Chapter 5
Other Solution Methods

5.1 Introduction

In Chaps. 3 and 4 we became familiar with two different ways of approximating the Green functions related to the scattering problems by finite series expansions in terms of appropriate eigensolutions of the Helmholtz and vector-wave equation. Both of the described ways produce the same expressions. The thus approximated Green functions result in corresponding series expansions of the scattered field with expansion coefficients calculated via the T-matrix from the known expansion coefficients of the primary incident field at the scatterer surface. Demonstrating that the T-matrix is a decisive element of the relevant Green function and that some important properties of the T-matrix like symmetry and unitarity are related to corresponding properties of the Green function can be considered to be the most important results of these two chapters. But there still exist other solution methods for the scattering problem of our interest which have been derived historically from other principles and assumptions used in the foregoing two chapters. Surprisingly, this holds for the T-matrix method itself. It was originally developed by use of the so-called "Extended Boundary Condition". In this chapter we will therefore answer the question of how such methods fit into the developed Green function formalism, or, alternatively, how we have to change the formalism appropriately to end up with some other solution methods. Thereby, it is not our intention to provide a description of selected solution methods which is as complete as possible. In fact, we are more interested in demonstrating that some of the solution methods developed originally from other principles and assumptions can be mapped onto the Green function formalism, and that this formalism provides therefore a sound mathematical basis to analyse the advantages and disadvantages as well as the capabilities of different solution methods. The following considerations are mainly restricted to the scalar case. An exception from this is made when dealing with the so-called "Lippmann-Schwinger" equations which will be derived for the scalar as well as the dyadic Green functions and interaction operators at the end of this chapter.

T. Rother and M. Kahnert, *Electromagnetic Wave Scattering on Nonspherical Particles*, Springer Series in Optical Sciences 145, DOI: 10.1007/978-3-642-36745-8_5,

5.2 T-Matrix Methods

To begin with, let us consider the way originally used by Waterman to derive the T-matrix of the outer Dirichlet problem (and only this problem is of our interest here). The final result will be identical with that one derived in Chap. 3 or 4 if choosing the weighting functions in our approach appropriately. As already mentioned in the introduction Waterman employed the "Extended Boundary Condition" (EBC) to derive the T-matrix. The resulting method is sometimes also called "Null-Field method". This latter notation expresses quite good the essential nature of the EBC and the original objective Waterman intended to achieve with it. Only after a couple of years it became obvious that the methods discussed in Sects. 1.3.1 and 2.2.3 of this book provide the same results. Surprisingly, we have to state that, despite the discovery of the equivalence of Rayleigh's method described in Chap. 1 and Waterman's EBC method for deriving the T-matrix, we can find statements even in the recent literature which prefer the EBC method for it is assumed that this method does not suffer from Rayleigh's hypothesis underlying Rayleigh's method. To understand this point of view we will take a closer look at the EBC method. The problem of Rayleigh's hypothesis is shifted to the next chapter.

Another choice of weighting functions will lead us to a different solution technique known as "Point Matching methods" (PMM) or "Collocation methods". These methods have been used quite often for solving boundary value problems in the history and can be considered to be special realizations of the general T-matrix approach. Moreover, these methods play an essential role in the context of Rayleigh's hypothesis. But on the other hand, one can observe that the conventional PMM become of less importance nowadays because of their numerical instabilities and restricted range of applicability if more realistic scenarios are considered.

5.2.1 The Extended Boundary Condition Method

Before we will come to the methodical details we want to start with some historical considerations since it casts an interesting light on the roots of the EBC in electromagnetic wave scattering theory.

The first paper (to the best of our knowledge!) on the T-matrix method with the title "Matrix Formulation of Electromagnetic Scattering" was published by Waterman in IEEE in 1965 (for the details see the reference chapter). This paper is aimed to present a method which does not suffer from numerical instabilities at the internal eigenresonances if electromagnetic wave scattering on an ideal metallic scatterer is considered. This scattering problem corresponds mathematically to the outer Dirichlet problem. What was the reason for those numerical instabilities? In the literature one can find the hint (in J. J. H. Wang: "Generalized Moment Methods in Electromagnetics", 1991, Sect. 6.6, for example) that such a numerical instability (or resonance) has been observed first in the papers of Mei and Van Bladel ("Scattering by

Perfectly-Conducting Rectangular Cylinders"), and of Andreasen ("Comments on 'Scattering by Perfectly-Conducting Rectangular Cylinders"'). But reading these two papers we can state already a problem with this resonance phenomenon. It can be found **only** in the first cited paper of Mei and Van Bladel at a certain size parameter. In this paper the authors employed a conventional boundary integral equation method (this method will be explained in more detail in Sect. 5.4 of this chapter) to solve the electromagnetic wave scattering problem on an ideal metallic cylinder with a rectangular cross-section. The cited paper of Andreasen is just a comment to the paper of Mei and Van Bladel in which he advised the authors of the existence of a resonance in one of their figures. Moreover, he discussed therein that he used a comparable solution method which does not exhibit this resonance and that it is actually not awaited at this parameter. This comment was commented afterwards by Mei, in which he stated that, performing the calculations presented in their first paper once again, the resonance phenomenon disappeared and the obtained results became in good agreement with the results of Andreasen even for the critical parameter. Thus, there was no longer observed any resonance phenomenon. But since this time there is still an uncertain feeling among many authors concerning such resonances which is especially related to the following argumentation: The boundary integral equation method used by Mei and Van Bladel assumes that the tangential projections of the total magnetic field must vanish identically if approaching the surface of an ideal metallic scatterer from inside. This is, of course, not true for the tangential projections of the magnetic field of internal eigenresonances since producing an equivalent surface current at the inner boundary surface of the resonator. The usual physical understanding of what we call an ideal metallic resonator assumes now that there is no relation between the induced surface current which is equivalent to a possibly existing internal resonance and the induced surface current which is equivalent to a possibly existing scattered field outside the resonator. Or, in other words: The inner region of an ideal metallic resonator is totally decoupled from its outer region, i.e., there is no scattering experiment from outside which will allow us to analyse an internal eigenresonance. Concerning the resonance phenomenon it was then argued that the method used by Mei and Van Bladel as well as several other boundary integral equation methods are not able to distinguish between these two induced surface currents, and that this situation may produce numerical instabilities. This argumentation forced Waterman to replace the conventional boundary integral equation method by a method which seems to be able to avoid such resonance phenomena. To achieve this goal he introduced the EBC. By the way, the EBC was discovered independently of Waterman by Ewald and Oseen in the field of molecular optics. There it was called the "Extinction Theorem". Only later on it was discovered by Agarwal that both expressions are equivalent (see the book of Nieto-Vesperinas in Sect. 10.9 of the reference chapter). Let us now see how Waterman's approach works in detail if applying it to the Green function of the outer Dirichlet problem and if he really reached his initial goal with this method.

