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SURFACE GREEN'S FUNCTION OF THE HELMHOLTZ EQUATION IN SPHERICAL COORDINATES

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Abstract—The surface Green's function belonging to the non-spherical exterior boundary value problem of Helmholtz's equation in spherical coordinates is derived. This is performed in two ways, first by applying the Separation of Variables method, and, second, by using the Method of Lines as a special Finite-Difference technique. With this Green's function we are able to resolve some contradictions concerning conceptual aspects of the Separation of Variables method, the Finite-Difference methods, and the Boundary Integral Equation methods which have been developed for rigorously solving non-separable boundary value problems. The necessary mathematical background, the relation to Waterman's T matrix, and simplifications due to certain symmetry properties of the boundary surface will be discussed. In this paper we focus on the scalar problem. The extension to the vector case for electromagnetic wave scattering is in preparation and will be published later.

1. INTRODUCTION

A large variety of different numerical methods exist for solving so-called "non-separable" boundary value problems (BVP) related to the Helmholtz equation. "Non-separable" denotes the fact that a certain condition is imposed on a surface which doesn't coincide with a constant coordinate line in a coordinate system in which the Helmholtz equation becomes separable. So far it has been assumed that in such cases the Separation of Variables method (SVM) can not be applied, and that other methods have to be employed. A critical evaluation of this point of view is one subject of this paper. Each of the methods developed so far has a certain range of applicability and several strengths and drawbacks in comparison to other methods. In this paper we will focus on two classes of numerical methods which are widely used to rigorously solving the non-separable BVP. These are the Finite-Difference methods (FD) and the Boundary Integral Equation methods (BIE) which have traditionally been treated separately. FD methods are based on the description of the BVP in terms of partial differential equations. They apply a discretization scheme to some (Method of Lines (MoL) [1]) or to all spatial coordinates (conventional FD methods, see e.g. Ref. [2]) of the corresponding partial differential equation. BIE methods, such as Waterman's T matrix approach, start from Green's theorem in conjunction with the Helmholtz equation and the related free-space Green's function [3]. But there is no essential difference in the general solution scheme of both approaches, as we

will demonstrate in this paper. Furthermore, it is common to the SVM, the BIE, and the FD methods that they have to approximate the surface potential to fulfil the condition imposed on the boundary surface [4]. The validity of such approximations is the subject of controversial discussions about the so-called Rayleigh hypothesis [5,6]. It is another goal of this paper to examine some aspects of this discussion. But our main goal is to bridge the gap between the SVM, the FD, and the BIE methods by condensing these three approaches into a common mathematical formalism. This can be achieved by generalizing the surface Green's function (SGF) concept of Morse and Feshbach [7] to non-separable boundary surfaces. The SGF is related to the volume Green's function (VGF) where the latter is the solution of the inhomogeneous Helmholtz equation with a delta source outside a bounded domain but for a homogeneous boundary condition on the boundary surface. Thus this VGF depends on the geometry of the boundary surface and must not be confused with the conventional free-space Green's function G_0. By use of Green's theorem, the surface integral over the SGF and a given potential on the boundary surface yields the exterior solution. Since such a representation can be obtained for the SVM as well as the FD and BIE methods the SGF provides an appropriate methodical link between them.

However, this unified description of the non-separable boundary value problem is not only of methodical interest. It also provides us with a more thorough understanding of the over-all accuracy of different approaches and reveals interesting new aspects of the FD methods. It further allows us to discuss as to what extent conceptual advantages of BIE methods, regarding especially the fulfilment of the radiation condition and the simplification of the orientational averaging process (as it may become necessary in light scattering analysis, for instance), may be applied to FD methods. In addition, we consider the relation between discrete symmetries of the boundary surface and symmetry relations of the corresponding solution of the Helmholtz equation. Discrete symmetries have been investigated in the T matrix description [8] and in other BIE based methods [9]. They have been demonstrated to drastically reduce CPU-time by several orders of magnitude [10], and to extend the range of size parameters that can be computed in light scattering applications [11]. In this paper we will derive symmetry relations for the SGF and discuss their relation to symmetry relations in the BIE formulation.

In Sec. 2 we briefly review the SGF concept of Morse and Feshbach [7] for a spherical boundary surface. This is followed by a review of the role of Green's theorem in two different BIE methods, namely, the null-field method [12], and the BIE method by Kleinman et

al. [13] and Ramm [14] which avoids the use of the null-field equation. In Sec. 3 we generalize the SGF concept to non-spherical boundary surfaces and discuss the important issue of convergence of the approximate solution of the exterior BVP. In this section we will also show how the generalized SVM approach can be obtained from the null-field equation. In Sec. 4 we demonstrate the derivation of the SGF by use of the MoL as a special FD technique and consider its limiting behaviour for an increasing number of discretization lines. The relation between discrete symmetries of the boundary surface and the symmetry relations of the SGF, and the equivalence of these symmetry relations to known symmetry relations in the BIE methods are considered in Sec. 5. Concluding remarks are given in Sec. 6.

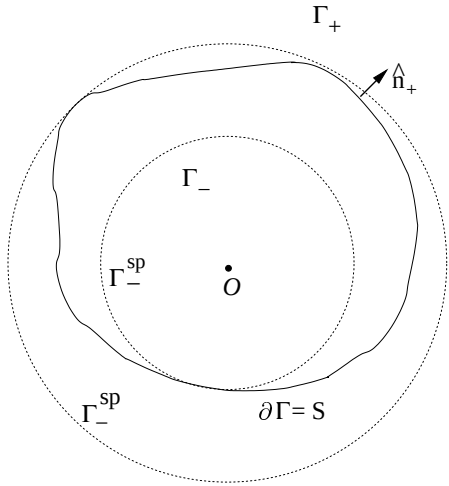

Figure 1. Geometry of the exterior boundary value problem. Γ_+^{sp} and Γ_-^{sp} denote the smallest circumscribing and the largest inscribing sphere, respectively.

2. THE EXTERIOR BOUNDARY VALUE PROBLEM IN SPHERICAL COORDINATES AND BOUNDARY INTEGRAL EQUATION METHODS

2.1. Formulation of the Boundary Value Problem

The geometry of the exterior BVP is depicted in Fig. 1. Let Γ_- denote a bounded domain in $\mathbb{R}^3$ having the boundary surface $\partial\Gamma$. Generally, this surface is assumed to fulfil a certain smoothness condition (Lyapunov surfaces) to meet the criteria for the mathematical proof of

completeness and linear independence of the radiating and regular spherical wave functions on this boundary surface. However, various applications have demonstrated that this assumption can be relaxed in many cases, and that stable and reliable results can also be obtained for other surfaces. We denote the exterior domain by Γ_+. Each point $\mathbf{x} \in \mathbb{R}^3$ shall be represented by spherical coordinates (r, θ, ϕ). The corresponding Cartesian coordinate system has its origin in Γ_-. We wish to find the solution of the homogeneous Helmholtz equation

$$(\nabla^2 + k^2)u(\mathbf{x}) = 0; \quad \mathbf{x} \in \Gamma_+ \tag{1}$$

in the exterior domain which satisfies the radiation condition

$$\lim_{r\to\infty} r \cdot \left\{ \frac{\partial u}{\partial r} - iku \right\} = 0, \tag{2}$$

and the inhomogeneous Dirichlet condition

$$u(\bar{\mathbf{x}}) = f(\bar{\mathbf{x}}); \quad \bar{\mathbf{x}} \in \partial\Gamma \tag{3}$$

on the boundary surface. Such a solution is called a radiating solution of Eq. (1). The surface potential f is assumed to be a known analytic function. For a given boundary surface with the parametric representation $R = R(\boldsymbol{\theta}, \phi)$ the outward directed normal vector $\hat{\mathbf{n}}_+$ is given by

$$\hat{\mathbf{n}}_+ = R^2(\theta,\phi)\sin\theta \left[\hat{\mathbf{r}} - \frac{1}{R(\theta,\phi)} \frac{\partial R(\theta,\phi)}{\partial \theta} \hat{\boldsymbol{\theta}} - \frac{1}{R(\theta,\phi)\sin\theta} \frac{\partial R(\theta,\phi)}{\partial \phi} \hat{\boldsymbol{\phi}} \right], \tag{4}$$

where $\hat{\mathbf{r}}$, $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\phi}}$ are the unit vectors in spherical coordinates. In what follows, we are exclusively dealing with the exterior BVP, i.e., k will henceforth represent the free-space wave number.

As already mentioned in the introduction the SGF is related to the VGF, where the latter is a solution of the inhomogeneous Helmholtz equation

$$(\nabla^2_{\mathbf{x}} + k^2)G(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x}, \mathbf{x}'), \quad \mathbf{x}, \mathbf{x}' \in \Gamma_+ \tag{5}$$

which fulfils the radiation condition at infinity and the condition

$$G(\mathbf{x}, \mathbf{x}') = 0, \quad \mathbf{x} \in \partial\Gamma \tag{6}$$

on the boundary surface. The formal solution of the BVP (1) can be represented in terms of this VGF by employing Green's theorem,

formulated for the exterior domain Γ_+,

$$\int_{\Gamma_+} \left[\psi(\mathbf{x})\nabla^2\phi(\mathbf{x}) - \phi(\mathbf{x})\nabla^2\psi(\mathbf{x})\right] \mathrm{d}V(\mathbf{x}) = \oint_{\partial\Gamma} \left[\psi(\bar{\mathbf{x}})\frac{\partial\phi(\bar{\mathbf{x}})}{\partial\hat{n}_-} - \phi(\bar{\mathbf{x}})\frac{\partial\psi(\bar{\mathbf{x}})}{\partial\hat{n}_-}\right] \mathrm{d}S(\bar{\mathbf{x}}), \quad (7)$$

where directional derivatives with respect to the inward pointing normal vector $\hat{\mathbf{n}}_-$ on the boundary surface are defined as

$$\frac{\partial\phi}{\partial\hat{n}_-} := \nabla_{\bar{x}}\phi \cdot \hat{\mathbf{n}}_-. \quad (8)$$

Substituting $\psi = u$ and $\phi = G$ into Eq. (7), we obtain in conjunction with Eq. (5)

$$u(\mathbf{x}) = \oint_{\partial\Gamma} f(\bar{\mathbf{x}})\frac{\partial G(\bar{\mathbf{x}}, \mathbf{x})}{\partial\hat{n}_-}\mathrm{d}S(\bar{\mathbf{x}}). \quad (9)$$

Obviously we do not need to know the VGF itself, but only its directional derivative on the boundary surface. By defining the SGF $G_{\partial\Gamma}$ according to

$$G_{\partial\Gamma}(\bar{\mathbf{x}}, \mathbf{x}) := \frac{\partial G(\bar{\mathbf{x}}, \mathbf{x})}{\partial\hat{n}_-}, \quad (10)$$

we can rewrite Eq. (9) as

$$u(\mathbf{x}) = \oint_{\partial\Gamma} f(\bar{\mathbf{x}})G_{\partial\Gamma}(\bar{\mathbf{x}}, \mathbf{x})\,\mathrm{d}S(\bar{\mathbf{x}}). \quad (11)$$

This equation clearly exhibits one advantage of the Green's function concept for solving the homogeneous Helmholtz equation with an inhomogeneous boundary condition. Once the corresponding SGF is known the solution of the BVP is "simply" obtained by integration over a given surface potential multiplied by the SGF. In this way we are able to separate the surface potential from the geometrical properties of the bounded domain Γ_-. This is analogous to the decoupling of the physical and geometrical properties of the scatterer from its orientation with respect to the incident field, a well-known advantage of the BIE methods if applied to light scattering analysis. By contrast, such a decoupling can not be achieved in conventional FD methods which makes orientational averaging a very time-consuming task.

However, to exploit the above-mentioned advantage of the SGF concept we first have to be able to compute the SGF. For separable geometries this was already done by use of the SVM, as described in Ref. [7]. This will be demonstrated in the next chapter.

2.2. Solution in the Limiting Case of a Spherical Boundary Surface and the Related Surface Green's Function

Apart from a few situations in which one obtains a closed analytical expression for the Green's function (free-space Green's function, for instance) a series expansion of this function in terms of the eigensolutions of the corresponding homogeneous partial differential equation is usually employed. So far this has only been done for separable boundary surfaces since in this case the linearly independent and complete set of eigenfunctions form an orthogonal basis (for details, see Refs. [7, 15]). Before we abandon this restriction we will demonstrate how to represent the SGF related to the exterior BVP of the Helmholtz equation in spherical coordinates if the surface potential f is given on a spherical boundary surface with radius R. Then, by use of the SVM, the solution of Eq. (1) can be expressed by the series expansion

$$\begin{gathered} u(r,\theta,\phi) = \sum_{l,n} a_{n,l} \cdot h_n^{(1)}(kr) \cdot Y_{n,l}(\theta,\phi); \\ n = 1, 2, \ldots \quad \text{and} \quad l = 0, \pm 1, \ldots, \pm n \end{gathered} \tag{12}$$

where $h_n^{(1)}(kr)$ denote the spherical Hankel functions of the first kind. The spherical harmonics $Y_{n,l}(\theta,\phi)$ are given by

$$Y_{n,l}(\theta,\phi) = \left[\frac{(2n+1)}{4\pi} \cdot \frac{(n-l)!}{(n+l)!}\right]^{\frac{1}{2}} (-1)^l P_{n,l}(\cos\theta) \cdot e^{jl\phi} \tag{13}$$

where the $P_{n,l}$ denote the associated Legendre polynomials. They form an orthonormal basis on a spherical surface, i.e., they obey the orthogonality relation

$$\int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \sin\theta \,\mathrm{d}\theta \, Y^*_{n',l'}(\theta,\phi) \cdot Y_{n,l}(\theta,\phi) = \delta_{ll'} \cdot \delta_{nn'}. \tag{14}$$

Applying an integration

$$\int_0^{2\pi} \mathrm{d}\bar{\phi} \int_0^{\pi} \sin\bar{\theta} \,\mathrm{d}\bar{\theta} \, Y^*_{n',l'}(\bar{\theta},\bar{\phi}) \tag{15}$$

to both sides of Eq. (12) yields (in conjunction with condition (3))

$$a_{n,l} = \left[h_n^{(1)}(kR)\right]^{-1} \cdot \int_0^{2\pi} \mathrm{d}\bar{\phi} \int_0^{\pi} \sin\bar{\theta} \,\mathrm{d}\bar{\theta} \, f(\bar{\theta},\bar{\phi}) \, Y^*_{n,l}(\bar{\theta},\bar{\phi}). \tag{16}$$

Inserting this result into Eq. (12) provides the solution in any point $\mathbf{x}$ outside the sphere,

$$u(r,\theta,\phi) = \sum_{l,n} \frac{h_n^{(1)}(kr)}{h_n^{(1)}(kR)} \cdot Y_{n,l}(\theta,\phi) \int_0^{2\pi} \mathrm{d}\bar{\phi} \int_0^{\pi} \sin\bar{\theta}\,\mathrm{d}\bar{\theta}\, f(\bar{\theta},\bar{\phi})\, Y_{n,l}^*(\bar{\theta},\bar{\phi}). \tag{17}$$

Interchanging summation and integration, and comparing this expression with Eq. (11) yields for the SGF

$$G_{\partial\Gamma}(R,\bar{\theta},\bar{\phi}/r,\theta,\phi) = \sum_{l,n} \frac{h_n^{(1)}(kr)}{h_n^{(1)}(kR)} \cdot Y_{n,l}(\theta,\phi) \cdot Y_{n,l}^*(\bar{\theta},\bar{\phi}), \tag{18}$$

and we may rewrite Eq. (17) as

$$u(r,\theta,\phi) = \int_0^{2\pi} \mathrm{d}\bar{\phi} \int_0^{\pi} \sin\bar{\theta}\,\mathrm{d}\bar{\theta}\, f(\bar{\theta},\bar{\phi})\, G_{\partial\Gamma}(R,\bar{\theta},\bar{\phi}/r,\theta,\phi). \tag{19}$$

We point out that the coefficients given in Eq. (16) are nothing but the series expansion coefficients of the surface potential f in terms of spherical harmonics when applying a least-squares scheme [16]. The series in Eq. (17), on the other hand, converges uniformly up to the spherical boundary so that the above mentioned interchange of summation and integration is justified. We will return to this aspect in Sec. 3.

