shape coefficients.

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