Beside the radiation condition we required additionally the fulfilment of boundary condition (2.280) at the scatterer surface for the scalar Green function G_{Γ_+} related to the outer Dirichlet problem. This condition was replaced by Waterman by the

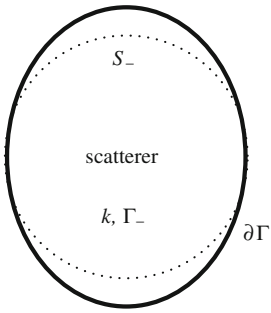

Fig. 5.1 S_- denotes the outer boundary surface of the subregion inside the scatterer to which the EBC is primarily applied

condition

$$G_{\Gamma_+}(\mathbf{x}, \mathbf{x}') = 0; \quad \mathbf{x} \in \Gamma_-; \ \mathbf{x}' \in \Gamma_+. \tag{5.1}$$

To avoid misunderstandings it should be mentioned that in the original paper of Waterman this was done for the total electric field and not for the scalar Green function. Condition (5.1) is obviously an extension of the former condition into the region Γ_- inside the scatterer. It is exactly the reason for calling this new condition the "Extended Boundary Condition". Waterman had demonstrated in his paper that the usually required vanishing of the tangential projections of the total electric field at the surface of an ideal metallic scatterer can be inferred from the vanishing of the electric field everywhere inside the scatterer. Since the magnetic field can be calculated by use of the "$\nabla\times$" operation if applied to the electric field the magnetic field it is also forced to vanish everywhere inside the scatterer. And this happens independent of whether there exist an internal resonance or not. According to Waterman, it is moreover sufficient to require that condition (5.1) is applied only to a subregion of Γ_-, for example to the region bounded by the spherical surface S_- (see Fig. 5.1). Using the procedure of continuing the field inside the subregion analytically he concluded the vanishing of this field everywhere inside the scatterer. But this procedure is described only verbal in his paper. This description ends with the remark that we "... assume, without further comment, that this analytic continuation procedure is valid". In the book of Doicu et al. already mentioned in Sect. 2.3.3 one can find a more precise mathematical justification for Waterman's assumption. So, let us also assume that it is correct. We place the source point $\mathbf{x}'$ outside the smallest spherical surface circumscribing the scatterer, as frequently done in the foregoing chapters. If the observation point is now placed somewhere in the subregion bounded by S_- we may write

$$G_{\Gamma_+}(\mathbf{x}, \mathbf{x}') := G_0^<(\mathbf{x}, \mathbf{x}') + \oint_{\partial\Gamma} G_0^<(\mathbf{x}, \bar{\mathbf{x}}) \cdot \tilde{W}_{\partial\Gamma}(\bar{\mathbf{x}}, \tilde{\mathbf{x}}) \cdot G_0^<(\tilde{\mathbf{x}}, \mathbf{x}')\, dS(\bar{\mathbf{x}})\, dS(\tilde{\mathbf{x}}) \tag{5.2}$$

as defining equation for the new interaction operator $\tilde{W}_{\partial\Gamma}$. It differs from definition (4.1) in using $G_0^<$ instead of $G_0^>$ in the boundary integral term on the right-hand side. Since $\mathbf{x}$ is somewhere inside S_- the usage of $G_0^<$, in contrast to the usage of $G_0^>$ in (4.1), is now justified without any doubt. Just to remember: $G_0^<$ solves the homogeneous Helmholtz equation and obeys the regularity requirement everywhere inside S_-. Combining (5.1) and (5.2) we get the integral equation

$$-G_0^<(\mathbf{x},\mathbf{x}') = \oint_{\partial\Gamma} G_0^<(\mathbf{x},\bar{\mathbf{x}}) \cdot \tilde{W}_{\partial\Gamma}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \cdot G_0^<(\tilde{\mathbf{x}},\mathbf{x}')\, dS(\bar{\mathbf{x}})\, dS(\tilde{\mathbf{x}}) \tag{5.3}$$

for observation points $\mathbf{x}$ inside S_-. This will allow us to determine the interaction operator $\tilde{W}_{\partial\Gamma}$. In Waterman's original paper there is used the induced surface current at the scatterer surface instead of the interaction operator introduced in (5.2). The interrelation between the induced surface current and the interaction operator will be clarified later on in Chap.7, as already mentioned in Sect. 4.3.1. Replacing $G_0^<$ by the (again finite!) approximation (2.278) (5.3) becomes

$$\begin{aligned} -(ik_0) \sum_{i=0}^{N} \psi_i(k_0,\mathbf{x}) \cdot \tilde{\varphi}_i(k_0,\mathbf{x}') \\ = (ik_0)^2 \sum_{i,k=0}^{N} \oint_{\partial\Gamma} \psi_i(k_0,\mathbf{x}) \cdot \tilde{\varphi}_i(k_0,\bar{\mathbf{x}}) \cdot \tilde{W}_{\partial\Gamma}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \cdot \psi_k(k_0,\tilde{\mathbf{x}}) \\ \cdot \tilde{\varphi}_k(k_0,\mathbf{x}')\, dS(\bar{\mathbf{x}})\, dS(\tilde{\mathbf{x}}). \end{aligned} \tag{5.4}$$

The equal sign is obviously justified if

$$(ik_0) \oint_{\partial\Gamma} \tilde{\varphi}_i(k_0,\bar{\mathbf{x}}) \cdot \tilde{W}_{\partial\Gamma}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \cdot \psi_k(k_0,\tilde{\mathbf{x}})\, dS(\bar{\mathbf{x}})\, dS(\tilde{\mathbf{x}}) = -\delta_{i,k} \tag{5.5}$$

holds. Next, we assume the following bilinear expansion for the interaction operator

$$\tilde{W}_{\partial\Gamma}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) = (ik_0)^{-1} \sum_{\alpha,\beta=0}^{N} \left[\tilde{W}_{\partial\Gamma}\right]_{\alpha,\beta} \cdot g_\alpha(\bar{\mathbf{x}}) \cdot h_\beta(\tilde{\mathbf{x}}). \tag{5.6}$$

$g_\alpha(\bar{\mathbf{x}})$ and $h_\beta(\tilde{\mathbf{x}})$ therein are not yet specified but linearly independent expansion functions at the scatterer surface. Inserting this expansion into (5.5) provides

$$\sum_{\alpha,\beta=0}^{N} \oint_{\partial\Gamma} \tilde{\varphi}_i(k_0,\bar{\mathbf{x}}) \cdot \left[\tilde{W}_{\partial\Gamma}\right]_{\alpha,\beta} \cdot g_\alpha(\bar{\mathbf{x}}) \cdot h_\beta(\tilde{\mathbf{x}}) \cdot \psi_k(k_0,\tilde{\mathbf{x}})\, dS(\bar{\mathbf{x}})\, dS(\tilde{\mathbf{x}}) = -\delta_{i,k}. \tag{5.7}$$

with the definition of the matrix elements of the two matrices $\mathbf{A}_{\partial\Gamma}^{(\tilde{\varphi}_0^*,g)}$ and $\mathbf{B}_{\partial\Gamma}^{(h^*,\psi_0)}$ according to

$$\left[A_{\partial\Gamma}^{(\tilde{\varphi}_0^*,g)}\right]_{i,k} := \oint_{\partial\Gamma} \tilde{\varphi}_i(k_0,\bar{\mathbf{x}}) \cdot g_k(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}) \tag{5.8}$$

and

$$\left[B_{\partial\Gamma}^{(h^*,\psi_0)}\right]_{i,k} := \oint_{\partial\Gamma} h_i(k_0,\tilde{\mathbf{x}}) \cdot \psi_k(k_0,\tilde{\mathbf{x}})\, dS(\tilde{\mathbf{x}}) \tag{5.9}$$

(please, note that this definition agrees with the scalar product definition (1.34) since we have used $h_i^*(k_0,\tilde{\mathbf{x}})$ in (5.9), for example, as weighting functions thus producing $h_i(k_0,\tilde{\mathbf{x}})$ in the boundary integral term!) we may write instead of (5.7) the matrix equation

$$\mathbf{A}_{\partial\Gamma}^{(\tilde{\varphi}_0^*,g)} \cdot \tilde{\mathbf{W}}_{\partial\Gamma} \cdot \mathbf{B}_{\partial\Gamma}^{(h^*,\psi_0)} \;=\; -\mathbf{E}. \tag{5.10}$$