2.3. Boundary Integral Equation Methods

In this chapter we will discuss conceptual aspects of two conventional BIE methods, Waterman's null-field approach (also known as the T matrix method) [12, 17] and the approach by Kleinman et al. [13] and Ramm [14]. This will demonstrate how we can use Green's theorem together with the boundary condition on the surface of the bounded domain Γ_- to derive the solution of the exterior BVP in the presence of a non-spherical boundary surface. Even though the final solution scheme is still the same the two approaches essentially differ in what quantities they substitute for ψ and ϕ into Green's theorem.

The null-field approach makes use of the free space Green's function G_0 which solves the inhomogeneous Helmholtz equation

$$(\nabla_{\mathbf{x}}^2 + k^2) G_0(\mathbf{x},\mathbf{x}') = \delta(\mathbf{x},\mathbf{x}') \tag{20}$$

subject to the radiation condition. The point source $\mathbf{x}'$ is assumed to be located in Γ_+. By substituting $\psi = u$ and $\phi = G_0$ into the identity

(7) we obtain in conjunction with the wave equations for u and G_0 and condition (3)

$$\oint_{\partial\Gamma}\left[f(\bar{\mathbf{x}})\frac{\partial G_0(\bar{\mathbf{x}},\mathbf{x})}{\partial\hat{n}_-}-G_0(\bar{\mathbf{x}},\mathbf{x})\frac{\partial u(\bar{\mathbf{x}})}{\partial\hat{n}_-}\right]\mathrm{d}S(\bar{\mathbf{x}})=\begin{cases}u(\mathbf{x}): & \mathbf{x}\in\Gamma_+\\ 0: & \mathbf{x}\in\Gamma_-\end{cases}. \tag{21}$$

Note that the volume integration in Eq. (7) is performed for Γ_+. For historical reasons, many authors refer to the lower branch of this equation as the extended boundary condition (EBC). Other authors avoid the term EBC and prefer to use the term null-field equation (NFE), since a condition usually refers to additional independent equations that are needed to solve Maxwell's equations. For instance, the Maxwell equation

$$\nabla\cdot\mathbf{D}=\rho \tag{22}$$

is only defined in those points in which the vector field $\mathbf{D}$ is differentiable. On boundary surfaces this is usually not the case. Therefore, additional equations that specify the continuity or discontinuity of the tangential and perpendicular components of $\mathbf{D}$ on the boundary surface need to be specified in order to solve Eq. (22). The boundary conditions are therefore additional conditions that are independent of Maxwell's equations in differential form. The NFE, on the other hand, is a consequence of Green's theorem and thus not an independent condition. We will therefore prefer the term NFE instead of EBC for the lower branch of Eq. (21). The NFE essentially establishes a relation between the known surface potential and the directional derivative of the solution on the boundary surface.

A somewhat different relation, at first glance, was derived by Kleinman et al. [13] and Ramm [14]. Let $\{\varphi_\alpha\}_{\alpha=1}^{\infty}$ be a set of radiating solutions of Helmholtz's equation. Substitution of $\psi=u$ and $\phi=\varphi_\alpha$ into Eq. (7) yields

$$\oint_{\partial\Gamma}\left[u(\bar{\mathbf{x}})\frac{\partial\varphi_\alpha(\bar{\mathbf{x}})}{\partial\hat{n}_-}-\varphi_\alpha(\bar{\mathbf{x}})\frac{\partial u(\bar{\mathbf{x}})}{\partial\hat{n}_-}\right]\mathrm{d}S(\bar{\mathbf{x}})=0. \tag{23}$$

With the Dirichlet boundary condition

$$u(\bar{\mathbf{x}})=f(\bar{\mathbf{x}})\quad\text{for}\quad\bar{\mathbf{x}}\in\partial\Gamma \tag{24}$$

we obtain

$$\oint_{\partial\Gamma}\varphi_\alpha(\bar{\mathbf{x}})\frac{\partial u(\bar{\mathbf{x}})}{\partial\hat{n}_-}\,\mathrm{d}\mathbf{S}(\bar{\mathbf{x}})=\oint_{\partial\Gamma}f(\bar{\mathbf{x}})\frac{\partial\varphi_\alpha(\bar{\mathbf{x}})}{\partial\hat{n}_-}\,\mathrm{d}S(\bar{\mathbf{x}}). \tag{25}$$

This equation again establishes a relation between the known surface potential f and the directional derivative of the solution on the boundary surface that needs to be determined.

Before continuing with the discussion of the solution scheme, we will show that there is no difference between the NFE and Eq. (25). For this we have to employ the well known expansion of the free-space Green's function in terms of spherical wave functions, i.e.,

$$G_0(\bar{\mathbf{x}},\mathbf{x}) = \begin{cases} \displaystyle\sum_{j=1}^{\infty} \psi_j(\bar{\mathbf{x}})\,\varphi_j(\mathbf{x}): & \bar{\mathbf{x}} \in \partial\Gamma, \text{ and } \mathbf{x} > \Gamma_+^{sp} \\ \displaystyle\sum_{j=1}^{\infty} \psi_j(\mathbf{x})\,\varphi_j(\bar{\mathbf{x}}): & \bar{\mathbf{x}} \in \partial\Gamma, \text{ and } \mathbf{x} < \Gamma_-^{sp} \end{cases}. \tag{26}$$

The index j is defined in terms of the pair (l,n) (see [13], for instance). φ and ψ denote the radiating and regular wave functions, i.e., the product of the spherical harmonics with the spherical Hankel functions of first kind or the spherical Bessel functions, respectively. This expansion converges uniformly for $\mathbf{x}$ outside Γ_+^{sp} or inside Γ_-^{sp} if the observation point $\bar{\mathbf{x}}$ is on the boundary surface. Γ_+^{sp} denotes the smallest circumscribing and Γ_-^{sp} the largest inscribing sphere of the bounded domain Γ_-. Inserting this expansion into the NFE and interchanging summation and integration yields

$$\sum_{j=1}^{\infty}(A_j - B_j)\psi_j(\mathbf{x}) = 0 \tag{27}$$

with

$$A_j = \oint_{\partial\Gamma} f(\bar{\mathbf{x}}) \frac{\partial\varphi_j(\bar{\mathbf{x}})}{\partial\hat{n}_-}\,\mathrm{d}S(\bar{\mathbf{x}}) \tag{28}$$

and

$$B_j = \oint_{\partial\Gamma} \varphi_j(\bar{\mathbf{x}}) \frac{\partial u(\bar{\mathbf{x}})}{\partial\hat{n}_-}\,\mathrm{d}S(\bar{\mathbf{x}}). \tag{29}$$

From this we can deduce relation (25) since $\{\psi_j\}_{j=1}^{\infty}$ is a set of linearly independent functions for $\mathbf{x}$ on any sphere inside Γ_-^{sp}. Consequently, $(A_j - B_j)$ must become zero for every j. From this result it becomes clear that both approaches are equivalent.

Now, by use of Eq. (25) or the NFE, we are able to determine an approximation of $\partial u/\partial\hat{n}_-$ on the boundary surface. Let's assume that

$\{\xi_\beta\}_{\beta=1}^{\infty}$ is a linearly independent and complete system of functions in $L^2(\partial\Gamma)$. Then, by use of the expansion

$$\frac{\partial u_N}{\partial \hat{n}_-} = \sum_{\beta=1}^{N} c_\beta^{(N)} \xi_\beta \tag{30}$$

as an approximation of $\partial u/\partial \hat{n}_-$ on the boundary surface, we obtain the linear equation system

$$\sum_{\beta=1}^{N} [a]_{\alpha,\beta}\, c_\beta^{(N)} = f_\alpha, \quad \alpha = 1, \ldots, N \tag{31}$$

to determine the unknown expansion coefficients $c_\beta^{(N)}$, with f_α given by

$$f_\alpha = \oint_{\partial\Gamma} f(\bar{\mathbf{x}}) \frac{\partial \varphi_\alpha(\bar{\mathbf{x}})}{\partial \hat{n}_-}\, \mathrm{d}S(\bar{\mathbf{x}}). \tag{32}$$

The matrix elements $[a]_{\alpha,\beta}$ are then given by

$$[a]_{\alpha,\beta} = \oint_{\partial\Gamma} \varphi_\alpha(\bar{\mathbf{x}})\, \xi_\beta(\bar{\mathbf{x}})\, \mathrm{d}\mathbf{S}(\bar{\mathbf{x}}). \tag{33}$$

Inserting this result into the upper branch of Eq. (21) results in an approximation of the solution of the BVP in the exterior domain.

3. THE SURFACE GREEN'S FUNCTION FOR NON-SPHERICAL BOUNDARY SURFACES

3.1. Questions and Answers

There are three questions in the context of the considerations given in the previous chapter which are of general importance not only for the derivation of the SGF but also for every specific realization of the solution schematically discussed above.

Question 1: We assumed $\{\xi_\beta\}_{\beta=1}^{\infty}$ to be a linearly independent and complete system on $\partial\Gamma$. When is this assumption justified?

Question 2: Is there a relation between the BIE method and the SVM?

Question 3: What can we say about the convergence of the finite series given in Eq. (30) and the resulting approximate solution u_N in the exterior domain if the truncation parameter N tends to infinity?

To begin with question 1 we can make the following statement:

Let $\{\varphi_i\}_{i=1}^{\infty}$ and $\{\psi_i\}_{i=1}^{\infty}$ denote the sets of radiating and regular wave functions belonging to the Helmholtz equation. Let's assume that $\partial\Gamma$ is given by a Lyapunov surface (this includes C^2 surfaces, e.g., ellipsoidal or Chebyshev surfaces which are widely used in practical applications). Then $\{\varphi_i\}_{i=1}^{\infty}$ and $\{\partial\varphi_i/\partial\hat{n}\}_{i=1}^{\infty}$ are linearly independent and complete systems in $L^2(\partial\Gamma)$. Furthermore, if k^2 is not an eigenvalue of the interior Dirichlet and Neumann problem then the systems $\{\psi_i\}_{i=1}^{\infty}$ and $\{\partial\psi_i/\partial\hat{n}\}_{i=1}^{\infty}$ are also linearly independent and complete in $L^2(\partial\Gamma)$. Throughout this paper it is assumed that these requirements are fulfilled. The proof of this statement is essentially based on the existence and uniqueness of the solution of the exterior and interior Dirichlet and Neumann problem of Helmhotz's equation which requires certain smoothness assumptions of the boundary surface. More detailed discussions of these aspects can be found, e.g., in Refs. [6, 13, 18, 19].

The second question can be answered with "yes". One result of our discussion in Sec. 2.2 was the fact that the solution could be represented by an infinite series expansion in terms of radiating wave functions, and that this solution depends solely on our ability to find the expansion coefficients of the given potential f on the spherical surface. This was done by applying a least-squares approach. Now, by use of Green's theorem, one can establish a similar relation for non-spherical surfaces, as already demonstrated by Kleinman et al. [13]. We start with an approximation of the surface potential by use of the finite series expansion

$$f_N(\bar{\mathbf{x}}) = \sum_{i=1}^{N} c_i^{(N)} \varphi_i(\bar{\mathbf{x}}). \tag{34}$$

On the other hand, we wish to find an approximate solution of the directional derivative $\partial u/\partial\hat{n}_-$ on the boundary surface in the form of the expansion

$$\frac{\partial u_N(\bar{\mathbf{x}})}{\partial\hat{n}_-} = \sum_{i=1}^{N} d_i^{(N)} \frac{\partial\varphi_i(\bar{\mathbf{x}})}{\partial\hat{n}_-}. \tag{35}$$

The unknown coefficients of this solution will be determined by solving Eq. (25) with f replaced by f_N. Making use of the formula

$$\oint_{\partial\Gamma} \left[\varphi_i(\bar{\mathbf{x}}) \frac{\partial\varphi_j(\bar{\mathbf{x}})}{\partial\hat{n}_-} - \varphi_j(\bar{\mathbf{x}}) \frac{\partial\varphi_i(\bar{\mathbf{x}})}{\partial\hat{n}_-} \right] \mathrm{d}S(\bar{\mathbf{x}}) = 0 \tag{36}$$

(which can simply be obtained from Green's theorem if applied to the two radiating wave functions φ_i and φ_j) results in

$$\sum_{i=1}^{N} \left[c_i^{(N)} - d_i^{(N)}\right] \oint_{\partial\Gamma} \varphi_i(\bar{\mathbf{x}}) \frac{\partial \varphi_j(\bar{\mathbf{x}})}{\partial \hat{n}_-} \mathrm{d}S(\bar{\mathbf{x}}) = 0, \quad \text{for } j = 1, \ldots, N. \tag{37}$$

The statement we made in connection with question 1 implies that each finite matrix of the form

$$\oint_{\partial\Gamma} \varphi_i(\bar{\mathbf{x}}) \frac{\partial \varphi_j(\bar{\mathbf{x}})}{\partial \hat{n}_-} \mathrm{d}S(\bar{\mathbf{x}}), \quad i, j = 1, \ldots, N \tag{38}$$

is invertible [13]. From this we find the relation

$$d_i^{(N)} = c_i^{(N)} \quad \text{for any} \quad i, j = 1, \ldots, N. \tag{39}$$

Making use of this result and inserting the expansions (34) and (35) into the upper branch of Eq. (21) provides

$$u_N(\mathbf{x}) = \sum_{i=1}^{N} c_i^{(N)} \oint_{\partial\Gamma} \left[\varphi_i(\bar{\mathbf{x}}) \frac{\partial G_0(\bar{\mathbf{x}}, \mathbf{x})}{\partial \hat{n}_-} - G_0(\bar{\mathbf{x}}, \mathbf{x}) \frac{\partial \varphi_i(\bar{\mathbf{x}})}{\partial \hat{n}_-}\right] \mathrm{d}S(\bar{\mathbf{x}}), \quad \mathbf{x} \in \Gamma_+. \tag{40}$$

The surface integral in Eq. (40) is nothing but the radiating wave function φ_i, as can be seen by substituting $\psi = \varphi_i$ and $\phi = G_0$ into Green's theorem. Thus we finally obtain

$$u_N(\mathbf{x}) = \sum_{i=1}^{N} c_i^{(N)} \varphi_i(\mathbf{x}), \quad \mathbf{x} \in \Gamma_+. \tag{41}$$

This establishes the equality of the expansion coefficients of the approximate solution u_N in the exterior domain and those of the approximation of the surface potential f given in Eq. (34). On the other hand, this equality is the very essence of the SVM. Thus we are able to deduce the SVM *ansatz* from the BIE approach. Furthermore, this result refutes Waterman's assumption that a representation of the solution according to Eq. (41) is not appropriate to satisfy the boundary condition on the boundary surface [17].

