A T-matrix method based on a plane-wave spectrum

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A computational scheme is proposed to generate a T matrix for an arbitrarily-shaped homogeneous particle. The method models the internal field within the particle as a directional spectrum of plane waves. A system of equations for the plane-wave coefficients is obtained by application of the model to a discrete-dipole representation of the particle.

INTRODUCTION

The work presented here represents a revisiting and re-examination of the discrete-dipole moment method (DDMM) for the calculation of the T matrix of arbitrarily-shaped particles[1]. This method retained the DD representation of the particle as a lattice of dipole elements, yet the distribution of dipole moment within the particle was modeled via an expansion of spherical wave harmonics. In general, the moment method was considerably faster than the corresponding direct DDA-to-T matrix route (DDA for discrete-dipole approximation), the latter of which involves solution of the DDA equations for each order/degree/mode component of a generalized, vector harmonic incident wave expansion. However, the DDMM method, as originally formulated, is difficult to translate into a working code; even though it relies on the DD model of the particle, the method would involve a major modification of the standard DDA codes to implement.

A simpler yet somewhat equivalent approach is outlined here. As opposed to the spherical wave harmonic basis, the dipole distribution within the particle is modeled by a discrete set of plane wave components, with each component corresponding to a specific propagation direction and polarization state. This approach is based on the idea that a regular solution to the Maxwell equations -- which will correspond to the field existing within the modeled particle interior -- can be expressed as an integral over vector plane waves [2]. A plane wave spectrum has been used to represent a Gaussian beam [3], yet the author is not aware of the use of plane wave methods to describe the internal field in the particle scattering problem.

FORMULATION

The analysis begins with the standard discrete-dipole representation of a homogeneous particle. The particle, of refractive index m, is represented as a cubic lattice of N_d dipole elements, with grid spacing $2a$. The scattered field from the entire particle is given by the superposition of fields scattered from each element:

$$\mathbf{E}_{sca,i}(\mathbf{r}) = \sum_{i=1}^{N_d} \sum_{m=-1}^{1} a_m^i \, \mathbf{N}_{m11}^{(3)}(\mathbf{r} - \mathbf{r}_i), \tag{1}$$

in which $\mathbf{N}_{m11}^{(3)}$ is the vector wave harmonic (VWH) of degree m, order 1, and TM mode, and a_m^i denote the sought dipole elements for lattice site i. The interaction equations for

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the dipole elements appear as

$$\frac{1}{\overline{a}}\, a_m^i - \sum_{\substack{j=1\\ j\neq i}}^{N_d} \sum_{k=-1}^{1} H_{mk}^{i-j}\, a_k^j = p_{m,\gamma_0}(\mathbf{k}_0)\, f^i(\mathbf{k}_0), \tag{2}$$

in which $\overline{a}$ denotes the dipole polarizability, which is a function of the refractive index m and the dimensionless lattice size $\mathrm{k}\, a = 2\pi a/\lambda$, H^{i-j} is a translation matrix from site j to i, $\mathbf{k}_0$ is a unit vector denoting the direction of the incident plane wave and described by the azimuth and polar angles (α_0, β_0) relative to a target--based frame, p_{m,γ_0} are the plane-wave VWH dipole expansion coefficients (degree m, order 1, and TM mode) for the incident field, with subscript $\gamma_0 = 1, 2$ denoting an incident polarization angle, relative to the $\hat{\mathbf{z}} - \mathbf{k}_0$ plane, of 0 or $\pi/2$, and f^i is the phase factor,

$$f^i(\alpha_0,\ \beta_0) = \exp\left[\mathrm{i}\mathsf{k}((x_i\, \cos\alpha_0 + y_i\, \sin\alpha_0)\sin\beta_0 + z_i\, \cos\beta_0)\right]. \tag{3}$$

Note that a dipole--limit VWH formulation of the DDA equations is employed, in which index m denotes the dipole azimuth degrees $-1, 0, 1$, as opposed to a Cartesian--based dipole-moment formulation; the two formulations are completely equivalent in the end [4, 1].