From this, we get in a straightforward way the matrix equation

$$\tilde{\mathbf{W}}_{\partial\Gamma} = -\mathbf{A}_{\partial\Gamma}^{(\tilde{\varphi}_0^*,g)^{-1}} \cdot \mathbf{B}_{\partial\Gamma}^{(h^*,\psi_0)^{-1}} \tag{5.11}$$

to determine the expansion coefficients $\left[\tilde{W}_{\partial\Gamma}\right]_{\alpha,\beta}$ of the bilinear expansion of the interaction operator $\tilde{W}_{\partial\Gamma}$. Once we know approximation (5.6) we are able to present the corresponding approximation of the Green function $G_{\Gamma_+}(\mathbf{x},\mathbf{x}')$ for observation points $\mathbf{x}$ outside the smallest spherical surface circumscribing the scatterer (i.e., for observation points in Γ_+!). For these observation points we write instead of (5.2)

$$\begin{aligned} G_{\Gamma_+}(\mathbf{x},\mathbf{x}') &= G_0(\mathbf{x},\mathbf{x}') \\ &\quad + \oint_{\partial\Gamma} G_0^{>}(\mathbf{x},\bar{\mathbf{x}}) \cdot \tilde{W}_{\partial\Gamma}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \cdot G_0^{<}(\tilde{\mathbf{x}},\mathbf{x}')\, dS(\bar{\mathbf{x}})\, dS(\tilde{\mathbf{x}}), \end{aligned} \tag{5.12}$$

i.e., $G_0^{<}(\mathbf{x},\bar{\mathbf{x}})$ in the boundary integral term of (5.2) is now replaced without any problems by $G_0^{>}(\mathbf{x},\bar{\mathbf{x}})$. Utilizing the expansions of $G_0^{<}$ and $G_0^{>}$ as well as the bilinear expansion (5.6) we obtain

$$\begin{aligned} G_{\Gamma_+}^{(N)}(\mathbf{x},\mathbf{x}') &= G_0(\mathbf{x},\mathbf{x}') \\ &\quad + (ik_0) \cdot \sum_{i,k,\alpha,\beta=0}^{N} \oint_{\partial\Gamma} \varphi_i(k_0,\mathbf{x}) \cdot \tilde{\psi}_i(k_0,\bar{\mathbf{x}}) \left[\tilde{W}_{\partial\Gamma}\right]_{\alpha,\beta} \\ &\quad \cdot g_\alpha(\bar{\mathbf{x}}) \cdot h_\beta(\tilde{\mathbf{x}}) \cdot \psi_k(k_0,\tilde{\mathbf{x}}) \cdot \tilde{\varphi}_k(k_0,\mathbf{x}')\, dS(\bar{\mathbf{x}})\, dS(\tilde{\mathbf{x}}). \end{aligned} \tag{5.13}$$

This expression can be rewritten into

$$\begin{aligned} G_{\Gamma_+}^{(N)}(\mathbf{x},\mathbf{x}') &= G_0(\mathbf{x},\mathbf{x}') \\ &\quad + (ik_0) \cdot \sum_{i,k=0}^{N} \left[W_{\partial\Gamma_+}\right]_{i,k} \cdot \varphi_i(k_0,\mathbf{x}) \cdot \tilde{\varphi}_k(k_0,\mathbf{x}'). \end{aligned} \tag{5.14}$$

With the definitions

$$\left[C_{\partial\Gamma}^{(\tilde{\psi}_0^*,g)}\right]_{i,k} := \oint_{\partial\Gamma} \tilde{\psi}_i(k_0,\bar{\mathbf{x}}) \cdot g_k(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}) \tag{5.15}$$

and

$$\left[D_{\partial\Gamma}^{(h^*,\psi_0)}\right]_{i,k} := \oint_{\partial\Gamma} h_i(k_0,\tilde{\mathbf{x}}) \cdot \psi_k(k_0,\tilde{\mathbf{x}})\, dS(\tilde{\mathbf{x}}) \tag{5.16}$$

of the elements of the matrices $\mathbf{C}_{\partial\Gamma}^{(\tilde{\psi}_0^*,g)}$ and $\mathbf{D}_{\partial\Gamma}^{(h^*,\psi_0)}$ we can calculate the new elements $\left[W_{\partial\Gamma_+}\right]_{i,k}$ in (5.14) from

$$\mathbf{W}_{\partial\Gamma_+} = -\mathbf{C}_{\partial\Gamma}^{(\tilde{\psi}_0^*,g)} \cdot \mathbf{A}_{\partial\Gamma}^{(\tilde{\varphi}_0^*,g)^{-1}} \cdot \mathbf{B}_{\partial\Gamma}^{(h^*,\psi_0)^{-1}} \cdot \mathbf{D}_{\partial\Gamma}^{(h^*,\psi_0)}. \tag{5.17}$$

But since both matrices $\mathbf{B}_{\partial\Gamma}^{(h^*,\psi_0)}$ and $\mathbf{D}_{\partial\Gamma}^{(h^*,\psi_0)}$ are obviously identical we end up with the simpler matrix equation

$$\mathbf{W}_{\partial\Gamma_+} = -\mathbf{C}_{\partial\Gamma}^{(\tilde{\psi}_0^*,g)} \cdot \mathbf{A}_{\partial\Gamma}^{(\tilde{\varphi}_0^*,g)^{-1}}. \tag{5.18}$$

This result agrees with that one obtained by Waterman in his 1965 paper (see Eqs. (7) and (14) therein!) if using the radiating eigensolutions $\varphi_\alpha(k_0,\bar{\mathbf{x}})$ and $\varphi_\beta(k_0,\tilde{\mathbf{x}})$ of the scalar Helmholtz equation as expansion functions $g_\alpha(\bar{\mathbf{x}})$ and $h_\beta(\tilde{\mathbf{x}})$ in the bilinear expansion (5.6). On the other hand, if choosing $\varphi_i^*(k_0,\mathbf{x})$ as weighting functions in (2.21) and (2.22), and if taking symmetry relation (4.46) additionally into account, then an intercomparison of (5.18) with (2.19) reveals the equality of both expressions. From this, we can infer the equality of approximation (5.14) and (4.8). Thus, we can state that, if choosing the expansion and weighting functions appropriately, the EBC method as well as Rayleigh's method may result in the same approximation of the Green function related to the outer Dirichlet problem.

