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"Hybrid" *T*-matrix methods

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Abstract

The *T*-matrix method is widely used for the calculation of scattering by particles of sizes on the order of the illuminating wavelength. Although the extended boundary condition method (EBCM) is the most commonly used technique for calculating the *T*-matrix, a variety of methods can be used.
Because the *T*-matrix depends only on the properties of the scatterer and the wavelength and not on other properties of the incident field, the *T*-matrix method is especially well-suited to repeated calculations involving varying illumination. Thus, it can be highly desirable to express the scattering properties of a given arbitrary particle as a *T*-matrix. However, the standard EBCM is only applicable to homogeneous scatterers, necessitating the use of other, more general methods.
We consider some general principles of "hybrid" *T*-matrix methods—calculating *T*-matrices using other techniques for calculating scattering—and consider some specific methods. In particular, we discuss the application of time-domain methods which offer the possibility of simultaneous multiple-wavelength or multiple-size calculations.

1 Introduction

The *T*-matrix method in wave scattering involves writing the relationship between the wave incident upon a scatterer, expanded in terms of orthogonal eigenfunctions,

$$U_{\text{inc}} = \sum_{n}^{\infty} a_n \psi_n^{(\text{inc})}, \tag{1}$$

where a_n are the expansion coefficients for the incident wave, and the scattered wave, also expanded in terms of orthogonal eigenfunctions,

$$U_{\text{scat}} = \sum_{k}^{\infty} p_k \psi_k^{(\text{scat})}, \tag{2}$$

where p_k are the expansion coefficients for the scattered wave, is written as a simple matrix equation

$$p_k = \sum_{n}^{\infty} T_{kn} a_n \tag{3}$$

or, in more concise notation,

$$\mathbf{P} = \mathbf{TA} \tag{4}$$

where T_{kn} are the elements of the T-matrix. The T-matrix method can be used for scalar waves or vector waves in a variety of geometries, with the only restrictions being that the geometry of the problem permits expansion of the waves as discrete series in terms of orthogonal eigenfunctions, that the response of the scatterer to the incident wave is linear, and that the expansion series for the waves can be truncated at a finite number of terms. In general, one calculates the T-matrix, although it is conceivable that it might be measured experimentally.

The T-matrix depends only on the properties of the particle—its composition, size, shape, and orientation—and the wavelength, and is otherwise independent of the incident field. This means that for any particular particle, the T-matrix only needs to be calculated once, and can then be used for repeated calculations. This is a significant advantage over many other methods of calculating scattering where the entire calculation needs to be repeated [1]. Some cases provide even more efficiency: if the waves are expanded in spherical functions, the averaging of scattering over various orientations of the particle compared to the direction of the incident wave can be performed analytically [2].

In the spherical geometry of elastic light scattering by a particle contained entirely within some radius r_0, the eigenfunction expansions of the fields are made in terms of vector spherical wavefunctions (VSWFs). These wavefunctions are the electric and magnetic multipole fields; the field representations are multipole expansions (references [1] to [6] discuss these in more depth).

For other geometries, other sets of eigenfunctions, such as cylindrical wavefunctions (for scatterers of infinite length in one dimension), or a Floquet expansion (planar periodic scatterers), are more appropriate. There is no requirement that the modes into which the incident and scattered fields are expanded be the same, or even similar. For example, the null-field method with discrete sources [7] uses an expansion in multipoles centred on multiple origins. In all of these cases, the T-matrix method remains applicable.

2 Non-EBCM calculation of the *T*-matrix

Methods other than the EBCM can be used to calculate the T-matrix. In general, one would calculate the scattered field, given a particular incident field. The most direct way in which to use this to produce a T-matrix is to solve the scattering problem when the incident field is equal to a single spherical mode – that is, a single VSWF such as $\mathbf{E}_{\mathrm{inc}}(\mathrm{r}) = \mathbf{RgM}_{11}(k\mathrm{r})$, $\mathbf{E}_{\mathrm{inc}}(\mathrm{r}) = \mathbf{RgN}_{11}(k\mathrm{r})$, $\mathbf{E}_{\mathrm{inc}}(\mathrm{r}) = \mathbf{RgM}_{21}(k\mathrm{r})$, etc, and repeat this for all VSWFs that need to be considered (up to $n = N_{\mathrm{max}}$). The expansion coefficients for the scattered field can be found in each case, if necessary, by using the orthogonal eigenfunction transform (the generalised Fourier transform), and each scattering calculation gives a single column of the T-matrix.