Next, we will discuss question 3 which concerns the convergence behaviour of our approximate solution. There is some confusion about

this aspect in the literature, as already stated by Millar [6], and, more recently, by Dallas [20]. One origin of this confusion is the fact that convergence issues pertaining to the expansion of the approximate solution u_N in the exterior domain are often mixed up with convergence issues related to the expansion of the free-space Green's function given in Eq. (26). We emphasize that the derivation given above demonstrates that the free-space Green's function is not really needed for obtaining an approximate solution in terms of a finite series. In contrast to our approach Waterman employed the expansion of the free-space Green's function to represent the solution by a formal infinite series in the domain exterior to the circumscribed sphere. In this domain this formal infinite series converges uniformly. But this convergence should not be confused with the convergence behaviour of the approximate solution for which one has to truncate the formal infinite series. Dallas recently presented a proof for the least-squares convergence of the far-field pattern in Waterman's special T matrix scheme [20]. This proof was restricted to ellipsoidal surfaces. Beyond the far-field case and the special surface geometry considered by Dallas no proofs concerning the convergence behaviour of Waterman's approximate solution exist. This holds in particular in the near-field zone for the region outside Γ_+^{sp}. Another source of confusion is the term "T matrix method". Very often this designation is used in reference to Waterman's approach alone. However, there are a variety of different solution methods which can be represented by use of a transition matrix, as demonstrated, e.g., in Ref. [21]. Now, to answer question 3, we can make the following statement: If the coefficients in Eq. (34) are determined in a least-squares sense uniform convergence of Eq. (41) in Γ_+ for $N \to \infty$ is guaranteed no matter whether Rayleigh's hypothesis is fulfilled or not. The proof of this statement has been known for several years (see, e.g., Refs. [6, 19]). The derivation of the SGF we will present in the next section is performed in this least-squares sense.

In the next section we explicitly write down the least-squares approximation of an analytic function on $\partial\Gamma$ and derive the corresponding SGF of the exterior BVP if a complete and linearly independent (but not necessarily orthogonal) system of functions is given. These considerations are completed by establishing a relation between a T matrix and the SGF.

3.2. General Least-Squares Approach and the Corresponding Surface Green's Function

Let f be an analytic and in general complex-valued function given on the surface $\partial\Gamma$. $\{\varphi_i\}_{i=1}^{\infty}$ is assumed to be a linearly independent and

complete system of functions in $L^2(\partial\Gamma)$. We will approximate f by the finite series

$$f_N(\bar{\mathbf{x}}) = \sum_{i=1}^{N} c_i^{(N)} \varphi_i(\bar{\mathbf{x}}). \tag{42}$$

The expansion coefficients should be determined such that the mean square error

$$M = \|f - f_N\|_{2,\partial\Gamma}^2 = \left\langle f - \sum_{i=1}^{N} c_i^{(N)} \varphi_i \,\middle|\, f - \sum_{i=1}^{N} c_i^{(N)} \varphi_i \right\rangle \tag{43}$$

is minimized, i.e., the relation

$$\frac{\partial M}{\partial c_i^{(N)}} = 0 \tag{44}$$

holds for every $i = 1, \ldots, N$. The scalar product in Eq. (43) is given by

$$\langle g \mid f \rangle = \oint_{\partial\Gamma} f(\bar{\mathbf{x}}) \cdot g^*(\bar{\mathbf{x}}) \mathrm{d}S(\bar{\mathbf{x}}). \tag{45}$$

Eq. (43) can be rewritten as

$$\begin{aligned} M = &\langle f \mid f \rangle - \sum_{i=1}^{N} c_i^{(N)} \langle f \mid \varphi_i \rangle - \sum_{i=1}^{N} \left(c_i^{(N)}\right)^* \langle \varphi_i \mid f \rangle \\ &+ \sum_{i=1}^{N} \sum_{j=1}^{N} \left(c_i^{(N)}\right)^* c_j^{(N)} \langle \varphi_i \mid \varphi_j \rangle. \end{aligned} \tag{46}$$

When applying Eq. (44) to this expression, and taking the conjugate-complex of it, we obtain the linear equation system

$$\sum_{i=1}^{N} c_i^{(N)} \cdot \langle \varphi_j \mid \varphi_i \rangle = \langle \varphi_j \mid f \rangle, \quad j = 1, \ldots, N \tag{47}$$

with

$$\langle \varphi_j \mid f \rangle = \oint_{\partial\Gamma} f(\bar{\mathbf{x}}) \cdot \varphi_j^*(\bar{\mathbf{x}}) \, \mathrm{d}S(\bar{\mathbf{x}}) \tag{48}$$

and the coefficient matrix $\mathbf{A}_{\partial\Gamma}$ with elements given by

$$[A_{\partial\Gamma}]_{j,i} = \langle \varphi_j \mid \varphi_i \rangle = \oint_{\partial\Gamma} \varphi_i(\bar{\mathbf{x}}) \cdot \varphi_j^*(\bar{\mathbf{x}}) \, \mathrm{d}S(\bar{\mathbf{x}}). \tag{49}$$

From Eq. (47) we can determine the expansion coefficients $c_i^{(N)}$. Obviously, this equation system can also be derived by multiplying the expansion of the surface potential given in Eq. (42) with φ_j^* and subsequently integrating over $\partial\Gamma$. For Lyapunov surfaces the matrix $\langle \varphi_j \mid \varphi_i \rangle$ can be inverted for any fixed N, as proven, e.g., by Kleinman et al. [13]. On the other hand, if we look at the limiting case of a spherical surface, this matrix becomes diagonal and we obtain the result already discussed in Sec. 2.2. In this particular case of a spherical boundary surface the expansion coefficients do not depend on the truncation parameter N, i.e., they fulfil Sommerfeld's requirement of finality [16]. Mathematically speaking we say that in this case $\{\varphi_i\}_{i=1}^{\infty}$ form a Schauder basis.

To proceed with the derivation of the SGF we formally invert the linear equation system given in Eq. (47),

$$c_i^{(N)} = \sum_{j=1}^{N} \left[A_{\partial\Gamma}^{-1}\right]_{i,j} \cdot \langle \varphi_j \mid f \rangle, \tag{50}$$

where $\mathbf{A}_{\partial\Gamma}^{-1}$ denotes the inverse of $\langle \varphi_j \mid \varphi_i \rangle$. Inserting Eq. (50) into Eq. (41) and using Eq. (48) we finally obtain

$$u_N(\mathbf{x}) = \oint_{\partial\Gamma} f(\bar{\mathbf{x}}) G_{\partial\Gamma}^N(\bar{\mathbf{x}}, \mathbf{x}) \, \mathrm{d}S(\bar{\mathbf{x}}) \tag{51}$$

with the approximation of the SGF given by

$$G_{\partial\Gamma}^N(\bar{\mathbf{x}}, \mathbf{x}) = \sum_{i=1}^{N} \sum_{j=1}^{N} \left[A_{\partial\Gamma}^{-1}\right]_{i,j} \cdot \varphi_j^*(\bar{\mathbf{x}}) \varphi_i(\mathbf{x}). \tag{52}$$

It can be proven that this SGF converges at least weakly against the exact one, as shown in the appendix.

We now wish to establish a relation between the derived SGF and a general T matrix, including Waterman's special approach. For this we have to insert again the expansion given in Eq. (41) into the left hand side of Eq. (51). After multiplication with φ_α^* and integration over Γ_+^{sp} we obtain

$$c_\alpha^{(N)} = \frac{1}{h_\alpha} \cdot \oint_{\partial\Gamma} \oint_{\Gamma_+^{sp}} f(\bar{\mathbf{x}}) G_{\partial\Gamma}^N(\bar{\mathbf{x}}, \mathbf{x}) \varphi_\alpha^*(\mathbf{x}) \, \mathrm{d}S(\mathbf{x}) \, \mathrm{d}S(\bar{\mathbf{x}}), \tag{53}$$

where h_α is a normalization constant that ensures that

$$\frac{1}{h_\alpha} \cdot \oint_{\Gamma_+^{sp}} \varphi_\alpha(\mathbf{x}) \cdot \varphi_\alpha^*(\mathbf{x}) \, \mathrm{d}S(\mathbf{x}) = 1, \tag{54}$$

and $\alpha = 1, \ldots, N$. Next we substitute the approximation of the surface potential

$$f_N(\bar{\mathbf{x}}) = \sum_{\beta=1}^{N} d_\beta^{(N)} \xi_\beta(\bar{\mathbf{x}}) \tag{55}$$

into Eq. (53). This results in the linear relation

$$c_\alpha^{(N)} = \sum_{\beta=1}^{N} \left\{ \frac{1}{h_\alpha} \cdot \oint_{\partial\Gamma} \oint_{\Gamma_+^{sp}} \xi_\beta(\bar{\mathbf{x}}) G_{\partial\Gamma}^N(\bar{\mathbf{x}}, \mathbf{x}) \varphi_\alpha^*(\mathbf{x}) \, \mathrm{d}S(\mathbf{x}) \, \mathrm{d}S(\bar{\mathbf{x}}) \right\} \cdot d_\beta^{(N)} \tag{56}$$

between the expansion coefficients of the solution in the exterior domain and the surface potential, as known from the T matrix approach. Therefore, with $\mathbf{c}^{(N)} = \left[c_1^{(N)}, \ldots, c_N^{(N)}\right]^t$ and $\mathbf{d}^{(N)} = \left[d_1^{(N)}, \ldots, d_N^{(N)}\right]^t$ we can rewrite Eq. (56) as

$$\mathbf{c}^{(N)} = \mathbf{T} \cdot \mathbf{d}^{(N)}, \tag{57}$$

where the elements of this general T matrix are given by

$$[T]_{\alpha,\beta} = \frac{1}{h_\alpha} \cdot \oint_{\partial\Gamma} \oint_{\Gamma_+^{sp}} \xi_\beta(\bar{\mathbf{x}}) G_{\partial\Gamma}^N(\bar{\mathbf{x}}, \mathbf{x}) \varphi_\alpha^*(\mathbf{x}) \, \mathrm{d}S(\mathbf{x}) \, \mathrm{d}S(\bar{\mathbf{x}}). \tag{58}$$

From this we can easily derive Waterman's special T matrix. If ξ_β is replaced by the set of regular wave functions ψ_β, and using Eq. (52) we obtain

$$c_\alpha^{(N)} = \sum_{j=1}^{N} \sum_{\beta=1}^{N} \left[A_{\partial\Gamma}^{-1}\right]_{\alpha,j} \oint_{\partial\Gamma} \psi_\beta(\bar{\mathbf{x}}) \varphi_j^*(\bar{\mathbf{x}}) \, \mathrm{d}S(\bar{\mathbf{x}}) \cdot d_\beta^{(N)}. \tag{59}$$

If we introduce the matrix $\mathbf{B}_{\partial\Gamma}$ with elements

$$[B_{\partial\Gamma}]_{j,\beta} = \oint_{\partial\Gamma} \psi_\beta(\bar{\mathbf{x}}) \varphi_j^*(\bar{\mathbf{x}}) \, \mathrm{d}S(\bar{\mathbf{x}}), \tag{60}$$

then we can rewrite Eq. (59) into

$$\mathbf{c}^{(N)} = \mathbf{A}_{\partial\Gamma}^{-1} \mathbf{B}_{\partial\Gamma} \cdot \mathbf{d}^{(N)}, \tag{61}$$

where $\mathbf{A}_{\partial\Gamma}^{-1}$ corresponds to $\mathbf{Q}^{-1}$, and $\mathbf{B}_{\partial\Gamma}$ to $\mathbf{ReQ}$ in Waterman's notation, respectively (see, e.g., Ref. [13]). We emphasize once more that Waterman's approach is not a least-squares approach.

3.3. The Surface Green's Function in Spherical Coordinates

To prepare the discussion of the symmetry properties in Sec. 5 we want to write down explicitly the expression for the SGF in spherical coordinates in the presence of a non-spherical and in general non-axisymmetric boundary surface. Assuming that the boundary surface has the parametric representation $R = R(\bar{\theta}, \bar{\phi})$ the scalar product defined in Eq. (45) reads

$$\langle g \mid f \rangle = \int_0^{2\pi} \int_0^{\pi} f(\bar{\boldsymbol{\theta}}, \bar{\phi}) \cdot g^*(\bar{\boldsymbol{\theta}}, \bar{\phi}) \sin(\bar{\theta}) \, \mathrm{d}\bar{\boldsymbol{\theta}} \, \mathrm{d}\bar{\boldsymbol{\phi}}. \tag{62}$$

The regular and radiating wave functions on this surface are given by

$$\psi_{n,l}(R, \bar{\boldsymbol{\theta}}, \bar{\boldsymbol{\phi}}) = j_n[kR(\bar{\boldsymbol{\theta}}, \bar{\boldsymbol{\phi}})] \cdot Y_{n,l}(\bar{\boldsymbol{\theta}}, \bar{\boldsymbol{\phi}}) \tag{63}$$

and

$$\varphi_{n,l}(R, \bar{\boldsymbol{\theta}}, \bar{\boldsymbol{\phi}}) = h_n^{(1)}[kR(\bar{\boldsymbol{\theta}}, \bar{\boldsymbol{\phi}})] \cdot Y_{n,l}(\bar{\boldsymbol{\theta}}, \bar{\boldsymbol{\phi}}) \tag{64}$$

respectively, with $n = 1, 2, \ldots,$ and $l = 0, \pm 1, \ldots, \pm n$. Under the assumptions discussed earlier they form a set of linearly independent and complete functions on $\partial\Gamma$. The approximation of the surface potential is represented by the finite series

$$f_N(\bar{\boldsymbol{\theta}}, \bar{\boldsymbol{\phi}}) = \sum_{n,l} c_{l,n}^{(L\mathrm{cut}, N\mathrm{cut})} \cdot \varphi_{n,l}(R, \bar{\boldsymbol{\theta}}, \bar{\boldsymbol{\phi}}). \tag{65}$$

Note that we have introduced the two convergence parameters $N\mathrm{cut}$ and $L\mathrm{cut}$. For this, the series expansion must be reorganised such that

$$\begin{aligned} l &= 0, \pm 1, \ldots, \pm L\mathrm{cut} \\ n &= |l|, |l| + 1, \ldots, |l| + N\mathrm{cut}. \end{aligned} \tag{66}$$

l is chosen to be the outer summation index, and independent of the summation index n. This is of some advantage for the numerical realization of the solution scheme especially if the boundary surface exhibits a certain symmetry. For the approximate solution of Helmholtz's equation in the exterior domain we obtain

$$u_N(r, \theta, \phi) = \int_0^{2\pi} \mathrm{d}\bar{\phi} \int_0^{\pi} \sin\bar{\theta} \, \mathrm{d}\bar{\theta} G_{\partial\Gamma}^{N\mathrm{cut}, L\mathrm{cut}}(R, \bar{\theta}, \bar{\phi}/r, \theta, \phi) \cdot f(\bar{\theta}, \bar{\phi}) \tag{67}$$

where

$$G_{\partial\Gamma}^{N\mathrm{cut}, L\mathrm{cut}}(R, \bar{\theta}, \bar{\phi}/r, \theta, \phi) = \sum_{l,l',n,n'} \left[A_{\partial\Gamma}^{-1}\right]_{l,l',n,n'} \varphi_{n',l'}^*(R, \bar{\boldsymbol{\theta}}, \bar{\boldsymbol{\phi}}) \cdot \varphi_{n,l}(r, \boldsymbol{\theta}, \phi) \tag{68}$$

being the SGF in spherical coordinates.

4. DERIVATION OF THE SURFACE GREEN'S FUNCTION BY USE OF THE METHOD OF LINES

In this section we will demonstrate how we can derive the SGF by use of a special FD technique, the so-called Method of Lines (MoL). A detailed description of the MoL and its application to separable and non-separable BVP's can be found, e.g., in Refs. [1, 22]. For simplicity we restrict the following considerations to axisymmetric boundary surfaces. In this case the MoL applies only a discretization scheme to the θ-dependent part of Eq. (1), but not to the r-dependent part. (For non-axisymmetric particles, both the polar and azimuthal coordinates would discretized.) The fact that the radial coordinate is not discretized allows us to analytically take the non-local radiation condition into account. This differs fundamentally from conventional FD techniques which apply a discretization procedure to all spatial coordinates, and, therefore, have to approximate the radiation condition by local absorbing boundaries.