Now, let us come back to the initially mentioned resonance phenomenon which was expected to be avoidable by use of the EBC. The above obtained result would then suggest that the same holds for the homogeneous Dirichlet condition valid solely at the scatterer surface. But looking at Sect. 3 of Waterman's 1965 paper shows us that this is not true. In this chapter, he discussed the corresponding eigenvalue problem of a nonspherical but ideal metallic resonator and its solution in terms of the appropriately modified EBC (see Eq. (17a) in this paper). The relevant matrix is identical with the matrix $\mathbf{C}_{\partial\Gamma}^{(\tilde{\psi}_0^*,g)}$ derived above. The values of k_0 for which its determinant becomes zero are the eigenvalues, i.e., the resonance frequencies of the problem. Fortunately, according to (5.18) for the scattering problem we just have to invert matrix $\mathbf{A}_{\partial\Gamma}^{(\tilde{\varphi}_0^*,g)}$, and not matrix $\mathbf{C}_{\partial\Gamma}^{(\tilde{\psi}_0^*,g)}$. Therefore, (5.18) will be not affected by a zero or nearly zero determinant of this matrix. But the situation changes if using the regular eigensolutions of the scalar Helmholtz equation instead of the radiating

ones in the bilinear expansion (5.6). This would correspond to choosing the regular eigensolutions as expansion functions for the induced surface current in Waterman's paper (see Eq. (6) therein). Then, we have to invert indeed even the critical matrix. But this will produce at least numerical problems near or at the eigenfrequencies, of course. Therefore, also if using the EBC to derive the T-matrix the occurrence of resonance phenomena depends strongly on the appropriate choice of expansion functions and can not be excluded from the beginning. That is exactly what was expressed more mathematically in Sect. 2.3.3 when considering the properties of the eigensolutions of Helmholtz's equation. There we pointed out that the regular eigensolutions are only linearly independent at the scatterer surface as long as k_0^2 is not an eigenvalue of the inner Dirichlet problem. Waterman has achieved his initial goal of avoiding resonances only by choosing the "correct" expansion functions, i.e., the radiating eigensolutions to approximate the induced surface current. But despite of this, with the EBC method he has offered a new solution technique for the scattering problem which became very successfully aftermath in many applications. We can therefore consider this 1965 paper as a milestone in the treatment of electromagnetic and acoustic wave scattering on nonspherical objects.

5.2.2 Point Matching Methods

This method is straightforward and very simple. Instead of (1.29) we can use the simpler boundary condition

$$\sum_{i=0}^{N} a_i^{(N)} \cdot \varphi_i(k_0, \mathbf{x}) = -\sum_{i=0}^{N} b_i \cdot \psi_i(k_0, \mathbf{x}); \quad \mathbf{x} \in \partial\Gamma \tag{5.19}$$

if the scalar outer Dirichlet problem is considered. But instead of this boundary condition we can also employ the transformation character of the T-matrix as a starting point. According to (2.17) we may write

$$\psi_i(k_0, \mathbf{x}) = \sum_{k=0}^{N} \left[\tilde{T}_{\partial\Gamma}\right]_{i,k} \cdot \varphi_k(k_0, \mathbf{x}); \quad i = 0, \ldots, N; \quad \mathbf{x} \in \partial\Gamma. \tag{5.20}$$

Both relations produces the same T-matrix, as already demonstrated in Chap. 1 and 2. For the conventional PMM it is simply required that both relations are fulfilled exactly only at $(N+1)$ selected points $\mathbf{x_j}$ $(j = 0, \ldots, N)$ at the scatterer surface $\partial\Gamma$. Then, we have the same number of matching points and unknown expansion coefficients $a_i^{(N)}$ in (5.19), for example. It is easy to see that this produces a T-matrix (2.19) of the size $(N+1) \times (N+1)$. The constituting matrices $\mathbf{A}_{\partial\Gamma}$ and $\mathbf{B}_{\partial\Gamma}$ are given by the values of the radiating and regular eigenfunctions at the selected surface points, i.e., by

$$[A_{\partial\Gamma}]_{i,j} = \varphi_j(k_0, \mathbf{x_i}) \tag{5.21}$$

$$[B_{\partial\Gamma}]_{i,j} = \psi_j(k_0, \mathbf{x_i}). \tag{5.22}$$

In accordance with (2.21) and (2.22) we obtain these matrix elements of the conventional PMM if choosing the scalar delta distribution at the scatterer surface defined in (3.6) as weighting functions,

$$g_i(\mathbf{x}) = \delta_{\partial\Gamma}(\mathbf{x} - \mathbf{x_i}); \quad i = 0, \ldots, N. \tag{5.23}$$

On the other hand, if considering the vectorial case of the outer Dirichlet problem we have to use

$$\vec{g}_{i,\tau}(\mathbf{x}) = \delta_{\partial\Gamma}(\mathbf{x} - \mathbf{x}_{\mathbf{i},\tau}) \cdot \hat{x}_1 + \delta_{\partial\Gamma}(\mathbf{x} - \mathbf{x}_{\mathbf{i},\tau}) \cdot \hat{x}_2 + \delta_{\partial\Gamma}(\mathbf{x} - \mathbf{x}_{\mathbf{i},\tau}) \cdot \hat{x}_3 \tag{5.24}$$

instead of (5.23) with $i = 0, \ldots, N$ and $\tau = 1, 2$. This produces again 2×2 block matrices, due to the additional τ-dependence.

The conventional PMM is not very stable and converges poorly even at the boundary surface but between the selected points, as it was experienced in many applications. But a slight change in the method results in drastic improvements. This change consists in choosing more matching points $\mathbf{x}_i$ along $\partial\Gamma$ than we have unknown expansion coefficients. The resulting overdetermined equation system is solved afterwards by employing a least-squares scheme. This can be done, for example, by use of the "Singular Value Decomposition" method. The thus modified conventional PMM is sometimes called the "generalized PMM".

5.3 The Method of Lines as a Special Finite-Difference Method

This section is concerned with a special Finite-Difference method. The method is called the "Method of Line" (MoL) for obvious reasons as we will see shortly. It was developed between 1950 and 1960 by Russian mathematicians, but sunk into oblivion until the advent of modern and powerful computers in science. Since 1980s it became of growing importance in several applications but especially in microwave technology and integrated optics. However, in all of these cases the application of the MoL was restricted to boundary value problems with boundary surfaces along constant coordinate lines in separable coordinate systems. Not till the beginning of the 1990s our group at the German Aerospace Center started with an upgrading of this method to the problem of light scattering on nonspherical particles in spherical coordinates as well as on infinitely extended cylinders with nonspherical cross-sections in cylindrical coordinates. Ultimately, these activities have led us to a new and more critical view on this special method and on the Finite-Difference methods in general. The reason for this rethinking will be explained in detail in this section. To anticipate the most important and somewhat provocative result: The Finite-Difference

methods are only a worsening of the Separation of Variables method and are not really advantageous if applied to the scattering problems discussed in this book. In what follows, we will show that there are tangible arguments supporting this opinion. But to avoid misunderstandings it should be emphasized that we do not want to claim that the Finite-Difference methods may produce wrong or incorrect results. They are, of course, a possible approach to solve the scattering problems of our interest. But these methods offer no evident advantages compared to other techniques. That these methods are widely used in the context of scattering, and that there still exist questionable point of views regarding the nature of this method are the essential reasons to include the MoL as a representative of the Finite-Difference methods in this book. Starting from a detailed discussion of the mathematical background, we will hopefully be able to provide a better understanding of the Finite-Difference methods thus supporting a more realistic estimate of their advantages and disadvantages in a certain application.

5.3.1 Discretization of the Scalar Helmholtz Equation and its Solution

Replacing the differential operator completely (conventional Finite-Difference methods) or partially (MoL) by appropriate difference schemes is the crucial step in all of the Finite-Difference techniques. In this way, the original partial differential equation will be substituted by a system of algebraic equations (conventional Finite-Difference methods) or a system of ordinary differential equations (MoL). So far, it is assumed that replacing the differential operator makes the essential methodical difference compared to those methods retaining the differential operator as it is but approximating the unknown function in terms of series expansions instead. The latter methods are sometimes called spectral methods. This at first glance simple concept in conjunction with the drastic improvements of our computational capabilities during the last decades are the main reasons for assuming the Finite-Difference methods to represent the most general and most easy to handle methods for solving scattering problems, for example. Appropriate arguments can be found frequently in recent papers and books. The preference of Finite-Difference methods is moreover supported by the fact that every solution technique is finally submitted to a certain discretization procedure if accomplished on a computer. But by use of the MoL, we will show now that such point of views deserve a correction. That is because, we can demonstrate that the original replacement of the differential operator can be transformed into an equivalent approximation of the unknown function in terms of a series expansion. In doing so, the MoL will lead us to specific expansion functions. We will demonstrate later that these expansion functions are nothing but a worsening of the known eigensolutions of the scalar Helmholtz equation in spherical coordinates discussed earlier in Sect. 2.3. The following considerations are restricted to axisymmetric scatterer geometries for simplicity.

