Expansion of Arbitrary Electromagnetic Fields in Terms of Vector Spherical Wave Functions

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Since 1908, when Mie reported analytical expressions for the fields scattered by a spherical particle upon incidence of an electromagnetic plane-wave, generalizing his analysis to the case of an arbitrary incident wave has proved elusive. This is due to the presence of certain radially-dependent terms in the equation for the beam-shape coefficients of the expansion of the electromagnetic fields in terms of vector spherical wave functions. Here we show for the first time how these terms can be canceled out, allowing analytical expressions for the beam shape coefficients to be found for a completely arbitrary incident field. We give several examples of how this new method, which is well suited to numerical calculation, can be used. Analytical expressions are found for Bessel beams and the modes of rectangular and cylindrical metallic waveguides. The results are highly relevant for speeding up calculation of the radiation forces acting on spherical particles placed in an arbitrary electromagnetic field, such as in optical tweezers.

Gustav Mie, in his celebrated 1908 paper [1], used the vector spherical wave function (VSWF), or partial wave expansion (PWE), of a linear polarized plane-wave to generalize scattering theories to spherical particles of any size, from geometrical optics to the Rayleigh regime, and thus was able to clarify many phenomena, for example in atmospheric physics. He obtained analytical expressions for the expansion coefficients based on special mathematical identities related to a plane-wave. This beam expansion was necessary for applying boundary conditions at a spherical interface. Since then, with the arrival of lasers and optical waveguides, the diversity and complexity of possible incident fields has become enormous so that the restriction to an incident plane-wave has become unrealistic.

Different experiments, ranging from particle levitation and trapping [2, 3], to the ultrahigh-Q microcavities used in cavity QED experiments [4, 5], use different beams. For example, very high numerical aperture beams are used in optical tweezers and confocal microscopy [6, 7], evanescent fields in near-field microscopy [8, 9], and the waveguide modes of a fiber taper are employed to couple light to the whispering gallery modes of spherical microcavities [10]. Optical forces, absorption, Raman scattering and fluorescence can be greatly enhanced inside spherical microcavities at Mie resonances [11–13]. Laguerre-Gaussian, Hermite-Gaussian and Bessel beams [14, 15], and the internal electromagnetic field of hollow core photonic crystal fibers [16, 17], are used to trap and transport particles. The understanding of all these phenomena requires a precise knowledge of the VSWF coefficients of the incident beams. A generalized Lorenz-Mie theory was developed to handle the many variants of beams beyond classical plane-waves, and the expansion coefficients in these cases are known as beam shape coefficients (BSC) [20, 21].

over, because the VSWFs form an orthogonal complete basis, they can be used to study scattering and forces [22] on non-spherical particles, and are the starting point of the powerful T-matrix methods [23].

The calculation of BSCs for an arbitrary beam has always been a complicated task, requiring significant effort. Furthermore, there is a fundamental problem with these calculations: an expansion of any function in some basis is complete only when the expansion coefficients can be written in terms of scalar products, or integrals, with defined numerical values. This task has actually never been accomplished for the VSWFs of an arbitrary beam because the integral over the solid angle does not explicitly eliminate the radial dependence, at least up until now. So far as we are aware, the current literature lacks any mathematical proof that this radial function, which appears after integration over all solid angles for any type of beam that satisfies Maxwell’s equations, can exactly cancel out the spherical Bessel function that appears on the other side of the BSC equation. If this is not true, then the BSC could not be a constant independent of the radial coordinate – as required for a successful expansion.

This non-radial dependence of the BSC has been proven only for the case of plane-waves and for a high numerical aperture focused Gaussian beam [24]. Working with an electromagnetic mode inside a hollow cylindrical waveguide, we also have been able to obtain analytical expressions for constant BSCs that depend only on the position of the reference frame. This raises the fundamental question, whether it would be possible to prove that the spherical Bessel function would naturally emerge from the solid angle integral for any type of electromagnetic field. The purpose of this letter is to show, we believe for the first time, that this is indeed possible. The implications of this
result for computational light scattering is very noteworthy. We show how the new method can be used to calculate the BSCs for plane-waves, cylindrical and rectangular waveguide modes and Bessel beams.