In contrast to the methods which approximate the unknown solution u in terms of a series expansion (as it happens in the SVM and BIE approaches discussed in the previous chapters) the MoL has been considered to be a method which approximates the differential operator of the Helmholtz equation. As a consequence it has been assumed that the relative convergence phenomenon, which appears in the other methods due to the necessary series truncation, does not occur in the MoL [22]. In Ref. [4] it was shown that this point of view is not correct, and that the primary approximation of the differential operator within the MoL can be reformulated into a finite series expansion of the unknown solution, thus establishing the mathematical basis for the derivation of the SGF in a least-squares scheme. On the other hand, the MoL in its original formulation is equivalent to the conventional point matching technique which suffers from the problems associated with Rayleigh's hypothesis.

At the end of this section we will discuss the nature of the MoL in more detail. The behaviour of the MoL for an increasing number of discretization lines reveals the strong similarity between the MoL and the SVM. This allows us to draw general conclusions about the kind of problems in which we can benefit from an application of the MoL.

4.1. The Discretization Procedure for Axisymmetric Boundary Surfaces

Each solution of the BVP in spherical coordinates is 2π-periodic with respect to the ϕ-dependency. Thus, expanding the solution in a Fourier

series according to

$$u(r,\theta,\phi) = \sum_l \tilde{U}^{(l)}(r,\theta) e^{jl\phi} \tag{69}$$

we obtain from Eq. (1)

$$\begin{aligned} \tilde{\nabla}^2 \tilde{U}^{(l)} + k^2 r^2 \tilde{U}^{(l)} &= 0 \\ \tilde{\nabla}^2 &= r\frac{\partial^2}{\partial r^2} r + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} - \frac{l^2}{\sin^2\theta}. \end{aligned} \tag{70}$$

Furthermore, depending on the azimuthal mode l, the homogeneous Neumann and Dirichlet conditions

$$\frac{d\tilde{U}}{\partial\theta} = 0 \quad \text{for} \quad l = 0 \tag{71}$$

and

$$\tilde{U} = 0 \quad \text{for} \quad l \neq 0 \tag{72}$$

must be taken into account for $\theta = 0$ and $\theta = \pi$. To solve Eq. (70) we replace all derivatives with respect to θ by an equidistant discretization procedure in the interval $[0, \pi]$ where we have to distinguish between the two cases $l = 0$ and $l \neq 0$. In so doing, the homogeneous Neumann condition can only be fulfilled approximately, whereas the homogeneous Dirichlet condition can be reproduced exactly. The two different discretization schemes are depicted in Fig. 2. They result in two systems of coupled ordinary differential equations for the radial dependent part of the solution given by

$$\left\{ h_\theta^2 \left[r\frac{d^2}{dr^2} r + k^2 r^2 \right] \cdot \mathbf{E} - \mathbf{P}_z^{(0,l)} \right\} \cdot \left| \tilde{U}^{(0,l)} \right\rangle = 0. \tag{73}$$

$\mathbf{E}$ and h_θ denote the unit dyad and the equidistant discretization angle, and the N_d-dimensional "ket"-vector

$$\left| \tilde{U}^{(0,l)} \right\rangle = \left[\tilde{U}^{(0,l)}(r,\theta_1), \ldots, \tilde{U}^{(0,l)}(r,\theta_{Nd},) \right]^t = \left(\tilde{U}_1^{(0,l)}, \ldots, \tilde{U}_{Nd}^{(0,l)} \right)^t \tag{74}$$

is the transpose of the vector containing the radially dependent components $\tilde{U}(\mathbf{r})$ of the sought solution defined on each discretization line. The coupling is expressed by the two tridiagonal matrices $\mathbf{P}_z^{(0)}$ and $\mathbf{P}_z^{(l)}$ for which we have

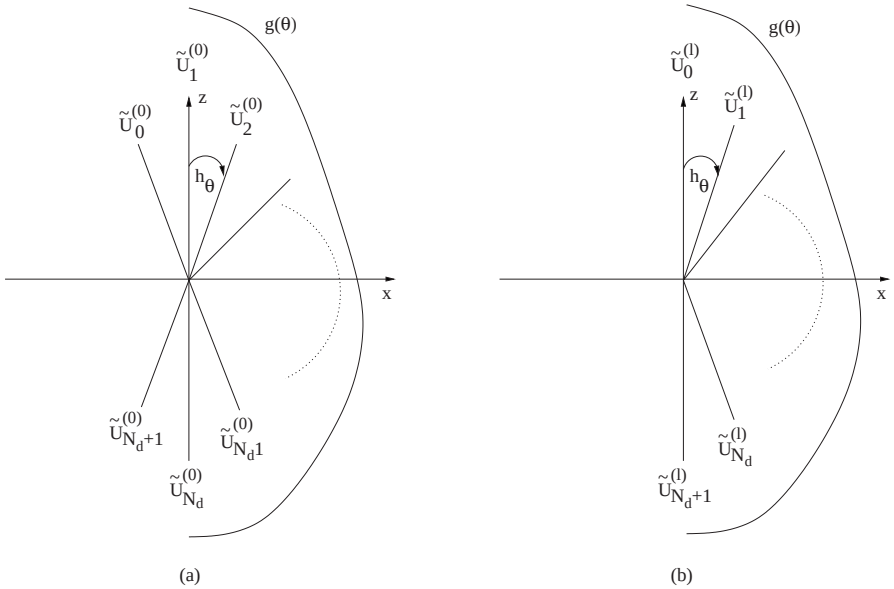

Figure 2. Equidistant discretization scheme with respect to the θ-coordinate for (a) homogeneous Neumann and (b) homogeneous Dirichlet conditions in $\theta = 0, \pi$. N_d denotes the number of discretization lines used in the interval $[0, \pi]$. $g(\theta)$ is the arbitrary but star-shaped surface somewhere in Γ_+ on which we want to solve the exterior BVP.

$$\mathbf{P}_z^{(0)} = \begin{pmatrix} 2 & -2 & 0 & 0 & \cdots & \cdots & 0 \\ -1 & (2+\kappa_2) & -(1+\kappa_2) & 0 & 0 & \cdots & 0 \\ 0 & -1 & (2+\kappa_3) & -(1+\kappa_3) & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \cdots & 0 & -1 & (2+\kappa_{Nd-1}) & -(1+\kappa_{Nd-1}) \\ 0 & \cdots & \cdots & \cdots & 0 & -2 & 2 \end{pmatrix} \tag{75}$$

and

$$\mathbf{P}_z^{(l)} = \begin{pmatrix} (2+\kappa_1+\gamma_1) & -(1+\kappa_1) & 0 & 0 & \cdots & \cdots & 0 \\ -1 & (2+\kappa_2+\gamma_2) & -(1+\kappa_2) & 0 & 0 & \cdots & 0 \\ 0 & -1 & (2+\kappa_3+\gamma_3) & -(1+\kappa_3) & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & -1 & (2+\kappa_{Nd-1}+\gamma_{Nd-1}) & -(1+\kappa_{Nd-1}) \\ 0 & 0 & \cdots & \cdots & 0 & -1 & (2+\kappa_{Nd}+\gamma_{Nd}) \end{pmatrix} \tag{76}$$

with

$$\gamma_i = \frac{h_\theta^2 l^2}{\sin^2 \theta_i} \tag{77}$$

$$\kappa_i = h_\theta \cdot \cot \theta_i. \tag{78}$$

The subindex i is running from $1, \ldots, N_d$. In what follows both cases are summarized in the common superindex (l). Obviously, we are operating from the beginning in a finite-dimensional vector space where the number of discretization lines becomes an additional convergence parameter.

The objective is to solve the system of coupled ordinary differential equations given by Eq. (73).

4.2. Representation of the Solution

The crucial step of the MoL consist in the diagonalization of the matrices $\mathbf{P}_z^{(0)}$ and $\mathbf{P}_z^{(l)}$, thus achieving a decoupling of the system (73). First we have to transform these matrices into symmetric ones by performing a similarity transformation. This can always be done for matrices of

the structure

$$\mathbf{P}^{(l)}_{nonsym.} = \begin{pmatrix} \alpha_1 & -\beta_2 & 0 & 0 & \cdots & \cdots & 0 \\ -\gamma_2 & \alpha_2 & -\beta_3 & 0 & 0 & \cdots & 0 \\ 0 & -\gamma_3 & \alpha_3 & -\beta_4 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \cdots & 0 & -\gamma_{Nd-1} & \alpha_{Nd-1} & -\beta_{Nd} \\ 0 & \cdots & \cdots & \cdots & 0 & -\gamma_{Nd} & \alpha_{Nd} \end{pmatrix} \tag{79}$$

with α_i being a real number and $\gamma_i \cdot \beta_i > 0$. These properties apply to the matrices given in Eqs. (75) and (76). The similarity transformation is then given by

$$\mathbf{P}^{(l)}_{sym.} = \mathbf{Z}^{(l)^{-1}} \cdot \mathbf{P}^{(l)}_{nonsym.} \cdot \mathbf{Z}^{(l)}, \tag{80}$$

where

$$\left[z^{(l)}\right]_{1,1} = 1 \quad \text{and} \quad \left[z^{(l)}\right]_{i,i} = \left(\frac{\gamma_2 \cdots \gamma_i}{\beta_2 \cdots \beta_i}\right)^{1/2} \tag{81}$$

are the elements of the diagonal matrices $\mathbf{Z}^{(l)}$ (see, e.g., Ref. [23]). Next we have to solve the eigenvalue problem

$$\left(\mathbf{P}^{(l)}_{z_{sym.}} - \lambda_i^{(l)} \cdot \mathbf{E}\right) \cdot \left|x_i^{(l)}\right\rangle = |0\rangle \tag{82}$$

to determine the orthogonal transformation matrix $\mathbf{T}^{(l)}$. Its columns are formed by the eigenvectors denoted with $\left|x_i^{(l)}\right\rangle$. $\lambda_i^{(l)}$ are the corresponding eigenvalues. Note that in spherical coordinates we can find the solution only numerically. Once we have calculated these quantities (which is numerically straightforward, as discussed in Ref. [1]) we are able to decouple the system of ordinary differential equations given above by introducing the transformed solution

$$|\hat{U}^{(l)}\rangle = \mathbf{Tr}^{(l)^{-1}} \cdot |\tilde{U}^{(l)}\rangle. \tag{83}$$

The transformation matrices and their inverse are given by

$$\mathbf{Tr}^{(l)} = \mathbf{Z}^{(l)} \cdot \mathbf{T}^{(l)} \tag{84}$$

$$\mathbf{Tr}^{(l)^{-1}} = \mathbf{T}^{(l)^{-1}} \cdot \mathbf{Z}^{(l)^{-1}}, \tag{85}$$

For these matrices the relation

$$\mathbf{Tr}^{(l)^{-1}} \cdot \mathbf{Tr}^{(l)} = \mathbf{E} \tag{86}$$

holds. If we use the additional substitution $\rho = k \cdot r$ and $\hat{U}_i^{(l)} = \frac{1}{\sqrt{\rho}} \cdot B_i^{(l)}$ we finally obtain Bessel's differential equation for each of the radially dependent component of the transformed solution,

$$\frac{d^2 B_i^{(l)}(\rho)}{d\rho^2} + \frac{1}{\rho} \cdot \frac{dB_i^{(l)}(\rho)}{d\rho} + \left[1 - \frac{\nu_i^{(l)^2}}{\rho^2}\right] \cdot B_i^{(l)}(\rho) = 0, \tag{87}$$

with

$$\nu_i^{(l)^2} = \frac{\lambda_i^{(l)}}{h_\theta^2} + \frac{1}{4}. \tag{88}$$

This equation allows us to incorporate the radiation condition at infinity analytically. In so doing we get the following general solution in the transformed domain:

$$\hat{U}_i^{(l)}(\rho) = c_{l,i}^{(N_d)} \cdot \frac{H^{(1)}_{\nu_i^{(l)}}(\rho)}{\sqrt{\rho}}. \tag{89}$$

$H^{(1)}_{\nu_i^{(l)}}$ denotes the Hankel functions of the first kind. Their orders are related to the eigenvalues $\lambda_i^{(l)}$ according to Eq. (88). The exact fulfillment of the radiation condition at infinity is the main advantage of the MoL in comparison to conventional FD-methods. The latter apply an additional discretization scheme with respect to the radial coordinate to solve Eq. (87). This is only possible in a finite volume. Therefore, local absorbing boundaries must be introduced. Both the additional discretization and the absorbing boundaries result in an additional approximation of the radial part of the solution. However, the general representation of the solution we want to derive now is the same in both the MoL and the conventional FD-methods.

Since we are interested in solving the BVP in the original domain we have to invert Eq. (83), i.e., we have to calculate

$$\left|\tilde{U}^{(l)}\right\rangle = \mathbf{Tr}^{(l)} \cdot \left|\hat{U}^{(l)}\right\rangle. \tag{90}$$

Finally, using the boundary condition given in Eq. (3), we obtain an $N_d \times N_d$ system of equations from which we can determine the N_d unknown coefficients $c_{l,i}^{(N_d)}$. This conventional way for applying the MoL is equivalent to the point-matching technique. However, an inspection of the inversion shows that Eq. (90) can be reformulated as an expansion in terms of the eigenvectors $\left|x_i^{(l)}\right\rangle$, which we obtained

as the solutions of the eigenvalue problem in Eq. (82) (see Ref. [1]). Combining Eqs. (69), (89), and (90) we can therefore represent the general solution at the N_d discrete points along an arbitrary but star-shaped surface $r = g(\theta)$ lying in Γ_+ (i.e., in the intersections of the discretization lines with $g(\theta)$, see Fig. 2) as

$$|u(\phi)\rangle = \sum_{l=-i}^{i} \sum_{i=1}^{N_d} c_{l,i}^{(N_d)} \cdot e^{jl\phi} \cdot \left[\tilde{U}^{(l)}\right]_{i,i} \cdot \left|x_i^{(l)}\right\rangle, \tag{91}$$

with $\tilde{\mathbf{U}}^{(l)}$ being a diagonal matrix of the form

$$\left[\tilde{U}^{(l)}\right]_{i,i} = \mathrm{diag}\left\{ \frac{H_{\nu_i^{(l)}}^{(1)}(g_i)}{\sqrt{g_i}} \right\}, \quad i = 1, \ldots, N_d. \tag{92}$$

The radially dependent arguments are given by

$$g_i = k \cdot g(\theta_i). \tag{93}$$

Since the product of this diagonal matrix with the eigenvector given in Eq. (91) provides a new vector we can rewrite this equation as

$$|u(\phi)\rangle = \sum_{l,i} c_{l,i}^{(N_d)} \cdot \left|\tilde{x}_i^{(l)}(\phi)\right\rangle_g \tag{94}$$

where

$$\left|\tilde{x}_i^{(l)}(\phi)\right\rangle_g = e^{jl\phi} \cdot \tilde{\mathbf{U}}_i^{(l)} \cdot \left|x_i^{(l)}\right\rangle \tag{95}$$

There are two different elements in this representation that depend on the number of discretization lines N_d. One is the N_d-dimensional vector $\left|\tilde{x}_i^{(l)}(\phi)\right\rangle_g$, and the other is the number of expansion terms. One may ask if it is really necessary to consider all of the N_d expansion terms. It has been shown in Ref. [1] that in practical calculations the number of expansion terms can always be chosen much smaller than N_d. Therefore we introduce an additional convergence parameter $N\mathrm{cut}$ with $1 \leq N\mathrm{cut} \leq N_d$ which denotes the number of expansion terms used. Thus, instead of Eq. (94), we write

$$|u(\phi)\rangle = \sum_{l,i} c_{l,i}^{(L\mathrm{cut},N\mathrm{cut})} \cdot \left|\tilde{x}_i^{(l)}(\phi)\right\rangle_g. \tag{96}$$

Note, however, that the number of components of the expansion vectors is still N_d. Note also that the rearrangement has been performed according to Eq. (66) where we have to ensure now that the relation

$|l|+N\text{cut} \leq N_d$ holds. Eq. (96) demonstrates that the original approximation of the operator in the Helmholtz equation can be reformulated as an approximation of the sought solution. It also reveals the strong similarity of the MoL and the SVM. This allows us to derive a SGF within the framework of the MoL.

