A review of point-group symmetries in the T matrix and Green's functions formalisms

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Abstract

An overview of the exploitation of boundary symmetries in electromagnetic scattering problems is presented. The paper follows the historical development of methodologies, thus starting with method-specific formulations based on boundary-integral equation approaches, followed by more general treatments based on the T matrix formulation, and finally reviewing a unified treatment of symmetries within the self-consistent Green's function formalism.

1 Introduction

Boundary symmetries of particles allow us to simplify the solution to the Helmholtz equation in electromagnetic or acoustic scattering, which results in a reduction of computational costs and and increase in numerical stability. The symmetries can either be inherent in nature, as in the case of spherical raindrops, pristine ice crystals, or cubical dry sodium chloride aerosols, or enter through simplifying assumptions by choosing symmetric model particles. Numerical experiments have demonstrated that the use of symmetries can result in reductions of CPU-time requirements by several orders of magnitude. This has paved the way for applying non-axisymmetric model particles to realistic atmospheric scattering and radiative transfer problems (see e.g. Refs. [1, 2]).

2 Exploitations of symmetries in light scattering problems

The earliest applications of symmetries in electromagnetic scattering theory have focused on specific kinds of symmetries or specific solution methods. In the special case of spherically symmetric particles the scattering problem can be solved analytically [3]. Waterman [4] investigated selected reflection symmetries in his boundary-integral equation (BIE) approach. Mishchenko [5] derived the symmetry properties of the T matrix of axisymmetric particles independent of the method employed for computing the T matrix.

More general treatments of symmetries in electrostatics and in electromagnetic and acoustic scattering theory have been conducted since the 1990's. Symmetries in integral-equation formulations of boundary value problems were studied by Zakharov et al. and applied to problems of electrostatics [6]. Zagorodnov and Tarasov studied symmetry groups in a Green's function approach to boundary value problems [7] and presented applications to integral-equation solutions to the electromagnetic scattering problem [8].

Symmetry properties of the T matrix for arbitrary symmetry groups were studied systematically for reducible [9] and irreducible representations [10]. The main idea is to investigate the transformation properties of the basis functions (usually vector spherical wave functions) under symmetry operations R, and thereby derive matrix representations $\mathbf{R}$ for each symmetry operation R in the vector space on which the T matrix operates. The symmetry properties of the T matrix can then be expressed as commutator relations

$$[\mathbf{T}, \mathbf{R}] = \mathbf{0}, \tag{1}$$

where the commutator is defined as $[\mathbf{T},\mathbf{R}] = \mathbf{T}\cdot\mathbf{R} - \mathbf{R}\cdot\mathbf{T}$. These commutator relations reduce the number of nonzero, independent T matrix elements that need to be evaluated in numerical applications.

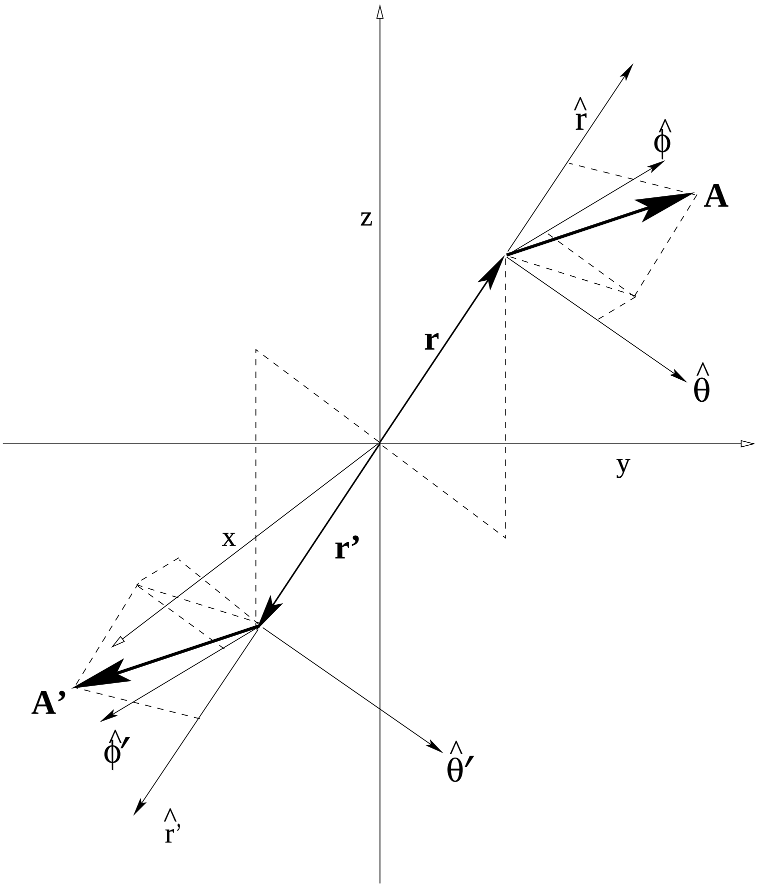

Figure 1: Transformation of a vector function under an inversion of all spatial coordinates.