The dimensionless BSCs $G_{pq}^{TE/TM}$ for an incident field $E = E(r), H = H(r)$ are defined in the equations [25, 26]

$$
\begin{bmatrix}
E \\
ZH
\end{bmatrix} = E_0 \sum_{p,q} \begin{bmatrix} G_{pq}^{TE} \\
G_{pq}^{TM}
\end{bmatrix} M_{pq} + \begin{bmatrix} -G_{pq}^{TM} \\
G_{pq}^{TE}
\end{bmatrix} N_{pq},
$$

where $E_0$ is an electric field dimension constant, $kN_{pq} = \hat{r} \times M_{pq}, M_{pq} = J_p(kr)X_{pq}(\hat{r}), J_p(kr)$ are spherical Bessel functions, $X(\hat{r}) = LY_{pq}(\hat{r})/\sqrt{p(p+1)}$ are the spherical harmonics, $Z = \sqrt{\mu/\varepsilon}, k = \omega \sqrt{\mu/\varepsilon}$ and $L = -ir \times \nabla$. Throughout this paper we use the terms inside $[]$ are parts of separate equations, i.e., (1) contains two equations, the first relating $E$ to $G^{TE}$ and $G^{TM}$ and the second, $ZH$ to $G^{pq}$. The usual procedure for obtaining the BSC’s involves multiply both sides of (1) by $X_{p'q'},$ take scalar products with the fields and integrate over the solid angle $\Omega$. Due to the orthogonality properties of the vector spherical harmonics [25, 26], one can easily show that

$$E_0 j_p(kr) \begin{bmatrix} G_{pq}^{TE} \\
G_{pq}^{TM}
\end{bmatrix} = \int d\Omega X_{p'q'}(\hat{r}) \cdot \begin{bmatrix} E(r) \\
ZH(r)
\end{bmatrix},$$

where $\Omega$ is the solid angle with respect to an arbitrary origin not related to any particular point of the incident beam. Equation (2) does not yield explicit expressions for the BSCs because the LHS still contains the radially-dependent spherical Bessel function. Our goal is to extract this function from the RHS and cancel it out with the one on the LHS, for any general incident electromagnetic field. To accomplish this we use the Fourier transform $F$ of the fields

$$\begin{bmatrix} E(r) \\
H(r)
\end{bmatrix} = \frac{1}{(2\pi)^{3/2}} \int d^3k' \begin{bmatrix} \mathcal{E}(k') \\
\mathcal{H}(k')
\end{bmatrix} e^{ik' \cdot r}.$$  

By this definition, one can show that $F(L\psi(r)) = L[F(\psi)]$ and that the angular momentum operator in reciprocal $k$-space $\hat{L}$ has the same form as in real $r$-space (is Hermitian) and is given by $\hat{L} = -i\hat{r} \times \nabla_k$ where $\nabla_k = (\partial_{k_x}, \partial_{k_y}, \partial_{k_z})$. Using this property and the expansion $e^{ik' \cdot r} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{lm}(\hat{r}) Y_{lm}^*(\hat{k'})$ and making $\mathcal{M}_{pq}(k) = j_p(kr)X_{pq}(\hat{r}), X_{pq}(\hat{k}) = LY_{pq}(\hat{k})/\sqrt{p(p+1)},$ we obtain

$$j_p(kr) \begin{bmatrix} G_{pq}^{TE} \\
G_{pq}^{TM}
\end{bmatrix} = \frac{i\pi}{E_0} \sqrt{\frac{2}{\pi}} \int d^3k' \mathcal{M}_{pq}^* \cdot \begin{bmatrix} \mathcal{E} \\
Z \mathcal{H}
\end{bmatrix}.$$  

Now, only Fourier transforms of the form $k^2 F(k') = \delta(k' - k)\mathcal{F}_k(\hat{k'})$ will represent a field $F(r)$ that satisfies the wave equation $\nabla^2 F + k^2 F = 0$ in three dimensions. So we define the $\hat{k}$-only dependent fields

$$\begin{bmatrix} \mathcal{E}(k') \\
\mathcal{H}(k')
\end{bmatrix} = \delta(k' - k) \begin{bmatrix} \mathcal{E}_k(\hat{k'}) \\
\mathcal{H}_k(\hat{k'})
\end{bmatrix}.$$  

Imposing this restriction one finally obtains that

$$\begin{bmatrix} G_{pq}^{TE} \\
G_{pq}^{TM}
\end{bmatrix} = \frac{i\pi}{E_0} \sqrt{\frac{2}{\pi}} \int d\Omega_{k'} X_{pq}^*(\hat{k'}) \begin{bmatrix} \mathcal{E}_k(\hat{k'}) \\
Z H_k(\hat{k'})
\end{bmatrix}.$$  

To calculate the coefficients placed at arbitrary position $r_0$ independent of the coordinate system of the fields one can use the translation property of Fourier transforms [26]. Since this form is free of any radially-dependent function, our goal has been achieved.