4.3. Representation of the Surface Green's Function

We already discussed in Sec. 3.2 that the expansion coefficients in Eq. (96) are determined by approximating the given surface potential $f(\bar{\theta}, \bar{\phi})$ on the boundary surface $R = R(\bar{\theta})$ in a least-squares sense. Therefore, starting from the expansion

$$|f_{N_d}(\bar{\phi})\rangle = \sum_{l,i} c_{l,i}^{(L\text{cut},N\text{cut})} \cdot |\tilde{x}_i^{(l)}(\bar{\phi})\rangle_R, \tag{97}$$

where $|f_{N_d}(\bar{\phi})\rangle = [f(\bar{\theta}_1, \bar{\phi}), \ldots, f(\bar{\theta}_{N_d}, \bar{\phi})]^t$ denotes the approximation of the surface potential in the N_d intersections of the discretization lines with the boundary surface $R(\bar{\theta})$, we obtain after scalar multiplication from the left with ${}_R\langle \tilde{x}_{i'}^{(l)}(\bar{\phi})|$

$$\langle \tilde{x}_{i'}^{(l)} | f_{N_d} \rangle_R = \sum_{l,i} \langle \tilde{x}_{i'}^{(l)} | \tilde{x}_i^{(l)} \rangle_R \cdot c_{l,i}^{(L\text{cut},N\text{cut})}. \tag{98}$$

The matrix elements of $\mathbf{A}_R$ on the right hand side of Eq. (98) are now defined by

$$\left[A_R\right]_{l,i,i'} = \langle \tilde{x}_{i'}^{(l)} | \tilde{x}_i^{(l)} \rangle_R = 2\pi \cdot \langle \tilde{x}_{i'}^{(l)} | \tilde{x}_i^{(l)} \rangle_{l_2}. \tag{99}$$

For the inhomogeneity on the left hand side of Eq. (98) we have

$$\langle \tilde{x}_{i'}^{(l)} | f_{N_d} \rangle_R = \int_0^{2\pi} e^{-jl\bar{\phi}} \cdot \langle \tilde{x}_{i'}^{(l)} | f_{N_d}(\cdot) \rangle_{l_2} \, \mathrm{d}\bar{\phi} \tag{100}$$

with $\langle \tilde{x}_{i'}^{(l)} | \tilde{x}_i^{(l)} \rangle_{l_2}$ and $\langle \tilde{x}_{i'}^{(l)} | f_{N_d}(\cdot) \rangle_{l_2}$ being the conventional algebraic scalar products of the corresponding N_d-component vectors. Formal inversion of Eq. (98) results in

$$c_{l,i}^{(L\text{cut},N\text{cut})} = \sum_{i'} \left[A_R^{-1}\right]_{l,i,i'} \cdot \langle \tilde{x}_{i'}^{(l)} | f_{N_d} \rangle_R. \tag{101}$$

Inserting these coefficients into Eq. (96) we arrive at the following representation of the approximate solution $|u\rangle$ on the star-shaped surface $g(\theta)$ in the exterior domain Γ_+:

$$|u(\phi)\rangle = \mathbf{G}_R^{(MoL)}(\phi/\bar{\phi}) \cdot |f_{N_d}(\bar{\phi})\rangle, \tag{102}$$

where the SGF is given by

$$\mathbf{G}_R^{(MoL)}(\phi/\bar{\phi}) = \sum_{l,i,i'} \left[A_R^{-1}\right]_{l,i,i'} \cdot \left|\tilde{x}_i^{(l)}(\phi)\right\rangle_g \cdot {}_R\left\langle \tilde{x}_{i'}^{(l)}(\bar{\phi})\right|. \tag{103}$$

Note that $\left|\tilde{x}_i^{(l)}(\phi)\right\rangle_g \cdot {}_R\left\langle \tilde{x}_{i'}^{(l)}(\bar{\phi})\right|$ is the dyadic product of the two vectors $\left|\tilde{x}_i^{(l)}(\phi)\right\rangle_g$ and $\left|\tilde{x}_{i'}^{(l)}(\bar{\phi})\right\rangle_R$.

With Eqs. (102) and (103) we have derived a representation of the approximate solution within the MoL which is equivalent to that of the BIE or SVM approaches given in Eqs. (67) and (68), and which benefits from the decoupling of the surface potential from the geometrical properties of the bounded domain Γ_- according to Eq. (11). We want to emphasize here that the same holds for the conventional FD methods in spherical coordinates if the additional approximation of the radial dependent solution is taken into account.

4.4. The Limiting Behaviour of the Surface Green's Function for an Infinite Number of Discretization Lines

If we compare the representation of the SGF in the SVM and in the MoL, i.e., the expressions given by Eq. (68) in conjunction with the simplifications due to the axisymmetric boundary surface and by Eq. (103), we find essential differences. One difference is the continuous nature of the eigenfunctions and semi-integer eigenvalues in the SVM as compared to the discrete nature of the eigenvectors and real eigenvalues according to Eq. (88) in the MoL. This also necessitates a different definition of the scalar product, which is necessary to approximate the surface potential. These differences first became obvious when it was shown [4] that the transformation of the initial approximation of the differential operators within the MoL can be reformulated into a corresponding approximation of the unknown solution, an aspect, which has totally been overlooked in all the previous discussions concerning the nature of the MoL (see Refs. [24, 25]). On the other hand, since both the SVM and the MoL claim to offer a rigorous approach to solving the nonspherical BVP, we may expect that there is a way to transform one method and its representation of the SGF into the other one. This is indeed possible, as can be seen by inspecting the limiting behaviour of the eigenvectors and eigenvalues in the MoL for an increasing number of discretization lines. For this we have to go back to Eq. (82). Unfortunately, in spherical coordinates the solution of this equation can be found only numerically. But for the corresponding BVP's in Cartesian and cylindrical coordinates we can find an analytical solution which depends on the number

of discretization lines. As a result, the transition $\lim_{N_d\to\infty}$ can be performed analytically. It was shown in Ref. [4] that in these cases the known eigenvalues and eigenvectors of the SVM can be reproduced exactly. Once we know this, we can try to verify this result in spherical coordinates by solving Eq. (82) numerically for an increasing number of discretization lines. It turns out that the eigenvectors $\left|x_i^{(l)}\right\rangle$ converge against the associated Legendre polynomials sampled at the N_d discrete points θ_i in the interval $[0, \pi]$, and that the eigenvalues $\nu_i^{(l)}$ approach the semi-integer orders of the spherical Hankel functions. Therefore, if we replace all the algebraic scalar products by an integral according to

$$\left\langle \tilde{x}_{i'}^{(l)} \middle| \tilde{x}_i^{(l)} \right\rangle_{l_2} = \int_0^\pi \sin\bar{\theta} P_{i',l}(\cos\bar{\theta}) \cdot P_{i,l}(\cos\bar{\theta})\, \mathrm{d}\bar{\theta} \tag{104}$$

both representations of the SGF become identical in the limit $\lim_{N_d\to\infty}$. This result also shows that one can not really benefit from an application of the MoL to solve the BVP in spherical coordinates. On the contrary, one has to take an additional inaccuracy into account, caused by the additional discretization procedure. This becomes even more important if one is interested in solving the eigenvalue problem for the homogeneous Dirichlet condition on the boundary surface $\partial\Gamma$, as demonstrated in Ref. [26]. Therefore, applying the SVM is always the better choice. It is only advantageous to apply the MoL in those cases in which we can not (or only with difficulties) calculate the eigenvalues and eigenvectors in the SVM. This may happen for partial differential equations other than the Helmholtz equation (Sturm-Liouville equation, for instance) or if the BVP is formulated in a more complicated coordinate system.

5. SURFACE GREEN'S FUNCTION FOR PARTICLES WITH DISCRETE SYMMETRIES

Discrete symmetries have been exploited with great success in theoretical chemistry, in particularly in electronic structure computations and in the classification of molecular vibrations [27]. In electromagnetics, they have been applied to potential theory [28, 29] as well as to the T matrix formulation of electromagnetic scattering theory [8] and to other BIE approaches [9].

Geometrical symmetries of objects of finite extent are represented by coordinate transformations, such as discrete rotations, reflection planes, rotation-reflection operations, or an inversion centre. These

coordinate transformations transform the coordinates of the object in such a way that the transformed object is indistinguishable from the original object. In electromagnetic scattering applications these geometrical symmetry properties must be reflected as symmetry relations of those quantities representing the optical properties of the particle, as, for example, the T matrix [8], or, as we will show shortly, the SGF.

The set of all symmetry elements of an object with discrete symmetries forms a finite group, a so-called point-group. The term originates from the fact that all symmetry operations in a point-group leave one point in space unchanged (in contrast to the space-groups used in solid state physics that also contain translations). The "degree of symmetry" of an object is expressed by the order M_o of the group. For instance, hexahedral ice crystals or the benzene molecule belong to the dihedral point-group $\mathcal{D}_{6h}$, which is of order 24, a trihedral prism belongs to the group $\mathcal{D}_{3h}$, which is only of order 12, whereas a cube belongs to the octahedral point-group $\mathcal{O}_h$, which is of order 48.

A recent numerical study using the null-field method [10] showed that for a particle belonging to a point-group of order M_o the computation time of the **Q** and **RgQ** matrices used in the computation of the T matrix can be reduced by a factor of M_o^2. This is due to a reduction by a factor of M_o of the number of **Q** and **RgQ** matrix elements that need to be computed, as well as a reduction by a factor of M_o of the surface area over which the numerical evaluation of the surface integrals in the null-field method needs to be carried out. This typically amounts to a reduction in CPU-time by 2–3 orders of magnitude, which is substantial. It was also found [30] that the CPU-time requirement for the procedure for computing the averaged optical properties for ensembles of randomly oriented particles [31–33] can be reduced by a factor of M_o.

Such a massive reduction in computation time has made it possible to conduct light scattering computations based on rigorous theory for ensembles of randomly oriented particles consisting of a large number of different sizes and geometries [30, 34].

Exploiting point-group symmetries can also lead to a significant extension of the range of size parameters in practical computations [11]. Thus it has become possible to rigorously compute the phase function of hexahedral prisms up to size parameters for which on can observe the famous halo peak at 22° [11], as can be seen in Fig. 3.

With these introductory remarks the advantages of exploiting discrete symmetries in electromagnetic scattering computations have been made abundantly clear. In the first two sections we will now derive the symmetry relations of the SGF and the corresponding geometry factors $\left[A_{\partial\Gamma}^{-1}\right]_{l,l',n,n'}$ under the assumption that the symmetry behav-

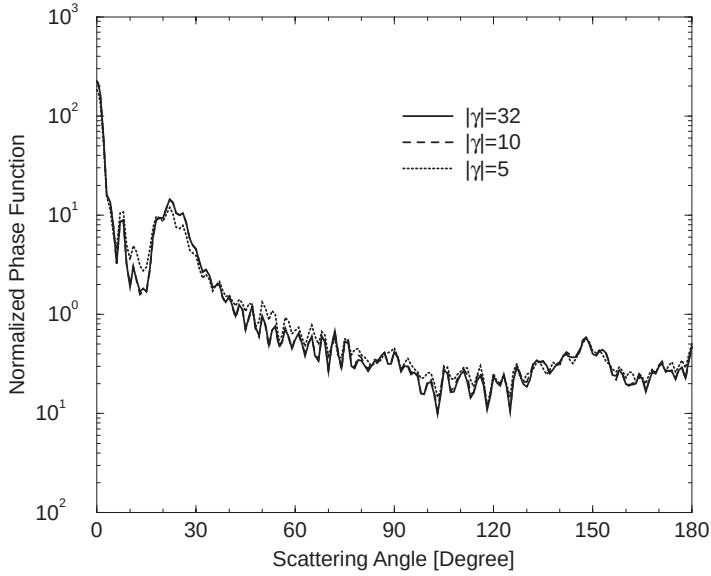

Figure 3. Normalized phase function of a finitely extended hexagonal ice cylinder with side length a. The parameters are $ka = 60$, $l = 30\,\mu$m, $\lambda = 0.5\,\mu$m, a refractive index of 1.313. Normal incidence with respect to the cylinder axis is considered. γ denotes the number on non-zero off-diagonals used in the computation. For details, see Ref. [11].

iour of the approximate solution is identical that of the exact solution. In the third section we will give the proof of this assumption for both the least-squares and Waterman's solution scheme.

5.1. Symmetry Relations of the Surface Green's Function

5.1.1. σ Symmetry

Let us assume that the potential on the surface be given by the inhomogeneous Dirichlet condition

$$u(\bar{\theta}, \bar{\phi}) = f[R(\bar{\theta}, \bar{\phi}), \bar{\theta}, \bar{\phi}]. \tag{105}$$

The solution u in the exterior domain is given in terms of f by Eq. (67). Now let us conduct a thought-experiment. What happens if we switch to a surface potential f' that is related to f according to

$$f'[R(\bar{\theta}, \bar{\phi}), \bar{\theta}, \bar{\phi}] = f[R(\pi - \bar{\theta}, \bar{\phi}), \pi - \bar{\theta}, \bar{\phi}]? \tag{106}$$

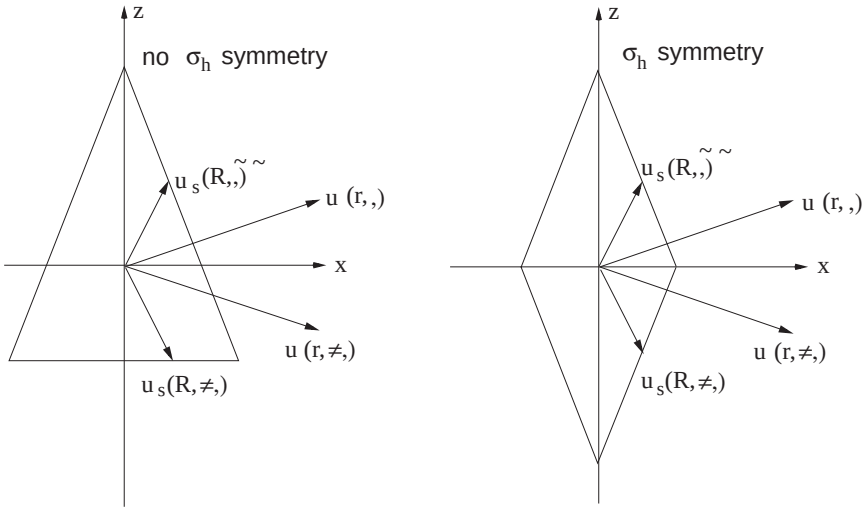

Figure 4. Particle without (left) and with (right) σ_h symmetry.