Separating the ϕ-dependent part of the scalar Helmholtz equation (2.46) by use of the Fourier series

$$u(r, \theta, \phi) = \sum_l e^{il\phi} \cdot \tilde{u}^{(l)}(r, \theta), \tag{5.25}$$

results in the modified partial differential equation

$$\begin{aligned} &\left(\tilde{\nabla}^2 + k^2 r^2\right) \tilde{u}^{(l)}(r, \theta) = 0 \\ &\tilde{\nabla}^2 = \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{\sin\theta} \frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta}\right) - \frac{l^2}{\sin^2\theta} \end{aligned} \tag{5.26}$$

for the unknown functions $\tilde{u}^{(l)}(r, \theta)$. Using this partial differential equation as a starting point is thus a consequence of the restriction to axisymmetric scatterers. Regarding the θ-dependence the functions $\tilde{u}^{(l)}(r, \theta)$ must obey conditions (2.68) and (2.69). To solve (5.26) by use of the MoL we replace all the derivatives with respect to θ by an equidistant discretization procedure within the interval $[0, \pi]$, i.e., we cover this interval with N_d radial lines starting from the origin. Please, note that the nonequidistant case is not of our interest here since providing no new insights. In contrast to the conventional Finite-Difference methods all derivatives with respect to the radial coordinate remain unaffected. Employing the discretization procedure with respect to θ we have to distinguish carefully the two cases with azimuthal modes $l = 0$ and $l \neq 0$. The two different discretization schemes are depicted in Figs. 5.2 and 5.3.

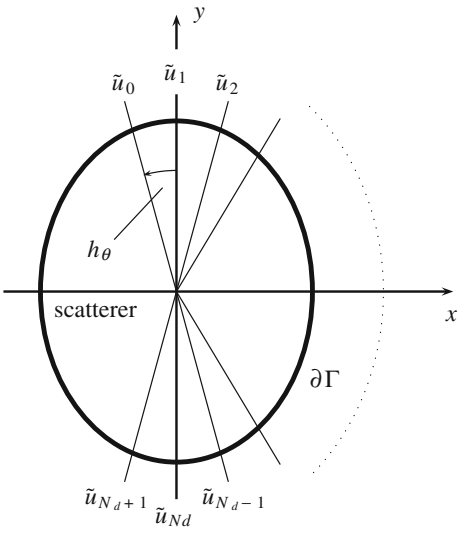

Fig. 5.2 Equidistant discretization procedure for $l = 0$ (homogeneous Neumann condition). We have $h_\theta = \pi/(N_d - 1)$; $\theta_i = (i-1)h_\theta$, and $i = 1, \ldots, N_d$

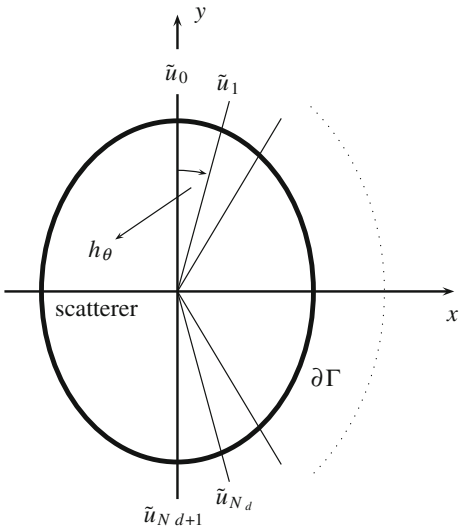

Fig. 5.3 Equidistant discretization procedure for $l \neq 0$ (homogeneous Dirichlet condition). We have $h_\theta = \pi/(N_d + 1)$; $\theta_i = i h_\theta$, and $i = 1, \ldots, N_d$

Obviously, at $\theta = 0, \pi$ the homogeneous Neumann condition is fulfilled only approximately whereas the homogeneous Dirichlet condition is reproduced exactly by use of this discretization procedure. We are now interested on the radial dependent solutions of (5.26) along the discretization lines. We assume further that each possible discretization line crosses the boundary surface of the scatterer only once. This is called a star-shaped scatterer geometry. All first derivatives with respect to θ may be replaced by an appropriate left-hand (subscript ls), right-hand (subscript rs), or central (subscript zt) discretization operator according to

$$\frac{\partial}{\partial\theta} \Rightarrow \frac{1}{h_\theta}\mathbf{D}_{ls}^{(\alpha)}, \quad \frac{1}{h_\theta}\mathbf{D}_{rs}^{(\alpha)}, \quad \text{or} \quad \frac{1}{h_\theta}\mathbf{D}_{zt}^{(\alpha)} \tag{5.27}$$

with superscript α denoting whether the homogeneous Neumann condition (NC) or the homogeneous Dirichlet condition (DC) is fulfilled at $\theta = 0, \pi$. These discretization operators are nothing but square matrices of the size $N_d \times N_d$. They read

$$\mathbf{D}_{ls}^{(\alpha)} = \begin{pmatrix} l_1 & 0 & 0 & 0 & \ldots & \ldots & 0 \\ -1 & 1 & 0 & 0 & 0 & \ldots & 0 \\ 0 & -1 & 1 & 0 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \ldots & \ldots & 0 & -1 & 1 & 0 \\ 0 & \ldots & \ldots & \ldots & 0 & l_2 & l_3 \end{pmatrix} \tag{5.28}$$

$$\mathbf{D}_{rs}^{(\alpha)} = \begin{pmatrix} r_1 & r_2 & 0 & 0 & \dots & \dots & 0 \\ 0 & -1 & 1 & 0 & 0 & \dots & 0 \\ 0 & 0 & -1 & 1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & \dots & 0 & 0 & -1 & 1 \\ 0 & \dots & \dots & \dots & 0 & 0 & r_3 \end{pmatrix} \tag{5.29}$$

$$\mathbf{D}_{zt}^{(\alpha)} = \begin{pmatrix} 0 & c_1 & 0 & 0 & \dots & \dots & 0 \\ -1 & 0 & 1 & 0 & 0 & \dots & 0 \\ 0 & -1 & 0 & 1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & \dots & 0 & -1 & 0 & 1 \\ 0 & \dots & \dots & \dots & 0 & c_2 & 0 \end{pmatrix}. \tag{5.30}$$

In dependence on the boundary condition at $\theta = 0, \pi$ the constants in these matrices are given by

–	l_1	l_2	l_3	r_1	r_2	r_3	c_1	c_2
NC	0	0	0	0	0	0	0	0
DC	1	−1	1	−1	1	−1	1	−1

The second derivative with respect to θ is replaced by the discretization operator

$$\frac{\partial^2}{\partial\theta^2} \Rightarrow \frac{1}{{h_\theta}^2}\,\mathbf{D}_z^{(\alpha)}. \tag{5.31}$$