To calculate these Fourier transforms numerically it could be convenient to use Laplace series [26], also known as spherical harmonic transforms [27]. Using the Laplace series expansion $[\mathcal{E}(\hat{k}'), Z H(\hat{k}')] = \sum_{p',q'} \langle e_{p',q'} | e_{p,q} | L(p,q) \rangle,$ one obtains

$$\begin{bmatrix} G_{pq}^{TE} \\
G_{pq}^{TM}
\end{bmatrix} = \frac{i\pi}{E_0} \sqrt{\frac{2}{\pi}} \sum_{p',q'} \langle e_{p',q'} | e_{p,q} \rangle \cdot \frac{\langle p',q' | L(p,q) \rangle}{\sqrt{p(p+1)}}.$$  

The $e_{p,m',n',p,m}$' coefficients can be calculated by several algorithms freely available in internet and the matrix $\langle p',q' | L(p,q) \rangle$ is shown in most quantum mechanics books.

**Plane wave:** The fields of a linearly polarized plane wave are given by $[E(r), Z H(r)] = E_0 [\hat{\varepsilon} \cdot \hat{k} \times \hat{\varepsilon}] e^{ikr},$ where $\hat{\varepsilon}$ is the unit polarization vector, therefore the angular Fourier transform is easily calculated, one obtains from equation (6) that

$$\begin{bmatrix} G_{pq}^{TE} \\
G_{pq}^{TM}
\end{bmatrix} = \frac{i\pi}{E_0} \sqrt{\frac{2}{\pi}} \sum_{p',q'} \langle e_{p',q'} | e_{p,q} \rangle \cdot \frac{\langle p',q' | L(p,q) \rangle}{\sqrt{p(p+1)}}.$$  

For the special case $\hat{k} = \hat{z}$ and for a circularly polarized wave with $\hat{\varepsilon} = \hat{\kappa} \pm i\hat{\gamma}$ we have

$$\begin{bmatrix} G_{pq}^{TE} \\
G_{pq}^{TM}
\end{bmatrix} = \frac{i\pi}{E_0} \sqrt{\frac{2}{\pi}} \sum_{p',q'} \langle e_{p',q'} | e_{p,q} \rangle \cdot \frac{\langle p',q' | L(p,q) \rangle}{\sqrt{p(p+1)}}.$$  

where $\delta_{n,m}$ is the Kronecker delta function. This is the result shown in Jackson’s book [25].

**General hollow waveguide mode:** The TM and TE modes of a hollow, cylindrical waveguide of arbitrary cross-sectional shape are given as function of $g(r) = g_p(\rho) e^{ik_z z},$ where $g_p(\rho)$ is the scalar solution of the transverse wave equation $(\partial_x^2 + \partial_y^2 + \gamma^2)g(\rho) = 0$ satisfying the boundary conditions at the waveguide surfaces [25].

$$\begin{bmatrix} E^{TM} \\
Z H^{TE}
\end{bmatrix} = \frac{k_z}{k} \hat{z} \times \begin{bmatrix} -Z H^{TM} \\
E^{TE}
\end{bmatrix}.$$  

$$E_0 \left[ \hat{z} \pm i \frac{k_z}{\gamma} \nabla \right] g(r),$$
where $k_z$ is the wavevector in the $z$ direction, $k^2 = k_z^2 + \gamma^2$, $\gamma$ is the transverse wavevector.

It should be useful to introduce the cylindrical coordinate system in the r-space and k-space. In the r-space we have $\rho = x\hat{x} + y\hat{y}$, $\rho^2 = \rho \cdot \rho$ and $\rho = \rho / \rho$. We have also $\phi = -y\hat{x} + x\hat{y}$ and $\hat{\phi} = \phi / \rho$. In the same way, in k-space we change $\rho \rightarrow \gamma$ and $\phi \rightarrow \phi_k$, obtaining an equivalent system of coordinates. So, the Fourier transforms of fields (10) and (11) are given by

$$\mathcal{E}_T = E_0 G(k') \left( \hat{z} - \frac{k_z}{\gamma} \right)$$

(12)

$$\mathcal{E}_M = E_0 \frac{k'}{2\pi} K^p_p \left( k_p' / k \right) G^p \gamma$$

(14)

$$G^p = \int dp' G_{r}(p') e^{-ipq}$$

(17)

**Rectangular hollow metallic waveguide mode:** In this case there are two scalar functions $g_m$ given by $g_T = \cos(k_m' x) \cos(k_n' y)$ and $g_M = \sin(k_m' x) \sin(k_n' y)$, where $k_m' = m\pi / a$ and $k_n' = m\pi / b$, $\phi_{m,n} = \arctan(k_m'/k_n')$, and $\gamma_{m,n} = \pi \sqrt{m^2/a^2 + n^2/b^2}$. The integral over $\phi_k$ given by $G^p_{r}$ in (17) -- where the plus sign is for the TE-waveguide mode and the minus sign is for the TM-waveguide mode -- is

$$G^p_{r} = \frac{(-1)^q \cos(q\phi_{m,n} - k_m' x_0 + k_n' y_0)}{\pi}$$

(18)

The BSCs can now be found substituting (18) in (14) and (15).