The new surface potential f' will give rise to a new solution u' in the exterior domain. If the particle surface has the symmetry property

$$R(\pi - \bar{\theta}, \bar{\phi}) = R(\bar{\theta}, \bar{\phi}) \tag{107}$$

(as the particle shown in Fig. 4 on the right hand side), then the new solution u' will be related to the old solution u according to

$$u'(r, \theta, \phi) = u(r, \pi - \theta, \phi). \tag{108}$$

For a particle not having the symmetry property given in Eq. (107) (as the particle shown in Fig. 4 on the left hand side), Eq. (108) will in general not hold. We now make the assumption that Eq. (109) also holds for the approximate solution $u_{N\mathrm{cut}}$, i.e.,

$$u'_{N\mathrm{cut}}(r, \theta, \phi) = u_{N\mathrm{cut}}(r, \pi - \theta, \phi). \tag{109}$$

Substitution of Eq. (67) into Eq. (109) yields

$$\begin{aligned} &\int_0^{2\pi} \mathrm{d}\bar{\phi} \int_0^{\pi} \sin\bar{\theta}\, \mathrm{d}\bar{\theta}\, G^{N\mathrm{cut},L\mathrm{cut}}_{\partial\Gamma}(R, \bar{\theta}, \bar{\phi}/r, \theta, \phi) f(R, \pi - \bar{\theta}, \bar{\phi}) \\ = &\int_0^{2\pi} \mathrm{d}\bar{\phi} \int_0^{\pi} \sin\bar{\theta}\, \mathrm{d}\bar{\theta}\, G^{N\mathrm{cut},L\mathrm{cut}}_{\partial\Gamma}(R, \bar{\theta}, \bar{\phi}/r, \pi - \theta, \phi) f(R, \bar{\theta}, \bar{\phi}). \end{aligned} \tag{110}$$

The surface potential in Eq. (110) is arbitrary. If we make the specific choice

$$f\big(R(\bar{\theta},\bar{\phi}),\bar{\theta},\bar{\phi}\big) = \frac{1}{\sin\bar{\theta}}\delta(\pi+\bar{\theta}-\theta')\delta(\bar{\phi}-\phi') \tag{111}$$

then we obtain

$$G_{\partial\Gamma}^{N\mathrm{cut},L\mathrm{cut}}(R,\theta',\phi'/r,\theta,\phi) = G_{\partial\Gamma}^{N\mathrm{cut},L\mathrm{cut}}(R,\pi-\theta',\phi'/r,\pi-\theta,\phi). \tag{112}$$

This is the symmetry relation of the SGF of a particle having a reflection plane that coincides with the xy-plane. By convention, reflection symmetries are called σ-symmetries. In the presence of a discrete rotational symmetry, one denotes a reflection plane that lies perpendicular to the rotational symmetry axis by σ_h ("horizontal"), and a reflection plane that contains the rotational symmetry axis by σ_v ("vertical").

5.1.2. C_N Symmetry

We now assume that the particle has an N-fold discrete rotational symmetry, i.e., a rotation of the particle by an angle $2\pi/N$ with respect to ϕ brings the particle into an orientation that is indistinguishable from the original orientation. The rotational symmetry axis is assumed to coincide with the z-axis. Thus we have the symmetry property

$$R(\bar{\theta},\bar{\phi}+\frac{2\pi}{N}) = R(\bar{\theta},\bar{\phi}). \tag{113}$$

In analogy to our investigation of σ symmetry, we now consider two surface potentials f and f' that are related to one another according to

$$f'[R(\bar{\theta},\bar{\phi}),\bar{\theta},\bar{\phi}] = f[R(\bar{\theta},\bar{\phi}+\frac{2\pi}{N}),\bar{\theta},\bar{\phi}+\frac{2\pi}{N}]. \tag{114}$$

Due to C_N symmetry of the boundary, the exterior solutions u and u' belonging to the surface potentials f and f', respectively, will be related to one another according to

$$u'(r,\theta,\phi) = u\left(r,\theta,\phi+\frac{2\pi}{N}\right). \tag{115}$$

As before, we now invoke the assumption

$$u'_{N\mathrm{cut}}(r,\theta,\phi) = u_{N\mathrm{cut}}\left(r,\theta,\phi+\frac{2\pi}{N}\right). \tag{116}$$

Combining Eqs. (113)–(116) in connection with Eq. (67) yields

$$\int_0^{2\pi} \mathrm{d}\bar{\phi} \int_0^{\pi} \sin\bar{\theta}\, \mathrm{d}\bar{\theta} G_{\partial\Gamma}^{N\mathrm{cut},L\mathrm{cut}}(R,\bar{\theta},\bar{\phi}/r,\theta,\phi) f\left(R,\bar{\theta},\bar{\phi}+\frac{2\pi}{N}\right)$$
$$= \int_0^{2\pi} \mathrm{d}\bar{\phi} \int_0^{\pi} \sin\bar{\theta}\, \mathrm{d}\bar{\theta} G_{\partial\Gamma}^{N\mathrm{cut},L\mathrm{cut}}\left(R,\bar{\theta},\bar{\phi}/r,\theta,\phi+\frac{2\pi}{N}\right) f(R,\bar{\theta},\bar{\phi}). \tag{117}$$

With the specific choice

$$f\big(R(\bar{\theta},\bar{\phi}),\bar{\theta},\bar{\phi}\big) = \frac{1}{\sin\bar{\theta}}\delta(\bar{\theta}-\theta')\delta\left(\bar{\phi}-\frac{2\pi}{N}-\phi'\right) \tag{118}$$

we finally obtain the C_N symmetry relation of the SGF

$$G_{\partial\Gamma}^{N\mathrm{cut},L\mathrm{cut}}(R,\theta',\phi'/r,\theta,\phi) = G_{\partial\Gamma}^{N\mathrm{cut},L\mathrm{cut}}\left(R,\theta',\phi'+\frac{2\pi}{N}/r,\theta,\phi+\frac{2\pi}{N}\right). \tag{119}$$

5.1.3. Dihedral Symmetry

As a further example we consider the case that the particle has an additional two-fold rotational symmetry axis that lies perpendicular to the main rotational symmetry axis. Such a symmetry element is called a dihedral symmetry. We assume that the particle is oriented such that this dihedral axis lies along the y-axis. The boundary surface thus has the symmetry property

$$R(\pi-\bar{\theta},2\pi-\bar{\phi}) = R(\bar{\theta},\bar{\phi}). \tag{120}$$

We consider again two different surface potentials f and f' that are related to one another according to

$$f'\left[R(\bar{\theta},\bar{\phi}),\bar{\theta},\bar{\phi}\right] = f\left[R(\pi-\bar{\theta},2\pi-\bar{\phi}),\pi-\bar{\theta},2\pi-\bar{\phi}\right]. \tag{121}$$

Due to dihedral symmetry of $\partial\Gamma$, the solutions in the exterior domain are now related to one another according to

$$u'(r,\theta,\phi) = u(r,\pi-\theta,2\pi-\phi). \tag{122}$$

Again, we assume

$$u'_{N\mathrm{cut}}(r,\theta,\phi) = u_{N\mathrm{cut}}(r,\pi-\theta,2\pi-\phi). \tag{123}$$

Combination of Eqs. (67) and (120)–(123) yields

$$\int_0^{2\pi} \mathrm{d}\bar{\phi} \int_0^{\pi} \sin\bar{\theta}\, \mathrm{d}\bar{\theta}\, G_{\partial\Gamma}^{N\mathrm{cut},L\mathrm{cut}}(R,\bar{\theta},\bar{\phi}/r,\theta,\phi) f(R,\pi-\bar{\theta},2\pi-\bar{\phi})$$
$$= \int_0^{2\pi} \mathrm{d}\bar{\phi} \int_0^{\pi} \sin\bar{\theta}\, \mathrm{d}\bar{\theta}\, G_{\partial\Gamma}^{N\mathrm{cut},L\mathrm{cut}}(R,\bar{\theta},\bar{\phi}/r,\pi-\theta,2\pi-\phi) f(R,\bar{\theta},\bar{\phi}). \tag{124}$$

With the specific choice

$$f\big(R(\bar{\theta},\bar{\phi}),\bar{\theta},\bar{\phi}\big) = \frac{1}{\sin\bar{\theta}} \delta(\pi+\bar{\theta}-\theta')\delta(2\pi+\bar{\phi}-\phi') \tag{125}$$

we arrive at

$$G_{\partial\Gamma}^{N\mathrm{cut},L\mathrm{cut}}(R,\theta',\phi'/r,\theta,\phi) = G_{\partial\Gamma}^{N\mathrm{cut},L\mathrm{cut}}(R,\pi-\theta',2\pi-\phi'/r,\pi-\theta,2\pi-\phi). \tag{126}$$

This is the symmetry relation of the SGF for a boundary surface with dihedral symmetry.

5.1.4. C_∞ Symmetry

Axial symmetry (denoted by C_∞) is just a special case of C_N symmetry. Assuming that the rotational symmetry axis lies along the z-axis, we have $R(\bar{\theta},\bar{\phi}) = R(\bar{\theta},\bar{\phi}+\bar{\phi}_1)$ for any $\bar{\theta},\bar{\phi},\bar{\phi}_1$. For the SGF this leads to the symmetry relation

$$G_{\partial\Gamma}^{N\mathrm{cut},L\mathrm{cut}}(R,\theta',\phi'/r,\theta,\phi) = G_{\partial\Gamma}^{N\mathrm{cut},L\mathrm{cut}}(R,\theta',\phi'+\phi_1/r,\theta,\phi+\phi_1) \quad \text{for any } \phi_1. \tag{127}$$

5.1.5. K Symmetry

Another special case is spherical symmetry (denoted by K). In this case we can derive an analytical expression for the SGF given in Eq. (68) since the relation

$$\big[A_{\partial\Gamma}^{-1}\big]_{l,l',n,n'} = \frac{1}{|h_n^{(1)}(kR)|^2} \cdot \delta_{l,l'}\delta_{n,n'} \tag{128}$$

holds. Let γ be the angle between the point (R,θ',ϕ') on the spherical boundary and the observation point (r,θ,ϕ). Then the addition theorem of the spherical harmonics

$$P_n(\cos\gamma) = \frac{4\pi}{2n+1} \sum_{l=-n}^{n} Y_{n,l}^*(\theta',\phi') Y_{n,l}(\theta,\phi) \tag{129}$$

implies

$$G_{\partial\Gamma}^{N\text{cut},L\text{cut}}(R,\theta',\phi'/r,\theta,\phi)=\sum_{n=1}^{\infty}\left(\frac{2n+1}{4\pi}\right)\frac{h_n^{(1)}(kr)}{h_n^{(1)}(kR)}P_n(\cos\gamma). \quad (130)$$

Thus the SGF only depends on the angle γ between the point (R,θ',ϕ') on the spherical boundary and the observation point (r,θ,ϕ).

5.2. Equivalent Symmetry Relations of the Geometry Factors $\mathbf{A}_{\partial\Gamma}^{-1}$

We will now investigate the symmetry relations of the surface Green's function for σ (Eq. (112)), C_N (Eq. (119)), and dihedral (Eq. (126)) symmetry in conjunction with the explicit expression of the SGF given in Eq. (68). This will result in explicit symmetry relations of the geometry factors $\mathbf{A}_{\partial\Gamma}^{-1}$.

5.2.1. σ Symmetry

From Eq. (68) we see that the symmetry relation given in (112) is equivalent to

$$\begin{aligned}&\sum_{n,n',l,l'}\left[A_{\partial\Gamma}^{-1}\right]_{l,l',n,n'}h_{n'}^{(1)}(kR)h_n^{(1)}(kr)Y_{n',l'}^*(\bar\theta,\bar\phi)Y_{n,l}(\theta,\phi)\\ &=\sum_{n,n',l,l'}\left[A_{\partial\Gamma}^{-1}\right]_{l,l',n,n'}h_{n'}^{(1)}(kR)h_n^{(1)}(kr)Y_{n',l'}^*(\pi-\bar\theta,\bar\phi)Y_{n,l}(\pi-\theta,\phi).\end{aligned} \quad (131)$$

Using

$$Y_{n,l}(\pi-\theta,\phi)=(-1)^{n+l}Y_{n,l}(\theta,\phi) \quad (132)$$

and splitting up the sums, we find that Eq. (131) is equivalent to

$$\begin{aligned}&\sum_{\substack{n,n',l,l'\\(n+n'+l+l')\text{even}}}\left[A_{\partial\Gamma}^{-1}\right]_{l,l',n,n'}h_{n'}^{(1)}(kR)h_n^{(1)}(kr)Y_{n',l'}^*(\bar\theta,\bar\phi)Y_{n,l}(\theta,\phi)\\ &+\sum_{\substack{n,n',l,l'\\(n+n'+l+l')\text{odd}}}\left[A_{\partial\Gamma}^{-1}\right]_{l,l',n,n'}h_{n'}^{(1)}(kR)h_n^{(1)}(kr)Y_{n',l'}^*(\bar\theta,\bar\phi)Y_{n,l}(\theta,\phi)\\ &=\sum_{\substack{n,n',l,l'\\(n+n'+l+l')\text{even}}}\left[A_{\partial\Gamma}^{-1}\right]_{l,l',n,n'}h_{n'}^{(1)}(kR)h_n^{(1)}(kr)Y_{n',l'}^*(\bar\theta,\bar\phi)Y_{n,l}(\theta,\phi)\end{aligned}$$

$$- \sum_{\substack{n,n',l,l' \\ (n+n'+l+l')\text{odd}}} \left[A^{-1}_{\partial\Gamma}\right]_{l,l',n,n'} h^{(1)}_{n'}(kR) h^{(1)}_{n}(kr) Y^{*}_{n',l'}(\bar{\theta},\bar{\phi}) Y_{n,l}(\theta,\phi). \tag{133}$$

Equation (133) is equivalent to

$$\sum_{\substack{n,n',l,l' \\ (n+n'+l+l')\text{odd}}} \left[A^{-1}_{\partial\Gamma}\right]_{l,l',n,n'} h^{(1)}_{n'}(kR) h^{(1)}_{n}(kr) Y^{*}_{n',l'}(\bar{\theta},\bar{\phi}) Y_{n,l}(\theta,\phi) = 0. \tag{134}$$

Multiplication of Eq. (134) by $Y^{*}_{n'',l''}(\theta,\phi)$ and integration over θ and ϕ over a spherical surface including the bounded domain yields with the orthogonality of the spherical harmonics on this spherical surface

$$\sum_{\substack{n',l' \\ (n'+n''+l'+l'')\text{odd}}} \left[A^{-1}_{\partial\Gamma}\right]_{l'',l',n'',n'} h^{(1)}_{n'}(kR) h^{(1)}_{n''}(kr) Y^{*}_{n',l'}(\bar{\theta},\bar{\phi}) = 0$$
$$\text{for any} \quad n'' = 0, 1, \ldots \quad \text{and} \quad l'' = -n'', \ldots, n''. \tag{135}$$

The previous step can be reversed so that Eqs. (134) and (135) are equivalent. Due to the linear independence of the radiating wave functions $h^{(1)}_{n'}(kR) Y^{*}_{n',l'}(\bar{\theta},\bar{\phi})$ on the Lyapunov surface $R(\bar{\theta},\bar{\phi})$, Eq. (135) is equivalent to

$$\left[A^{-1}_{\partial\Gamma}\right]_{l'',l',n'',n'} = 0 \quad \text{if} \quad (l''+l'+n''+n') \quad \text{odd}. \tag{136}$$

This is the symmetry relation for the geometry factors for a boundary surface with a reflection plane in the xy-plane. As we have emphasised throughout the derivation, all steps that led from Eq. (131) to Eq. (136) are reversible. Thus the symmetry relation of the geometry factors given in (136) is equivalent to that of the SGF given in (112).