Consider as an example an inversion I of the spatial coordinates given by $(x, y, z) \longrightarrow (-x, -y, -z)$. As shown in the figure a vector function given in spherical coordinates will transform according to

$$\begin{pmatrix} A_r(r,\theta,\phi) \\ A_\theta(r,\theta,\phi) \\ A_\phi(r,\theta,\phi) \end{pmatrix} \xrightarrow{I} \begin{pmatrix} A_r(r,\pi-\theta,\pi+\phi) \\ -A_\theta(r,\pi-\theta,\pi+\phi) \\ A_\phi(r,\pi-\theta,\pi+\phi) \end{pmatrix}. \tag{2}$$

By using the properties of the vector spherical wave functions $\mathbf{M}^{(j)}_{n,m,\tau}$ (where $\tau = 1, 2$ and $j = 1, \ldots, 4$) this leads to

$$\mathbf{M}^{(j)}_{n,m,\tau} \xrightarrow{I} (-1)^{n+\tau}\mathbf{M}^{(j)}_{n,m,\tau}, \quad j = 1, \ldots, 4. \tag{3}$$

Thus a matrix representation of the inversion operation is given in components by

$$I_{n,m,\tau;n',m',\tau'} = \delta_{n,n'}\,\delta_{m,m'}\,\delta_{\tau,\tau'}\,(-1)^{n+\tau}. \tag{4}$$

If the boundary surface is invariant under the inversion operation, then $\mathbf{T}= \mathbf{I}\cdot\mathbf{T}\cdot\mathbf{I}^{-1}$, or, analogous to Eq. (1), $[\mathbf{T},\mathbf{I}] = \mathbf{0}$. Using Eq. (4), this becomes in explicit form

$$T_{n,m,\tau;n',m',\tau'} = (-1)^{n+\tau+n'+\tau'}\,T_{n,m,\tau;n',m',\tau'}, \tag{5}$$

or equivalently

$$T_{n,m,\tau;n',m',\tau'} = 0, \text{ unless } (n+\tau+n'+\tau') \text{ even.} \tag{6}$$

This method can be used to derive representations and symmetry relations for any symmetry operation encountered in point groups [10].

The representations **R** in the basis of vector spherical wave functions are in general reducible. By means of group theoretical techniques one can construct a similarity transformation to transform the reducible into irreducible representations, thus bringing the matrix representations into block-diagonal form. It can be shown that this transformation also brings the T and Q matrix into irreducible block-diagonal form [10]. The main idea is to construct projection operators

$$\tilde{P}^{(\mu)}_{j,i} = \sum_{g\in\mathcal{G}} \chi^{(\mu)*}(g)\, R_{j,i}(g) \tag{7}$$

that project into the μ-th irreducible invariant subspace. Here $\mathcal{G}$ denotes the symmetry group, $R_{j,i}(g)$ denote the reducible representations of group element g, and $\chi^{(\mu)}(g)$ denote the characters of the irreducible representations, which can be computed by standard group-theoretical techniques [11, 12]without prior knowledge of the irreducible representations. By use of the operators (7) one constructs a similarity transformation into the irreducible basis in which all matrix quantities become block-diagonal.

It was demonstrated by use of irreducible representations in a BIE approach [8] that exploitation of symmetries can reduce CPU-time requirements by a factor of M_0^2, where M_0 represents the order of the symmetry group. Interestingly enough, the same was observed in Ref. [13], in which only reducible representations were exploited. A recent comparison of BIE computations that exploited reducible and irreducible representations, respectively, showed that the latter only saved and additional factor of 3–4 in computation time [10]. However, it was also shown [10] that the block-diagonalisation of the T and Q matrix favourably pre-conditions the Q matrix, thus increasing the numerical stability of the Q matrix inversion problem in T matrix computations.