**Cylindrical hollow metallic waveguide mode:** The scalar solution for the electromagnetic fields in terms of cylindrical coordinates with the origin on axis for the metallic waveguide are given by $g_T(\rho) = J_m(\gamma_{m,n} \rho) e^{\pm i \phi_k}$, where $J_m(\gamma_{m,n})$ are order $m$ Bessel functions, $J_m'(x)$ is the derivative of $J_m(x)$, $\gamma_{m,n} = \chi_{m,n} / R$ or $\gamma_{m,n} = \chi_{m,n} / R$, with $R$ being the radius of the cylinder, $\chi_{m,n}$ the $n$-th root of $J_m'(x)$ for the TM mode and $\chi_{m,n}$ being the $n$-th root of $J_m'(x)$ for the TE mode [25].

From now on we define the functions

$$\psi_m(k; r) = J_m(\gamma_{m,n} \rho) e^{\pm i \phi_k}$$

(19)

$$\Psi_m(k; r) = \sqrt{2} e^{\pm i \phi_k}$$

(20)

and remember the addition theorem [28] to express the scalar function in terms of a new coordinate system $r = r' + r_0$, written as a convolution

$$\psi_m(k; r) = \sum_{j = -\infty}^{\infty} \psi_{m-j}(k; r_0)$$

(21)

The Fourier transform of $\psi_m(k; r)$ can be written as

$$G_{r}(p') = \sqrt{2\pi} \sum_{j = -\infty}^{\infty} \psi_{m-j}(k; r_0)$$

(22)

$$G_{r} = (2\pi)^{3/2} \psi_m e^{i\phi_k}$$

(23)

The BSC's can now be found substituting (23) in (14) and (15). The on-axis case can be obtained by setting $\rho_0 = 0$, which implies that $J_{m+n}(\gamma_{m,n} \rho_0) = \delta_{m,n,q}$, and therefore

$$G_{r} = (2\pi)^{3/2} (-i)^{m} e^{i\phi_k}$$

(24)

As we can see the sum over $q$ in (11) will disappear.

**Bessel Beams:** We have calculated BSCs for two kind Bessel beams electromagnetic fields that obey Maxwell equations [29]. They are derived using vector potential and Lorenz gauge [30] and are given as function of $\psi$ already defined in (19) and (21).

$$E_I = E_0 \left( \psi_m \hat{z} + \frac{1}{k} \nabla \cdot \psi_m \hat{z} \right) - \frac{1}{k} \nabla \times \psi_m \hat{z}$$

(25)

$$E_{II} = E_0 \left( \psi_m \hat{e}_\pm + \frac{1}{k} \nabla \cdot \psi_{m-1} \hat{e}_\pm \right) - \frac{1}{k} \nabla \times \psi_{m-1} \hat{e}_\pm$$

(26)

The Fourier transform of these fields are given by

$$E_I = E_{0} \Psi_m \left[ -\hat{z} - k' \cdot \hat{z} \right]$$

(27)

$$E_{II} = E_{0} \Psi_m \left[ -\hat{e}_\pm - k' \cdot \hat{e}_\pm \right]$$

(28)

The $k'$ component is obviously null by orthogonality with angular momentum. Using again the addition theorem [21].
and making $c_{p,q}^m = \sqrt{p(p+1) - q(q+1)}$ one can show that the coefficients are given by (29) and (30).

In conclusion, we have shown that radially-independent amplitudes (the BSCs) of a complete set of vector spherical wave functions can be calculated explicitly for an arbitrary electromagnetic field. We have shown how this result can be used to determine the BSCs for several beam-types commonly employed in photonics, although of course the method is not restricted to applications within the field of optics. This new-found ability to evaluate the BSCs of the VSWFs analytically makes it much easier to explore rapidly the influence of experimental parameters in practical field scattering and optical tweezer systems. With this analytical breakthrough, the long-standing problem of evaluating the BSCs for an arbitrary field has been solved and the non-radial dependence of the BSCs proven, allowing one to avoid unnecessary approximations in the numerical evaluation of these quantities.

\[
\begin{align*}
\begin{bmatrix}
G_{pq}^{TE} & G_{pq}^{TM} \\
G_{pq}^{TM} & \pm i \frac{k}{\gamma} G_{pq}^{TE}
\end{bmatrix}
\end{bmatrix}_{II} =
\begin{bmatrix}
\gamma^2 q^2 K_{pq}^m P_{pq} \\
\frac{1}{2} \gamma^2 q^2 K_{pq}^m P_{pq} \\
\end{bmatrix}
\end{align*}
\]

(29)

(30)

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