5.2.2. C_N Symmetry

The derivation of the symmetry relation of the geometry factors for a boundary surface having C_N symmetry is quite analogous to the derivation in the previous section. One starts by substituting Eq. (68) into the C_N symmetry relation of the SGF given in Eq. (119). Using

$$Y_{n,l}(\theta,\phi + 2\pi/N) = Y_{n,l}(\theta,\phi) \exp(2\pi i l/N) \tag{137}$$

the orthogonality of the spherical harmonics, and the linear independence of the spherical wave functions on the boundary surface, one arrives at

$$\left[1-\exp(2\pi i(l''-l')/N)\right]\left[A^{-1}_{\partial\Gamma}\right]_{l'',l',n'',n'}=0$$
$$\text{for any } n',n''=0,1,\ldots;\ l'=-n',\ldots,n' \text{ and } l''=-n'',\ldots,n'' \quad (138)$$

and thus

$$\left[A^{-1}_{\partial\Gamma}\right]_{l'',l',n'',n'}=0 \quad \text{if} \quad (l''-l')\neq 0,N,2N,\ldots . \quad (139)$$

This is the symmetry relation of the geometry factors for a boundary having a discrete N-fold rotational symmetry axis along the z-axis. This symmetry relation is equivalent to the corresponding symmetry relation of the SGF given in Eq. (119).

5.2.3. Dihedral Symmetry

In complete analogy we start from Eq. (126) in conjunction with Eq. (68). Using Eq. (132), the relation

$$Y_{n,l}(\theta,2\pi-\phi)=Y_{n,-l}(\theta,\phi), \quad (140)$$

the orthogonality of the spherical harmonics, and the linear independence of the spherical wave functions on the boundary surface, we obtain the symmetry relation of the geometry factors for a dihedral symmetry axis along the y-axis

$$\left[A^{-1}_{\partial\Gamma}\right]_{-l'',-l',n'',n'}=(-1)^{l''+l'+n''+n'}\left[A^{-1}_{\partial\Gamma}\right]_{l'',l',n'',n'}. \quad (141)$$

Again, this relation is equivalent to the corresponding symmetry relation of the SGF given in (126).

5.2.4. C_∞ Symmetry

In the limit $N\to\infty$ we obtain from Eq. (139)

$$\left[A^{-1}_{\partial\Gamma}\right]_{l'',l',n'',n'}=\delta_{l'',l'}\left[A^{-1}_{\partial\Gamma}\right]_{l'',l',n'',n'}. \quad (142)$$

We can, of course, also derive this symmetry relation from the symmetry relation of the SGF given in Eq. (127).

5.2.5. K Symmetry

Using Eq. (128) the geometry factors of a sphere have the symmetry property

$$\left[A^{-1}_{\partial\Gamma}\right]_{l,l',n,n'}=\left[A^{-1}_{\partial\Gamma}\right]_{n}\delta_{l,l'}\delta_{n,n'}. \quad (143)$$

5.2.6. Comparison with the Symmetry Relations of the T Matrix

Symmetry relations of the T matrix for σ, C_N, and dihedral symmetry are given, respectively, by [8]

$$[T]^{(k,k')}_{n,l,n',l'} = 0 \quad \text{if} \quad (l + l' + n + n' + k + k') \quad \text{odd} \tag{144}$$

$$[T]^{(k,k')}_{n,l,n',l'} = 0 \quad \text{if} \quad (l - l') \neq 0, N, 2N, \ldots \tag{145}$$

$$[T]^{(k,k')}_{n,-l,n',-l'} = (-1)^{l+l'+n+n'} \, [T]^{(k,k')}_{n,l,n',l'} \, . \tag{146}$$

For the special case of axial symmetry, relation (145) becomes [8]

$$[T]^{(k,k')}_{n,l,n',l'} = \delta_{l,l'} \, [T]^{(k,k')}_{n,l,n',l} \tag{147}$$

and for spherical symmetry, the T matrix has the symmetry property [8]

$$[T]^{(k,k')}_{n,l,n',l'} = \delta_{l,l'} \delta_{n,n'} \delta_{k,k'} \, [T]_n \, . \tag{148}$$

The extra indices $k, k' = 1, 2$ come from the use of vector spherical functions. Analogous symmetry relations hold for the **Q** and **RgQ** matrices. The similarity between the symmetry relations of the T matrix given in (144), (145), (146), (147), and (148) and the corresponding relations of the geometry factors in (136), (139), (141), (142), and (143) is obvious.

5.3. Proof of Symmetry Relations for the Least-Squares and Waterman Solution Scheme

The approach taken in Sec. 5.1 was based on a simple and intuitively appealing thought experiment considering the relation between the surface potential f and the solution u for certain symmetries of the boundary surface. This approach required us to make the additional assumption that the approximate solution $u_{N\text{cut}}$ satisfies the same relations as the exact solution u. But we have no a priori guarantee that this assumption actually holds. Of course, it could be verified by numerical experiments for each method for determining the expansion coefficients of $u_{N\text{cut}}$. Another way is to derive the symmetry relations of the geometry factors $\mathbf{A}^{-1}_{\partial\Gamma}$ rigorously for each given method. In the following section we will sketch out a mathematically sound derivation of the symmetry relations of the geometry factors $\mathbf{A}^{-1}_{\partial\Gamma}$ in spherical coordinates for the least-squares approach and for Waterman's method. The proof proceeds in two steps. In the first step, we use Eq. (49) to derive the symmetry relations of the matrix $\mathbf{A}_{\partial\Gamma}$ for a given symmetry

property of the boundary surface. In the second step, we show that the inverse matrix, i.e., the geometry factors $\mathbf{A}_{\partial\Gamma}^{-1}$ possess the same symmetry property. We start with the first step.

5.3.1. σ Symmetry

Equation (49) reads in spherical coordinates

$$[A_{\partial\Gamma}]_{l,l',n,n'} = \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta \sin\theta \cdot z_n^{(\alpha)}\big(kR(\theta,\phi)\big) z_{n'}^{(\beta)*}\big(kR(\theta,\phi)\big) Y_{n,l}(\theta,\phi) Y_{n',l'}^*(\theta,\phi). \tag{149}$$

The radial functions $z_n^{(\alpha)}$ and $z_n^{(\beta)}$ denote spherical Bessel, Neumann, or Hankel functions. In a least-squares approach, $z_n^{(\alpha)} = z_n^{(\beta)}$, whereas in Waterman's approach, $z_n^{(\alpha)} = j_n$ and $z_n^{(\beta)} = h_n^{(1)}$. For the sake of conciseness we denote $z_n^{(\alpha)} z_{n'}^{(\beta)*} = Z_{n,n'}$.

The polar integral yields zero if the integrand is odd with respect to the point $\theta/2$. For σ symmetry, $R(\pi-\theta,\phi) = R(\theta,\phi)$. Since the sine is even with respect to the point $\theta/2$, the integrand is antisymmetric if the product of the spherical harmonics is antisymmetric. From Eq. (132) it follows that

$$[A_{\partial\Gamma}]_{l,l',n,n'} = 0 \quad \text{if} \quad l + l' + n + n' \quad \text{odd}. \tag{150}$$

5.3.2. C_N Symmetry

Using $R(\theta,\phi+2\pi/N)$=$R(\theta,\phi)$ and $Y_{n,l}(\theta,\phi) = P_{n,l}(\theta)\exp(il\phi)$ we obtain from Eq. (149)

$$\begin{aligned}
&\int_0^{2\pi} \mathrm{d}\phi' Z_{n,n'}\big(kR(\theta,\phi')\big) \exp[i(l-l')\phi'] \\
&= \sum_{k=0}^{N-1} \int_{2\pi k/N}^{2\pi(k+1)/N} \mathrm{d}\phi' Z_{n,n'}\big(kR(\theta,\phi')\big) \exp[i(l-l')\phi'] \\
&= \sum_{k=0}^{N-1} \int_0^{2\pi} \mathrm{d}\phi Z_{n,n'}\big(kR(\theta,\phi-2\pi k/N)\big) \exp[i(l-l')(\phi-2\pi k/N)] \\
&= \left\{\sum_{k=0}^{N-1} \exp[-i(l-l')2\pi k/N]\right\} \int_0^{2\pi} \mathrm{d}\phi Z_{n,n'}\big(kR(\theta,\phi)\big) \exp[i(l-l')\phi]
\end{aligned} \tag{151}$$

where we have made the substitution $\phi = \phi' - 2\pi k/N$. If $(l - l') = 0, N, 2N, \ldots$ then the sum in front of the integral yields N. Otherwise this geometric series yields

$$\frac{1 - \exp[i(l - l')2\pi]}{1 - \exp[i(l - l')2\pi/N]} = 0. \tag{152}$$

Thus

$$[A_{\partial\Gamma}]_{l,l',n,n'} = 0 \quad \text{if} \quad (l - l') \neq 0, N, 2N, \ldots . \tag{153}$$

5.3.3. Dihedral Symmetry

Using $(-1)^{n+l} Y_{n,-l}(\theta, \phi) = Y_{n,l}(\pi - \theta, 2\pi - \phi)$ we obtain from Eq. (149)

$$\begin{aligned}
&(-1)^{n+l+n'+l'} [A_{\partial\Gamma}]_{-l,-l',n,n'} \\
&\quad = (-1)^{n+l+n'+l'} \int_0^{2\pi} \mathrm{d}\phi' \int_0^{\pi} \mathrm{d}\theta' \sin\theta' Z_{n,n'}\big(kR(\theta', \phi')\big) \\
&\qquad \cdot Y_{n,-l}(\theta', \phi') Y^*_{n',-l'}(\theta', \phi') \\
&\quad = \int_0^{2\pi} \mathrm{d}\phi' \int_0^{\pi} \mathrm{d}\theta' \sin\theta' Z_{n,n'}\big(kR(\theta', \phi')\big) \\
&\qquad \cdot Y_{n,l}(\pi - \theta', 2\pi - \phi') Y^*_{n',l'}(\pi - \theta', 2\pi - \phi').
\end{aligned} \tag{154}$$

Using $R(\pi - \theta, 2\pi - \phi) = R(\theta, \phi)$ and substituting $\pi - \theta' = \theta$ and $2\pi - \phi' = \phi$, we immediately obtain

$$(-1)^{n+l+n'+l'} [A_{\partial\Gamma}]_{-l,-l',n,n'} = [A_{\partial\Gamma}]_{l,l',n,n'}. \tag{155}$$

5.3.4. C_∞ Symmetry

In the limit $N \to \infty$ we obtain from Eq. (153)

$$[A_{\partial\Gamma}]_{l,l',n,n'} = \delta_{l,l'} [A_{\partial\Gamma}]_{l,l,n,n'}. \tag{156}$$

5.3.5. K Symmetry

For spheres $R(\theta, \phi) = \text{const}$. Thus Eq. (149) in conjunction with the orthogonality property of the spherical harmonics yields

$$[A_{\partial\Gamma}]_{l,l',n,n'} = \delta_{l,l'} \delta_{n,n'} Z_{n,n}(kR). \tag{157}$$

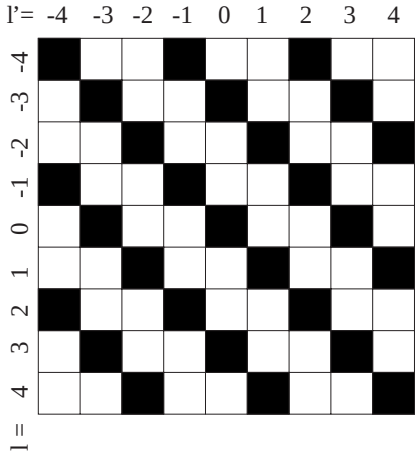

Figure 5. Multi-diagonal block structure of the matrix $\mathbf{A}_{\partial\Gamma}$ for C_3 symmetry and $L\text{cut} = 4$.

5.3.6. Symmetry Properties of the Inverse of the Matrix $\mathbf{A}_{\partial\Gamma}$

At this point we have derived symmetry relations of the matrix $\mathbf{A}_{\partial\Gamma}$ without the additional assumptions made in Sec. 5.1. It remains to derive symmetry relations of the inverse matrix $\mathbf{A}_{\partial\Gamma}^{-1}$ (the geometry factors) from the corresponding symmetry relations of the matrix $\mathbf{A}_{\partial\Gamma}$. This will complete the derivation of the symmetry relations of the geometry factors without making the assumption that the approximate solution satisfies the same symmetry relations as the exact solution. We will sketch out the proof for C_N symmetry. The proof for σ symmetry follows exactly the same idea. The case of K symmetry is trivial, since the matrix $\mathbf{A}_{\partial\Gamma}$ is diagonal. The case of C_∞ symmetry is also trivial, since the matrix $\mathbf{A}_{\partial\Gamma}$ is block-diagonal, and the inverse of a block-diagonal matrix is also block-diagonal.

We start by inspecting the matrix $\mathbf{A}_{\partial\Gamma}$. Figure 5 schematically shows the symmetry structure of the matrix $\mathbf{A}_{\partial\Gamma}$ for the example of C_3 symmetry with $L\text{cut} = 4$. Each black square represents a block matrix having a size of $N\text{cut} \times N\text{cut}$. The white squares, on the other hand, represent those block matrices that are equal to zero due to C_3 symmetry. The arrangement of the matrix elements corresponds to the arrangement of the sum expansion terms in Eq. (66). Thus each block matrix characterised by a row index l and a column index l' contains several elements with row indices $n = |l|, |l| + 1, \ldots, |l| + N\text{cut}$ and column indices $n' = |l'|, |l'| + 1, \ldots, |l'| + N\text{cut}$. To show for the C_N symmetry that $\mathbf{A}_{\partial\Gamma}^{-1}$ has the same symmetry structure as matrix $\mathbf{A}_{\partial\Gamma}$,

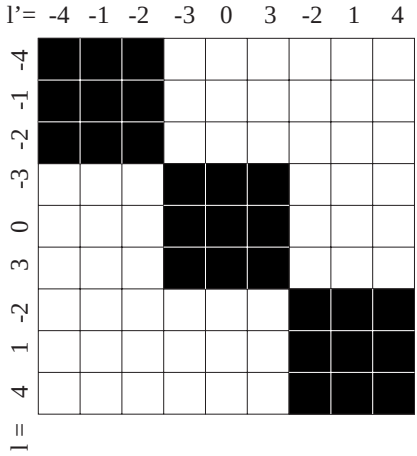

Figure 6. Diagonal block structure of the matrix $\mathbf{A}_{\partial\Gamma}$ after appropriate permutation of columns and rows. The size of each hyper matrix on the diagonal is determined by the parameters Lcut and Ncut.

we apply a permutation procedure to the latter, first to the rows and second to the columns, resulting in a block-diagonal structure with N hyper matrices on the main diagonal, as depicted in Fig. 6. The size of each hypermatrix is determined by Lcut and Ncut. Due to the permutation procedure, the components of the solution vector and of the inhomogeneity on the right hand side will also become rearranged. This system can simply be inverted by calculating the inverse of each hyper matrix, i.e., the solution can formally be written in exactly the same block diagonal form as we have obtained for the original system after permutation. Finally, after reversing the permutation, we arrive at an inverse matrix $\mathbf{A}_{\partial\Gamma}^{-1}$ that has exactly the same symmetry structure as the original matrix $\mathbf{A}_{\partial\Gamma}$.

For σ symmetry we can proceed in a completely analogous way by applying to the matrix $\mathbf{A}_{\partial\Gamma}$ a permutation procedure that brings the matrix into block diagonal form.