In general, the number of unknowns in Eq. (2) will scale with $x_V^3 = (\mathrm{k}a_V)^3$, where a_V is a volume-equivalent radius of the particle. The objective of the method proposed here is to reduce the number of unknowns, so that the computational overhead scales with the surface area of the particle as opposed to the volume. The approach taken in [1] was to represent the discrete distribution of dipole elements as a continuous distribution, modeled by an expansion of scalar spherical wave harmonics centered about the particle origin and evaluated for the particle medium. The rationale is that the distribution of dipole elements should satisfy the scalar Helmholtz equation for the particle material, and the spherical wave harmonics form a complete basis for a regular solution to the Helmholtz equation.

The approach taken here is to use a simpler set of basis functions to represent the dipole distribution. Specifically, the distribution of dipole elements are now modeled by a directional spectrum of plane waves, evaluated within the particle medium. This is expressed as

$$a_m^i \approx \sum_{\nu=1}^{M} \sum_{\gamma=1}^{2} \omega_\nu\, p_{m,\gamma}(\mathbf{k}_\nu)\, \hat{f}^i(\mathbf{k}_\nu)\, W_{\nu\gamma,\nu_0\gamma_0}, \tag{4}$$

in which $\mathbf{k}_\nu = (\alpha_\nu, \beta_\nu)$ describes the direction of the plane wave component, ω_ν is a weighting function, W is a matrix which is sought from the analysis, ν_0, γ_0 represents the incident direction and polarization, and $\hat{f}$ is a phase factor evaluated in the particle medium (i.e., wavenumber mk). A logical choice for the distribution of angles and weights is the Gauss quadrature points of a chosen order M_β for $\cos\beta$ and an even distribution of $2M_\beta$ points in α. The total number of directions will then be $M = 2M_\beta^2$

Following the DDMM procedure, a system of equations for W can be obtained by multiplying Eq. (2) by the conjugate of the basis function in Eq. (4) and contracting over all lattice positions. This results in

$$\sum_{\nu'=1}^{M} \sum_{\gamma'=1}^{2} A_{\nu\gamma\,\nu'\gamma'}\, W_{\nu'\gamma'\,\nu_0\gamma_0} = B_{\nu\gamma\,\nu_0\gamma_0} \tag{5}$$

with

$$A_{\nu\gamma\,\nu'\gamma'} = \omega_\nu\,\omega_{\nu'} \sum_{m=-1}^{1}\sum_{k=-1}^{1} \left(p_{m,\gamma}(\mathbf{k}_\nu)\right)^*\, p_{k,\gamma'}(\mathbf{k}_{\nu'}) \times \sum_{i=1}^{N_d} \hat{f}^{i*}(\mathbf{k}_\nu) \left(\frac{1}{a}\,\hat{f}^i(\mathbf{k}_{\nu'})\delta_{m-k} - \sum_{\substack{j=1\\ j\neq i}}^{N_d} H_{mk}^{i-j}\,\hat{f}^j(\mathbf{k}_{\nu'}) \right), \tag{6}$$

$$B_{\nu\gamma\,\nu_0\gamma_0} = \omega_\nu\,\left(p_{m,\gamma}(\mathbf{k}_\nu)\right)^*\, p_{m,\gamma_0}(\mathbf{k}_{\nu_0}) \sum_{i=1}^{N_d} \hat{f}^{i*}(\mathbf{k}_\nu)\, f^i(\mathbf{k}_{\nu_0}). \tag{7}$$

It is computationally simple and efficient to use existing DDA codes to generate the A matrix defined in Eq. (6) [4, 5]. In particular, the FFT convolution scheme can be used to perform the summation over lattice site j, followed by a direct sum over site i. In general, the operation count in generating the A matrix will scale as $M^2 N_d \ln(N_d)$. Standard inversion methods can then be used to obtain the W matrix from the solution of Eq. (5).