Therefore, the calculation of a T-matrix requires that $2N_{\mathrm{max}}(N_{\mathrm{max}} + 2)$ separate scattering problems are solved. This provides a criterion for deciding whether it is desirable to calculate a T-matrix: if more than $2N_{\mathrm{max}}(N_{\mathrm{max}} + 2)$ scattering calculations will be performed, then it is more efficient to calculate the T-matrix and use this for the repeated calculations than it is to use the original scattering method repeatedly. Repeated calculations are expected if orientation averaging is to be carried out, or if inhomogeneous illumination is to be considered, such as, for example, scattering by focussed beams, where there are generally 6 degrees of freedom, namely the three-dimensional position of the scatterer within the beam, and the three-dimensional orientation of the scatterer. Even if only a modest number of points are considered along each degree of freedom, the total number of scattering calculations required rapidly becomes very large, and even if the T-matrix takes many hours to calculate, the total time saved by doing so can make an otherwise computationally infeasible problem tractable.

Volume methods are of interest, since they can readily be used for inhomogeneous or anisotropic particles. The two most likely candidates are the finite-difference time-domain method (FDTD) [1, 8] and the discrete dipole approximation (DDA). In FDTD, the Maxwell equations are discretised in space and time, and, beginning from a known initial state, the electric and magnetic fields at each spatial grid point are calculated for successive steps in time. The number of grid points required is $O(N_{\max}^3)$ for three-dimensional scattering, and $O(N_{\max})$ time steps required, so FDTD solutions scale as $O(N_{\max}^4)$. Therefore, calculation of the T-matrix using FDTD should scale as $O(N_{\max}^6)$, which is the same scaling as the EBCM. However, the grid required must be closely spaced compared to the wavelength, and the space outside the scatterer must also be discretised, making FDTD substantially slower than EBCM, especially for smaller particles. However, FDTD is an extremely general technique, and has potential as a method for the calculation of T-matrices.

We should add that there is an additional consideration that makes FDTD potentially attractive as a method for calculating the T-matrix: FDTD does not assume that the incident wave is monochromatic. Consider the case when the illumination is a brief pulse with a Gaussian envelope. The frequency spectrum of the incident wave is Gaussian, and the scattering of a range of frequencies can be found by taking the Fourier transform of the scattered field [9]. Even if we are not interested in other than monochromatic illumination, we will frequently be interested in scattering by size distributions of particles. Since varying the frequency for a particular particle is equivalent to varying the size of the particle for a fixed incident frequency, the T-matrices for a range of particle sizes can be calculated simultaneously.

The other major volume method for computational scattering, the discrete dipole approximation (DDA), also known as the coupled-dipole method, has been recently applied to the calculation of the T-matrix by Mackowski [10], who obtained good results, with reasonable computational efficiency using a moment method to solve the DDA system of equations. There is no need to discuss his method in detail here, and the interested reader is referred to his recent description of the method [10].

Lastly we note our recent application of the point-matching method to the calculation of T-matrices [11], where we showed it to be a feasible alternative to the EBCM for particles devoid of symmetry. The point-matching method is an attractive candidate since a T-matrix implementation will generally include routines to calculate VSWFs, making the implementation of a point-matching T-matrix calculator simple. A wide range of possible point-matching methods exist, such as the multiple-multipole method (MMP), discrete sources method, etc [12].

3 Time-domain methods

As mentioned above, time-domain methods offer the possibility of simultaneously calculating the T-matrix for multiple wavelengths. If one can provide an incident field of which the spectral components in time and space are single electric or magnetic multipoles, the scattered field expansions can be found from the scattered field frequency space components. This would directly give a column of the T-matrices for each frequency component.

On the other hand, it might only be possible to use time-varying plane wave illumination in the time-domain code. In this case, as a first step, one would obtain a T-matrix relating an incident plane wave expansion to a scattered multipole expansion. Although the convergence properties of multipole expansions and plane wave expansion are very different when considering infinite regions, equivalent accuracy is obtainable with a finite set of components in a limited volume. Sufficient plane wave components must be used for this be valid. The plane wave expansion can be directly transformed into the equivalent spherical wave expansion. Presumably, the transformation matrix for this would be pre-calculated, reducing the conversion of the T-matrix to the desired form to a matrix-matrix multiplication.

Ideally, one would know beforehand the wavelengths at which the T-matrix is desired, allowing a suitable envelope w.r.t. time to be chosen for the incident wave. If the variation of refractive index with wavelength is assumed to be zero, variation of the T-matrix with wavelength is exactly equivalent to variation of the T-matrix with scatterer size for a fixed wavelength. This may prove to be a useful technique for scattering by polydisperse particles.

4 Conclusion

While the extended boundary condition method (EBCM) is the standard method for the calculation of the T-matrix of a scatterer, the T-matrix method itself is a very general technique, consisting of the representation of the scattering properties of a particle as a matrix transforming a truncated discrete eigenfunction expansion of an incident wave to that of the scattered wave. Accordingly, a diverse range of computational methods can be used for calculating T-matrices. These are of most value when considering inhomogeneous scatterers for which the EBCM cannot be used. In particular, time-domain methods offer the possibility of simultaneous calculation of the T-matrix at multiple wavelengths or, equivalently, multiple particle sizes.

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