In a recently published treatment [14] of symmetries (which was focused on the exterior problem) it was shown that one can derive general symmetry relations of the Green's function of an arbitrary linear boundary-value problem. From the general symmetry relations, one obtains for the special case of the Helmholtz equation symmetry relations for the surface Green's function $G_{\partial\Gamma}$ of the form

$$G_{\partial\Gamma}(\mathbf{x},\mathbf{x}_s) = G_{\partial\Gamma}(D_g(\mathbf{x}), D_g(\mathbf{x}_s)) \tag{8}$$

where $\mathbf{x}$ lies in the surrounding medium and $\mathbf{x}_s$ lies on the boundary surface. The D_g denote the representations in three-dimensional space of the symmetry group's elements g. Likewise, one obtains for the volume Green's function G_{Γ_+}

$$G_{\Gamma_+}(\mathbf{x}_0,\mathbf{x}) = G_{\Gamma_+}(D_g(\mathbf{x}_0), D_g(\mathbf{x})), \tag{9}$$

where $\mathbf{x}_0$ and $\mathbf{x}$ lie in the surrounding medium. For the interaction operator $W_{\partial\Gamma}$ one obtains

$$W_{\partial\Gamma}(\mathbf{x}_s,\mathbf{x}'_s) = W_{\partial\Gamma}(D_g(\mathbf{x}_s), D_g(\mathbf{x}'_s)), \tag{10}$$

where $\mathbf{x}_s$ and $\mathbf{x}'_s$ lie on the boundary surface. These three symmetry relations are shown to be equivalent [14]. The volume Green's function is related to volume-integral equation (VIE) methods, the surface Green's function to BIE methods, and the interaction operator to the T-matrix formulation. For instance, from the symmetry relations of the interaction operator, one can derive the commutator relations of the T-matrix. Thus one has a general description of symmetries in acoustic and electromagnetic scattering theory that comprises symmetries in VIE and BIE methods as well as in the T-matrix formalism. This treatment of symmetries is based on the self-consistent Green's function formulation of the electromagnetic and acoustic scattering problem [15, 16].

References

[1] M. Kahnert and A. Kylling. Radiance and flux simulations for mineral dust aerosols: Assessing the error due to using spherical or spheroidal model particles. *J. Geophys. Res.*, 109:D09203, doi:10.1029/2003JD004318, errata: doi:10.1029/2004JD005311, 2004.

[2] T. Nousiainen, M. Kahnert, and B. Veihelmann. Light scattering modeling of small feldspar aerosol particles using polyhedral prisms and spheroids. *J. Quant. Spectrosc. Radiat. Transfer*, 101:471–487, 2006.

[3] G. Mie. Beiträge zur Optik trüber Medien, speziell kolloidaler Metallösungen. *Ann. Phys.*, 25:377–445, 1908.

[4] P. C. Waterman. Matrix formulation of electromagnetic scattering. *Proc. IEEE*, 53:805–812, 1965.

[5] M. I. Mishchenko. Light scattering by randomly oriented axially symmetric particles. *J. Opt. Soc. Am. A.*, 8:871–882, 1991.

[6] E. V. Zakharov, S. I. Safronov, and R. P. Tarasov. Finite-order abelian groups in the numerical analysis of linear boundary-value problems of potential theory. *Comput. Maths. Math. Phys.*, 32:34–50, 1992.

[7] I. A. Zagorodnov and R. P. Tarasov. The problem of scattering from bodies with a noncommutative finite group of symmetries and its numerical solution. *Comput. Maths. Math. Phys.*, 37:1206–1222, 1997.

[8] I. A. Zagorodnov and R. P. Tarasov. Finite groups in numerical solution of electromagnetic scattering problems on non-spherical particles. In *Light Stattering by Nonspherical Particles: Halifax Contributions*, pages 99–102, Adelphi, MD, 2000. Army Research Laboratory.

[9] F. M. Schulz, K. Stamnes, and J. J. Stamnes. Point group symmetries in electromagnetic scattering. *J. Opt. Soc. Am. A*, 16:853–865, 1999.

[10] M. Kahnert. Irreducible representations of finite groups in the T matrix formulation of the electromagnetic scattering problem. *J. Opt. Soc. Am. A*, 22:1187–1199, 2005.

[11] J. D. Dixon. High speed computation of group characters. *Numerische Mathematik*, 10:446–450, 1965.

[12] J. J. Cannon. Computers in group theory: a survey. *Commun. ACM*, 12:3–11, 1969.

[13] F. M. Kahnert, J. J. Stamnes, and K. Stamnes. Application of the extended boundary condition method to homogeneous particles with point group symmetries. *Appl. Opt.*, 40:3110–3123, 2001.

[14] M. Kahnert. Boundary symmetries in linear differential and integral equation problems applied to the self-consistent Green's function formalism of acoustic and electromagnetic scattering. *Opt. Commun.*, 265:383–393, 2006.

[15] T. Rother. Self-consistent Green's function formalism for acoustic and light scattering, Part 1: Scalar notation. *Opt. Commun.*, 251:254–269, 2005.

[16] T. Rother. Self-consistent Green's function formalism for acoustic and light scattering, Part 2: Dyadic notation. *Opt. Commun.*, 251:270–285, 2005.