This operator can be calculated from the Taylor expansion

$$\tilde{u}^{(l)}(r, \theta_{i\pm1}) = \tilde{u}^{(l)}(r, \theta_i) \pm \frac{h_\theta}{1!}\left(\frac{\partial\tilde{u}^{(l)}}{\partial\theta}\right)_{\theta_i} \pm \frac{h_\theta^2}{2!}\left(\frac{\partial^2\tilde{u}^{(l)}}{\partial\theta^2}\right)_{\theta_i} \pm \cdots \tag{5.32}$$

of the function $\tilde{u}^{(l)}(r, \theta)$ of (5.25) at a fixed angle θ_i. Employing the Taylor series up to the second order results in

$$\left(\frac{\partial^2\tilde{u}^{(l)}}{\partial\theta^2}\right)_{\theta_i} = \frac{1}{{h_\theta}^2} \cdot \left(\tilde{u}^{(l)}(r, \theta_{i-1}) - 2 \cdot \tilde{u}^{(l)}(r, \theta_i) + \tilde{u}^{(l)}(r, \theta_{i+1})\right). \tag{5.33}$$

The corresponding discretization operator thus becomes

$$\mathbf{D}_z^{(\alpha)} = \begin{pmatrix} 2 & z_1 & 0 & 0 & \dots & \dots & 0 \\ -1 & 2 & -1 & 0 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & \dots & 0 & -1 & 2 & -1 \\ 0 & \dots & \dots & \dots & 0 & z_2 & 2 \end{pmatrix} \tag{5.34}$$

with constants

–	z_1	z_2
NC	-2	-2
DC	-1	-1

Next, we apply these discretization operators to (5.26). In this way, we obtain the following system of coupled ordinary differential equations for the radial dependent functions $\tilde{u}^{(l)}(r, \theta_i)$ on the discretization lines:

$$\left\{ h_\theta^2 \left[\frac{d}{dr} \left(r^2 \frac{d}{dr} \right) + k^2 r^2 \right] \cdot \mathbf{E} - \mathbf{P}^{(l)} \right\} \cdot \mid \tilde{u}^{(l)}(r) >= \mid 0 > . \tag{5.35}$$

Taking the two different cases $l = 0$ and $l \neq 0$ into account, and because of

$$\mathbf{P}^{(0)} = \mathbf{D}_z^{(NC)} - diag(\kappa) \cdot \mathbf{D}_{rs}^{(NC)} \tag{5.36}$$

and

$$\mathbf{P}^{(l)} = \mathbf{D}_z^{(DC)} - diag(\kappa) \cdot \mathbf{D}_{rs}^{(DC)} + diag(\gamma^{(l)}) \tag{5.37}$$

we get for the matrices $\mathbf{P}^{(l)}$ the expressions

$$\mathbf{P}^{(0)} = \begin{pmatrix} 2 & -2 & 0 & 0 & \dots & \dots & 0 \\ -1 & (2+\kappa_2) & -(1+\kappa_2) & 0 & 0 & \dots & 0 \\ 0 & -1 & (2+\kappa_3) & -(1+\kappa_3) & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & \dots & 0 & -1 & (2+\kappa_{Nd-1}) & -(1+\kappa_{Nd-1}) \\ 0 & \dots & \dots & \dots & 0 & -2 & 2 \end{pmatrix} \tag{5.38}$$

and

$$\mathbf{P}^{(l)} = \begin{pmatrix} (2+\kappa_1 & -(1+\kappa_1) & 0 & 0 & \dots & \dots & 0 \\ +\gamma_1^{(l)}) & & & & & & \\ -1 & (2+\kappa_2 & -(1+\kappa_2) & 0 & 0 & \dots & 0 \\ & +\gamma_2^{(l)}) & & & & & \\ 0 & -1 & (2+\kappa_3 & -(1+\kappa_3) & 0 & \dots & 0 \\ & & +\gamma_3^{(l)}) & & & & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & -1 & (2+\kappa_{Nd-1} & -(1+ \\ & & & & & +\gamma_{Nd-1}^{(l)}) & \kappa_{Nd-1}) \\ 0 & 0 & \dots & \dots & 0 & -1 & (2+ \\ & & & & & & \kappa_{Nd}+\gamma_{Nd}^{(l)}) \end{pmatrix} \tag{5.39}$$

$\gamma_i^{(l)}$ and κ_i therein are given by

$$\gamma_i^{(l)} = \frac{h_\theta^2 l^2}{\sin^2 \theta_i} \tag{5.40}$$

$$\kappa_i = h_\theta \cdot \cot \theta_i . \tag{5.41}$$

$\mathbf{E}$ is the unit matrix and h_θ denotes the equidistant discretization angle. The N_d-dimensional "ket" vector $|\, \tilde{u}^{(l)}(r) >$ is the transpose of the row vector with the radial dependent functions $\tilde{u}^{(l)}(r, \theta_i)$ as its components, i.e.,

$$|\, \tilde{u}^{(l)}(r) > = \left(\tilde{u}^{(l)}(r, \theta_1), \dots, \tilde{u}^{(l)}(r, \theta_{Nd},) \right)^{tp} . \tag{5.42}$$

This corresponds to the definition (1.24) introduced in Chap. 1.

The derived system of coupled but ordinary differential equations seems to offer no essential advantages compared to the original partial differential equation, at first glance. But it can be shown that both the tridiagonal coupling matrices (5.38) and (5.39) may be transformed into diagonal matrices thus resulting in a decoupling of the system of ordinary differential equations. This is a consequence of the special form of (5.38) and (5.39) since every nonsymmetric but tridiagonal matrix

$$\mathbf{P}^{(l)}_{unsym.} = \begin{pmatrix} \alpha_1 & -\beta_2 & 0 & 0 & \dots & \dots & 0 \\ -\gamma_2 & \alpha_2 & -\beta_3 & 0 & 0 & \dots & 0 \\ 0 & -\gamma_3 & \alpha_3 & -\beta_4 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & \dots & 0 & -\gamma_{Nd-1} & \alpha_{Nd-1} & -\beta_{Nd} \\ 0 & \dots & \dots & \dots & 0 & -\gamma_{Nd} & \alpha_{Nd} \end{pmatrix}, \tag{5.43}$$

with $\gamma_i \cdot \beta_i > 0$ may be brought into a symmetric form by use of an similarity transformation . This is achieved by

$$\mathbf{P}^{(l)}_{sym.} = \mathbf{Z}^{(l)^{-1}} \cdot \mathbf{P}^{(l)}_{unsym.} \cdot \mathbf{Z}^{(l)}. \tag{5.44}$$

$$\left[z^{(l)}\right]_{1,1} = 1, \quad \text{and} \quad \left[z^{(l)}\right]_{i,i} = \left(\frac{\gamma_2 \cdot \ldots \cdot \gamma_i}{\beta_2 \cdot \ldots \cdot \beta_i}\right)^{1/2} \tag{5.45}$$

are the elements of the diagonal transformation matrix $\mathbf{Z}^{(l)}$. The resulting elements of matrix (5.44) read

$$\left[p^{(l)}_{sym.}\right]_{i,i} = \alpha_i; \qquad \left[p^{(l)}_{sym.}\right]_{i,i+1} = \left[p^{(l)}_{sym.}\right]_{i+1,i} = -\left(\beta_{i+1} \cdot \gamma_{i+1}\right)^{1/2}. \tag{5.46}$$