We know from Secs. 5.1 and 5.2 that the symmetry relations of the geometry factors $\mathbf{A}_{\partial\Gamma}^{-1}$ are equivalent to the corresponding symmetry relations of the SGF. Thus we can conclude that for the least-squares approach and for Waterman's approach in spherical coordinates we have proven the symmetry properties of the SGF for σ and for C_N symmetry given in Eqs. (112) and (119), respectively, without the additional assumption needed in Sec. 5.1. The derivations of these symmetry properties of the geometry factors and of the SGF presented in this section where considerably more cumbersome than the derivations

presented in Sec. 5.1. However, we emphasise again that the additional assumption needed in Sec. 5.1, namely that the approximate solution exhibits the same symmetry properties as the exact solution, are not guaranteed to be satisfied for every method.

Finally, we note that the angular spheroidal functions transform under a σ, C_N, and dihedral coordinate transformation in the same way as the spherical harmonics [35]. Thus when formulating a least-squares approach or Waterman's approach in spheroidal coordinates [36], the SGF and the geometry factors will satisfy exactly the same symmetry relations as in spherical coordinates.

5.4. Classification of Particle Symmetries by Point-Groups

The procedure for obtaining symmetry relations of the surface Green's function and of the geometry factors has been explained here by use of a few concrete examples. It is clear how this procedure can be generalized to other symmetry elements. In general, however, it is not necessary to derive the symmetry relations of the Green's function or geometry factors for all symmetry elements of a particle. To understand this, we briefly review what we know about discrete symmetries of the T matrix.

The set of all symmetry elements of a particle forms a point-group. Within each point-group one can identify a subset of essential symmetry elements from which all other group elements can be obtained by combination. As explained in Ref. [8], only such a minimum subset of group elements yields *independent* symmetry relation of the T matrix. In close analogy to the reasoning in Ref. [8] we can deduce that only such a minimum subset of group elements yields *independent* symmetry relations of the geometry factors $\left[A^{-1}_{\partial\Gamma}\right]_{l,l',n,n'}$.

For example, a hexahedral prism belongs to the dihedral point-group $\mathcal{D}_{6h}$. This group contains several discrete rotations, reflection planes, rotation-reflection elements, the inversion element, and the unit element. However, all elements of the group can be represented by combinations of the main six-fold rotational symmetry element (denoted by C_6), the reflection plane perpendicular to the main symmetry axis (σ_h), and one of the six dihedral axes (D). The coordinate system can be chosen such that the C_6-axis coincides with the z-axis, the σ_h-plane coincides with the xy-plane, and the D-axis coincides with the y-axis. The symmetry relations of the geometry factors are then given by Eqs. (136), (139) (with $N = 6$), and (141). Other symmetry elements, such as the inversion center, σ_v planes containing the C_6-axis, other dihedral axes, etc., will also give rise to symmetry relations of the geometry factors. However, these symmetry relations can be de-

rived from those of the essential group elements and are therefore not *independent* symmetry relations.

The same must be true for the symmetry relations of the SGF, since they are equivalent to the corresponding relations of the geometry factors. For example, a set of independent symmetry relations of the SGF for a particle belonging to some dihedral point-group $\mathcal{D}_{Nh}$ is given by Eqs. (112), (119), and (126).

Symmetry relations of the geometry factors, as those in our examples given by (136), (139), and (141), can be used to reduce CPU and memory requirements in practical computations. On the other hand, the equivalent symmetry relations of the SGF given in (112), (119), and (126) are much more appealing to intuition and could simply be guessed from the symmetry properties of the surface parameterization $R(\bar{\theta}, \bar{\phi})$.

6. CONCLUSIONS

In this paper we derived the SGF belonging to the exterior boundary value problem of Helmholtz's equation in the presence of non-spherical boundary surfaces. For this we applied the SVM and the MoL in a least-squares sense. It was also demonstrated that from the BIE approach, which is essentially based on the application of Green's theorem, the SVM solution scheme can be deduced. Thus the SGF is able to provide a common mathematical basis for these three classes of solution techniques, the SVM, the BIE methods, and the MoL as a special FD technique. The considerations were restricted to Lyapunov surfaces to ensure that the expansion functions used in the approximation of the surface potential are complete and linearly independent on the boundary surface. The application of a least-squares scheme, on the other hand, ensures uniform convergence of the approximate solution in the exterior domain. Of course, the restrictions to Lyapunov surfaces and the least-squares scheme is not necessary (as shown in Sec. 3.2 when we considered the relation to Waterman's T matrix approach). In the past, practical applications of several solution schemes not based on the assumption of least-squares convergence have demonstrated that reliable and convergent results can also be obtained for such approaches. However, one has to keep in mind that one leaves the sound mathematical basis of the least-squares approaches, and that problems may occur that are more fundamental than purely technical or numerical difficulties.

Furthermore, the reformulation of the MoL to fit into the SVM scheme reveals interesting new aspects of this special FD method. So far, this method has been considered to approximate the differential

operator in Helmholtz's equation. It was assumed that this is in contrast to those methods which approximate the unknown solution by use of a finite series expansion. Now we can see that such a point of view can no longer be maintained. From the reformulation of the MoL we can also see that in the limiting case of an infinite number of discretization lines this special FD technique transforms into the known SVM scheme.

Last not least, we have demonstrated how certain symmetries of the boundary surface results in corresponding symmetry properties of the SGF and its geometry factors. This can simplify the numerical effort drastically since the calculation of unnecessary matrix elements can be avoided.

APPENDIX A. PROOF OF THE WEAK CONVERGENCE OF THE SGF DERIVED IN SEC. 3.2 OF THIS PAPER

Let $u_N(\mathbf{x}) = \sum_{n=1}^{N} a_n^{(N)} \varphi_n(\mathbf{x})$ be an approximate solution to the Dirichlet boundary-value problem, where the functions φ_n satisfy the Helmholtz equation in Γ_+ and the radiation condition at infinity. The system $\{\varphi_n\}_{n=1}^{\infty}$ is complete and linear independent in $L^2(\partial\Gamma)$. Let us determine the coefficients $a_n^{(N)}$ by minimizing the residual field $u_N - f$ in the least-square sense on $\partial\Gamma$, or, equivalently, by solving the normal system of equations

$$\sum_{n=1}^{N} \langle \varphi_m, \varphi_n \rangle_{2,\partial\Gamma} a_n^{(N)} = \langle \varphi_m, f \rangle, \quad m = 1, 2, \ldots, N.$$

With u being the exact solution to the Dirichlet boundary-value problem we see that u_N is the projection of u $(= f)$ onto the N-dimensional space $H_N = Sp\{\varphi_1, \varphi_2, \ldots, \varphi_N\}$; whence $\|u - u_N\|_{2,\partial\Gamma} \to 0$ as $N \to \infty$ follows. Now, using the estimate [19]

$$\|u - u_N\|_{\infty,\Lambda} \leq c \|u - u_N\|_{2,\partial\Gamma},$$

where Λ is any closed subset of Γ_+, we deduce that $u(\mathbf{x}) - u_N(\mathbf{x}) \to 0$ as $N \to \infty$, for each $\mathbf{x}$ in Γ_+. Consequently, with $G_{\partial\Gamma}(\bar{\mathbf{x}}, \mathbf{x}) = \partial G(\bar{\mathbf{x}}, \mathbf{x}) / \partial \hat{n}(\bar{\mathbf{x}})$ standing for the surface Green function we may use the representations

$$u_N(\mathbf{x}) = \int_{\partial\Gamma} G_{\partial\Gamma}^{N}(\bar{\mathbf{x}}, \mathbf{x}) f(\bar{\mathbf{x}}) dS(\bar{\mathbf{x}})$$

and

$$u(\mathbf{x}) = \int_{\partial\Gamma} G_{\partial\Gamma}(\bar{\mathbf{x}}, \mathbf{x}) f(\bar{\mathbf{x}}) dS(\bar{\mathbf{x}})$$

to conclude that

$$\left\langle f^{\star}, G^{N}_{\partial\Gamma}(\cdot,\mathbf{x}) - G_{\partial\Gamma}(\cdot,\mathbf{x})\right\rangle_{2,\partial\Gamma} \to 0$$

as $N \to \infty$, for each $\mathbf{x}$ in Γ_+. Since f is any continuous function defined on $\partial\Gamma$, we can choose $f = G^{N\star}_{\partial\Gamma}(\cdot,\mathbf{x})$, where $\mathbf{x}$ is some fixed point in Γ_+. In this context, the sequence $u_M(\mathbf{x}) = \int_{\partial\Gamma} G^{M}_{\partial\Gamma}(\cdot,\mathbf{x}) f dS$ converges, and, therefore, the term $u_N(\mathbf{x}) = \left\|G^{N}_{\partial\Gamma}(\cdot,\mathbf{x})\right\|^2_{2,\partial\Gamma}$ is bounded. The latter together with the fact that $C(\partial\Gamma)$ is dense in $L^2(\partial\Gamma)$ leads to the conclusion that $G^{N}_{\partial\Gamma}(\cdot,\mathbf{x}) \to G_{\partial\Gamma}(\cdot,\mathbf{x})$ weakly as $N \to \infty$ for each $\mathbf{x}$ in Γ_+.

REFERENCES

1. Rother, T. and K. Schmidt, "The discretized Mie-formalism for electromagnetic scattering," *Progress in Electromagnetic Research*, J. A. Kong (ed.), 91–183, EMW Publishing, Cambridge, MA, 1997.
2. Taflove, A., *Computational Electrodynamics — The Finite-Difference Time-Domain Method*, Artech House, Boston, 1995.
3. Tsang, L., J. A. Kong, and R. T. Shin, *Theory of Microwave Remote Sensing*, John Wiley & Songs, New York, 1995.
4. Rother, T., "General aspects of solving Helmholtz's equation underlying eigenvalue and scattering problems in electromagnetic wave theory," *J. Electromagn. Waves Appl.*, Vol. 13, 867–888, 1999.
5. Lippmann, B. A., "Note on the theory of gratings," *J. Opt. Soc. Amer.*, Vol. 43, 408, 1953.
6. Millar, R. F., "The Rayleigh hypothesis and a related least-squares solution to scattering problems for periodic surfaces and other scatterers," *Radio Sci.*, Vol. 8, 785–796, 1973.
7. Morse, P. M. and H. Feshbach, *Methods of Theoretical Physics*, McGraw-Hill Book Company, Inc., 1953.
8. Schulz, F. M., K. Stamnes, and J. J. Stamnes, "Point group symmetries in electromagnetic scattering," *J. Opt. Soc. Am. A*, Vol. 16, 853–865, 1999.
9. Zagorodnov, I. A. and R. P. Tarasov, "Finite groups in numerical solution of electromagnetic scattering problems on non-spherical particles," *Light Scattering by Nonspherical Particles: Halifax Contributions*, 99–102, Army Research Laboratory, Adelphi, MD, 2000.

10. Kahnert, F. M., J. J. Stamnes, and K. Stamnes, "Application of the extended boundary condition method to homogeneous particles with point group symmetries," *Appl. Opt.*, Vol. 40, 3110–3123, 2001.
11. Rother, T., K. Schmidt, and S. Havemann, "Light scattering on hexagonal ice columns," *J. Opt. Soc. Am. A*, Vol. 18, 2512–2517, 2001.
12. Waterman, P. C., "Matrix formulation of electromagnetic scattering," *Proc. IEEE*, Vol. 53, 805–812, 1965.
13. Kleinman, R. E., G. F. Roach, and S. E. G. Ström, "The null field method and modified Green function," *Proc. R. Soc. Lond. A*, Vol. 394, 121–136, 1984.
14. Ramm, A. G., *Scattering by Obstacles*, D. Reidel, Dordrecht, 1986.
15. Tai, C.-T., *Dyadic Green Functions in Electromagnetic Theory*, IEEE Press, Piscataway, 1993.
16. Sommerfeld, A., *Partial Differential Equations in Physics*, Academic Press, New York, 1949.
17. Waterman, P. C., "Symmetry, unitarity, and geometry in electromagnetic scattering," *Phys. Rev. D*, Vol. 3, 825–839, 1971.
18. Colton, D. and R. Kress, *Inverse Acoustic and Electromagnetic Scattering Theory*, Springer Verlag, Berlin, 1992.
19. Doicu, A., Y. Eremin, and T. Wriedt, *Acoustic and Electromagnetic Scattering Analysis Using Discrete Sources*, Academic Press, New York, 2000.
20. Dallas, A. G., "On the convergence and numerical stability of the second waterman scheme for approximation of the acoustic field scattered by a hard object," Technical Report, No. 2000-7, 1–35, Dept. of Mathematical Sciences, Univ. of Deleware, 2000.
21. Schmidt, K., T. Rother, and J. Wauer, "The equivalence of applying the extended boundary condition and the continuity conditions for solving electromagnetic scattering problems," *Optics Comm.*, Vol. 150, 1–4, 1998.
22. Pregla, R. and W. Pascher, "The methods of lines," *Numerical Techniques for Microwave and Millimeter Wave Passive Structures*, T. Itoh (ed.), 381–446, Wiley, New York, 1989.
23. Wilkinson, J. H., *The Algebraic Eigenvalue Problem*, Oxford University Press, Oxford, 1965.
24. Pregla, R., "About the nature of the method of lines," *Arch. Elektr. Bertragungstech.*, Vol. 41, 370–386, 1987.
25. Pregla, R., "Higher order approximations for the difference operator in the method of lines," *IEEE Microwave and Guided Wave*

Letters, Vol. 5, 53–55, 1995.

26. Dreher, A. and T. Rother, "New aspects of the method of lines," *IEEE Microwave and Guided Wave Letters*, Vol. 5, 408–410, 1995.
27. Bishop, D. M., *Group Theory and Chemistry*, Dover Publications, Mineola, 1993.
28. Zakharov, E. V., 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.*, Vol. 32, 34–50, 1992.
29. Zakharov, E. V., S. I. Safronov, and R. P. Tarasov, "Finite group algebras in iterational methods of solving boundary-value problems of potential theory," *Comput. Maths. Math. Phys.*, Vol. 33, 907–917, 1993.
30. Kahnert, F. M., J. J. Stamnes, and K. Stamnes, "Can simple particle shapes be used to model scalar optical properties of an ensemble of wavelength-sized particles with complex shapes?" *J. Opt. Soc. Am. A*, Vol. 19, 521–531, 2002.
31. Mishchenko, M. I., "Light scattering by randomly oriented axially symmetric particles," *J. Opt. Soc. Am. A.*, Vol. 8, 871–882, 1991.
32. Khlebtsov, N. G., "Orientational averaging of light-scattering observables in the T-matrix approach," *Appl. Opt.*, Vol. 31, 5359–5365, 1992.
33. Mackowski, D. W. and M. I. Mishchenko, "Calculation of the T matrix and the scattering matrix for ensembles of spheres," *J. Opt. Soc. Am. A*, Vol. 13, 2266–2278, 1996.
34. Kahnert, F. M., J. J. Stamnes, and K. Stamnes, "Using simple particle shapes to model the Stokes scattering matrix of ensembles of wavelength-sized particles with complex shapes: possibilities and limitations," *J. Quant. Spectrosc. Radiat. Transfer*, Vol. 74, 167–182, 2002.
35. Schulz, F. M., K. Stamnes, and J. J. Stamnes, "Scattering of electromagnetic waves by spheroidal particles: A novel approach exploiting the T-matrix computed in spheroidal coordinates," *Appl. Opt.*, Vol. 37, 7875–7896, 1998.
36. Kahnert, F. M., J. J. Stamnes, and K. Stamnes, "Surface-integral formulation for electromagnetic scattering in spheroidal coordinates," *J. Quant. Spectrosc. Radiat. Transfer*, in press.