Relation to the T matrix

By use of the addition theorem for VWH, the scattered field from the particle, given by Eq. (1), can be represented by a single outgoing VWH expansion centered about the origin of the particle. The expansion coefficients in this representation, for the VWH component of degree/order/mode k, l, q, are given by [1]

$$a_{klp} = \sum_{i=1}^{N_d}\sum_{m=-1}^{1} J_{klq\,m11}^{0-i}\,a_m^i, \tag{8}$$

where J is the regular harmonic translation matrix and L the truncation limit. In the far field, the transverse components of the scattered field in a direction $\mathbf{k}_s$, referenced to the target coordinate frame, will be given by

$$\mathbf{E}_{s,\gamma_s}(\mathbf{k}_s) = \frac{e^{\mathrm{i}k\,r}}{\mathrm{i}kr} \sum_{l=1}^{L}\sum_{k=-l}^{l}\sum_{q=1}^{2} \left(p_{klq,\gamma_s}(\mathbf{k}_s)\right)^*\, a_{klq}, \tag{9}$$

in which p_{klq,γ_s} is the plane-wave VWH coefficient and $\gamma_s = 1$ and 2 would correspond to the θ and ϕ components.

The plane-wave model in Eq. (4) can be substituted directly into Eq. (8) to obtain the VWH form for the scattered field. An alternative approach is to recognize that the plane-wave coefficients p_{klq} and the phase factor f are the eigenvectors and eigenvalues to the translation matrix [6];

$$p_{m11,\gamma}(\mathbf{k})\,f^i(\mathbf{k}) = \sum_{l=1}^{l}\sum_{k=-l}^{l}\sum_{q=1}^{2} J_{m11\,klq}^{i-0}\,p_{klq,\gamma}(\mathbf{k}). \tag{10}$$

By employing the above into Eq. (8) and using the matrix relations developed for the plane-

wave model, the far-field components of electric field will be given by

$$\mathbf{E}_s(\mathbf{k}_s) = \frac{e^{\mathrm{i}k\,r}}{\mathrm{i}k r}\sum_{\nu=1}^{M}\sum_{\gamma=1}^{2} B^*_{\nu\gamma\,\nu_s\gamma_s}\,W_{\nu\gamma\,\nu_0\gamma_0}$$

$$= \frac{e^{\mathrm{i}k\,r}}{\mathrm{i}k r}\sum_{\nu=1}^{M}\sum_{\gamma=1}^{2}\sum_{\nu'=1}^{M}\sum_{\gamma'=1}^{2} B^*_{\nu\gamma\,\nu_s\gamma_s}\,A^{-1}_{\nu\gamma\,\nu'\gamma'}\,B_{\nu'\gamma'\,\nu_0\gamma_0} = \frac{e^{\mathrm{i}k\,r}}{\mathrm{i}k r}\,S_{\nu_s\gamma_s\,\nu_0\gamma_0}. \quad (11)$$

The matrix S is recognized as a scattering amplitude matrix. The traditional T matrix can be obtained by use of Eq. (10) and the orthogonality relations of the p_{klq} functions. Assuming an integration over direction is accurately represented by the chosen quadrature scheme and weights, the T matrix will be given by

$$T_{mnp\,klq} = \sum_{\nu=1}^{M}\sum_{\gamma=1}^{2}\sum_{\nu'=1}^{M}\sum_{\gamma'=1}^{2} \left(p_{mnp,\gamma}(\mathbf{k}_\nu)\right)^*\,S_{\nu\gamma\,\nu'\gamma'}\,p_{klq,\gamma'}(\mathbf{k}_{\nu'}). \quad (12)$$

Preliminary results and directions

A code has been developed to test the veracity of the proposed method. Preliminary results indicate that the number of polar angles M_β (i.e., the number of quadrature points) needed for accurate agreement with exact DDA results is proportional to x_V. Viewed another way, M_β will be comparable to the VWH order truncation limit L for the T-matrix representation.

The plane-wave form in Eq. (4) offers some unique features when coupled with the DDA procedure. For certain particle shapes, e.g., a rectangular solid, the model becomes a separable function of x, y, and z, and this can reduce considerably the computational overhead in calculation of Eq. (6). It is also relatively simple to implement a surface integral form of the equations -- as opposed to a volume integration -- which will remove the need for a dipole polarizability. These topics, and the results of example calculations, will be presented at the meeting.

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