By applying a principal axis transformation to this symmetric matrix we are able to transform it into a diagonal matrix. For this, we have to consider the eigenvalue problem

$$\left(\mathbf{P}^{(l)}_{sym.} - \lambda^{(l)}_i \cdot \mathbf{E}\right) \cdot \vec{x}^{\,(l)}_i = \vec{0} \tag{5.47}$$

which must be solved for each azimuthal mode l independently. The resulting eigenvectors $\vec{x}^{\,(l)}_i$ form the columns of the required transformation matrix $\mathbf{H}^{(l)}$. Unfortunately, problem (5.47) can be solved only numerically in spherical coordinates. Fortunately, this solution provides no essential difficulties and can be performed with numerical standard methods. It is, however, not necessary to solve this problem numerically, as we will see shortly. But for a moment let us assume that we have solved the problem successfully. Then we are able to accomplish the decoupling of the system (5.35). For this, we define the transformed solution vector according to

$$|\,\tilde{u}^{(l)}(r)\,> = \mathbf{Tr}^{(l)^{-1}} \cdot |\,\tilde{u}^{(l)}(r)\,> \tag{5.48}$$

with

$$\mathbf{Tr}^{(l)} = \mathbf{Z}^{(l)} \cdot \mathbf{H}^{(l)} \tag{5.49}$$

$$\mathbf{Tr}^{(l)^{-1}} = \mathbf{H}^{(l)^{-1}} \cdot \mathbf{Z}^{(l)^{-1}} \tag{5.50}$$

being the overall transformation matrix of the diagonalization. This matrix is characterized by its property

$$\mathbf{Tr}^{(l)^{-1}} \cdot \mathbf{Tr}^{(l)} = \mathbf{Tr}^{(l)} \cdot \mathbf{Tr}^{(l)^{-1}} = \mathbf{E}. \tag{5.51}$$

Inserting the unit matrix $\mathbf{E} = \mathbf{Tr}^{(l)} \cdot \mathbf{Tr}^{(l)^{-1}}$ in between the expressions $\mathbf{P}^{(l)}$ and $|\,\tilde{u}^{(l)}(r)\,>$ of (5.35), multiplying the resulting equation with $\mathbf{Tr}^{(l)^{-1}}$ afterwards, taking the property

$$\mathbf{Tr}^{(l)^{-1}} \cdot \mathbf{P}^{(l)} \cdot \mathbf{Tr}^{(l)} = diag(\lambda^{(l)}) \tag{5.52}$$

into account, and, finally, substituting

$$\rho = k \cdot r \tag{5.53}$$

and

$$\bar{u}_i^{(l)}(\rho) = \frac{1}{\sqrt{\rho}} \cdot B_i^{(l)}(\rho) \tag{5.54}$$

provides the following ordinary differential equation for each of the component of the transformed and according to (5.54) substituted solution vector $|\, \bar{u}^{(l)}(\rho) >$:

$$\frac{d^2 B_i^{(l)}(\rho)}{d\rho^2} + \frac{1}{\rho} \cdot \frac{d B_i^{(l)}(\rho)}{d\rho} + \left[1 - \frac{\nu_i^{(l)^2}}{\rho^2} \right] \cdot B_i^{(l)}(\rho) = 0. \tag{5.55}$$

Here we have

$$\nu_i^{(l)^2} = \frac{\lambda_i^{(l)}}{h_\theta^2} + \frac{1}{4}, \quad i = 1, \ldots, N_d. \tag{5.56}$$

Equation (5.55) is nothing but Bessel's ordinary differential equation. Its solution was already discussed in Chap. 2. Therefore, if the radiation condition (2.76) must additionally be taken into account, we obtain

$$\bar{u}_i^{(l)}(\rho) = c_{l,i}^{(N_d)} \cdot \frac{H_{\nu_i^{(l)}}^{(1)}(\rho)}{\sqrt{\rho}} \tag{5.57}$$

as the general solution for each component of $|\, \bar{u}^{(l)}(\rho) >$. If the regularity is required we have on the other hand

$$\bar{u}_i^{(l)}(\rho) = c_{l,i}^{(N_d)} \cdot \frac{J_{\nu_i^{(l)}}(\rho)}{\sqrt{\rho}} \tag{5.58}$$

with unknown coefficients $c_{l,i}^{(N_d)}$ in both cases. The difference to the solutions given in (2.65) and (2.66) consists in the order of the Bessel and Hankel functions. In (5.57) and (5.58) these orders are defined via the eigenvalues of the eigenvalue problem (5.47) according to relation (5.56). Having determined the formal solution of the discretized Helmholtz equation in the transformed region we have to go back to the original region. This can be accomplished with the inverse of (5.48), i.e., by

$$|\, \tilde{u}^{(l)}(\rho) >= \mathbf{Tr}^{(l)} \cdot |\, \bar{u}^{(l)}(\rho) > . \tag{5.59}$$

Thus, we get for the general solution of the discretized Helmholtz equation (5.26) in the intersection points of the discretization lines with the scatterer surface $\partial\Gamma$

$$| u_{l,n}(\rho_i, \phi) >= c_{l,n}^{(N_d)} \cdot | \tilde{x}_{l,n} >= c_{l,n}^{(N_d)} \cdot e^{il\phi} \cdot \mathbf{U}_n^{(l)} \cdot \vec{x}_n^{(l)}. \tag{5.60}$$

$\mathbf{U}_n^{(l)}$ therein are diagonal matrices with elements

$$\left[U_n^{(l)}\right]_{i,i} = \frac{Z_{\nu_n^{(l)}}(\rho_i)}{\sqrt{\rho_i}}, \quad i = 1, \ldots, N_d, \tag{5.61}$$

and $Z_{\nu_n^{(l)}}$ are Bessel's functions $J_{\nu_n^{(l)}}$ or Hankel's functions of first kind $H^{(1)}_{\nu_n^{(l)}}$, depending on whether the regularity requirement or the radiation condition must be additionally fulfilled. Expression $\rho_i = k \cdot r_i$ denotes the the respective argument at the intersection point of the considered discretization line with the scatterer surface according to (5.53). The N_d-dimensional vectors $| \tilde{x}_{l,n} >$ are the eigenvectors $\vec{x}_n^{(l)}$ of the eigenvalue problem (5.47) but modified by the term $e^{il\phi} \cdot \mathbf{U}_n^{(l)}$. Note moreover that i in $e^{il\phi}$ represents the imaginary unit and not the summation index. The best way to convince oneself that (5.60) is indeed a consequence of Eq. (5.59) is to write down explicitly the inverse transformation for two discretization lines only. In doing so the transformation matrix $\mathbf{Tr}^{(l)}$ with eigenvectors $\vec{x}_n^{(l)}$ as its columns can considered to be a known quantity.

The following statement is the most important result of the procedure described just now: Vector $| u(\rho_i, \phi) >$ with a finite number of components defined at the intersection points of the discretization lines with the scatterer surface $\partial\Gamma$ can be represented by a finite series in terms of the eigenvectors $| \tilde{x}_{l,n} >$ given in (5.60) according to

$$| u(\rho_i, \phi) >= \sum_l \sum_{n=1}^{N} c_{l,n}^{(N)} \cdot | \tilde{x}_{l,n} >, \quad N \leq N_d. \tag{5.62}$$

The unknown expansion coefficients $c_{l,n}^{(N)}$ can be determined afterwards by applying the Rayleigh method described in Chap. 1. The modified eigenvectors $| \tilde{x}_{l,n} >$, in contrast to the original eigenvectors $\vec{x}_n^{(l)}$ of the eigenvalue problem (5.47), are not orthogonal, in general. Their orthogonality holds only if the scatter surface is a spherical one, due to the resulting constancy of the arguments ρ_i.

5.3.2 *The Limiting Behaviour of the Method of Lines*

What are the consequences of (5.62) for the conceptual interpretation of the MoL? This is what we try to find out in this subsection. The most remarkable aspect of (5.62) is the fact that it transforms the initial discretization of the differential operator of

Helmholtz's equation into an equivalent approximation of the unknown solution in terms of a finite series expansion. But that is exactly what is known from all the spectral methods, including the Separation of Variables method. Thus, the following question arises: What are the differences between the eigensolutions of the Helmholtz equation discussed in Sect. 2.3.1 and the eigenvectors $\vec{x}_n^{(l)}$ of the eigenvalue problem (5.47) we have to solve if employing the MoL? On the one hand, both eigensolutions differ in the order of the Bessel functions and Hankel functions of the first kind. Applying the Separation of Variables method these orders are given by semi-integer numbers (see Sect. 2.3.1). In the MoL the orders are calculated from the eigenvalues according to (5.56). At first glance, these orders are not even semi-integer numbers. On the other hand, both eigensolutions differ in the θ-dependence of the eigenvectors. In the Separation of Variables method this dependency is expressed by the associated Legendre polynomials. In the MoL we have the N_d-dimensional and orthogonal eigenvectors $\vec{x}_n^{(l)}$ instead. These are the only differences! Thus, we are faced with a strange situation. Both approaches the Separation of Variables method and the MoL result in an expansion of a continuously varying function $| f >$ with respect to θ at $\partial\Gamma$ or a discrete function $| f >$ defined at the intersection points θ_i along $\partial\Gamma$ into the corresponding eigenvectors of the respective method. At least for a spherical scatterer surface we may expect from both expansions that they will approximate the continuously varying or discrete function $| f >$ at this surface in the sense of the criteria discussed in Sect. 2.2.1, for example, if the relevant parameters are chosen appropriately. But then the above mentioned differences should disappear since both methods claim to solve the eigenvalue problems of Helmholtz's equation without further approximations. And this is what we can indeed demonstrate if going back to the eigenvalue problem (5.47). It determines the essential elements of the MoL, the orders of the components of the discrete expansion vectors and the expansion vectors itself. An "appropriate choice of the relevant parameters" means an increase of the number N_d of discretization lines within the interval $[0, \pi]$. We have therefore to prove if the relations

$$\lim_{N_d \to \infty} \vec{x}_n^{(l)} = P_n^l \tag{5.63}$$

$$\lim_{N_d \to \infty} \nu_n^{(l)} = n + \frac{1}{2} \tag{5.64}$$

hold for the eigenvectors and eigenvalues of the MoL. A numerical treatment of (5.47) in spherical coordinates reveals the correctness of these relations. For each arbitrary number N_d we obtain already eigenvectors $\vec{x}_n^{(l)}$ which agree by all but a constant factor with the associated Legendre polynomials P_n^l calculated at the discrete points θ_i. This factor is a consequence of the different normalization used in each of the methods. In the MoL, the normalization of the finite-dimensional eigenvectors is usually performed according to

$$< x_m^{(l)} \mid x_n^{(l)} >= \delta_{m,n}. \tag{5.65}$$

The Separation of Variables method employs (2.70), on the other hand. Unfortunately, the proof of (5.64) is not as simple. The dependence of the orders $\nu_n^{(l)}$ on the azimuthal modes l is one obvious difference. Remember: (5.47) must be solved independently for every azimuthal mode l! But such a dependence can also be generated in (2.83) and (2.84) if reordering the summation with respect to l and n,

$$\sum_{n=0}^{\infty} \sum_{l=-n}^{n} \cdots = \sum_{l} \sum_{n=|l|}^{\infty} \cdots ; \quad l = 0, \pm 1, \pm 2, \cdots . \tag{5.66}$$

To prove (5.64) numerically we fix mode l to a certain integer number and consider the dependence of the resulting orders $\nu_n^{(l)}$ on the number N_d of discretization lines. It bears out that for an increasing N_d the orders are represented better and better by the sequences

$$|l| + \frac{1}{2}, \ |l| + 1 + \frac{1}{2}, \ |l| + 2 + \frac{1}{2}, \cdots . \tag{5.67}$$

Thus, we can approve (5.64) at least numerically. But it is somehow unsatisfactory to rest on a pure numerical treatment. Therefore, we will deal with the equivalent two-dimensional problem in Cartesian coordinates which allows for an analytical treatment.

We look at the solution $f(x, y)$ of the two-dimensional Helmholtz equation

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) f(x, y) + k^2 f(x, y) = 0 \tag{5.68}$$

subject to the homogeneous Dirichlet conditions

$$f(0, y) = f(a, y) = 0 \tag{5.69}$$

at $x = 0, a$. The boundary conditions with respect to the variable y can be ignored. We apply the MoL to (5.68) by performing an equidistant discretization with respect to x which is in accordance with (5.69). The corresponding discretization scheme is depicted in Fig. 5.4. This procedure provides us with the following analytical expressions of the eigenvalues and eigenvectors:

$$\vec{x}_i = sin\left(\frac{ij\pi}{N_d + 1} \right) = sin\left(\frac{i\pi}{a} j h_x \right), \quad i, j = 1, \cdots, N_d \tag{5.70}$$

$$\lambda_i = \frac{4}{h_x^2} \cdot sin^2 \left[\frac{i\pi}{2(N_d + 1)} \right], \quad h_x = \frac{a}{N_d + 1}. \tag{5.71}$$

The derivation of these expressions is omitted here. It is a not to difficult exercise for the reader. In contrast to what happens in spherical coordinates the discretization procedure results directly into a symmetric and tridiagonal coupling matrix, i.e., there is no need to perform the similarity transformation (5.44). The lazy reader is

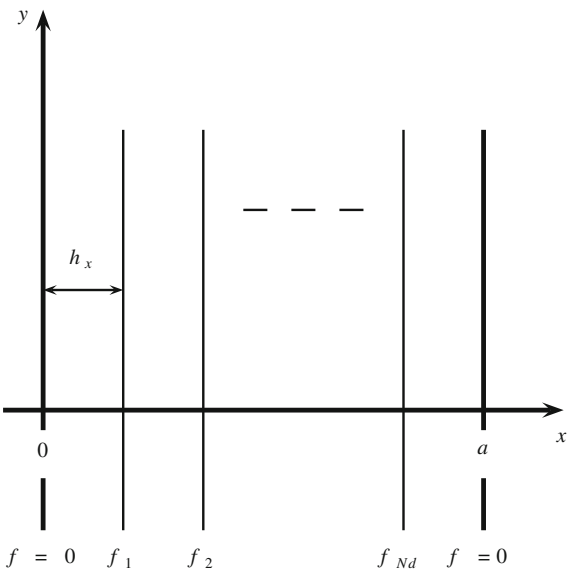

Fig. 5.4 Equidistant discretization scheme applied to the two-dimensional homogeneous Dirichlet problem of Helmholtz's equation in Cartesian coordinates

referred to the book of Pregla and Pascher cited in the reference chapter. Among others, he can find therein the derivation of the above given expressions. With (5.70) and (5.71) we know the decisive elements of the MoL. On the other hand, if applying the separation ansatz $f(x, y) = Y(y) \cdot X(x)$, we obtain the expressions

$$X_n(x) = sin\left(\frac{n\pi}{a}x\right) \tag{5.72}$$

and

$$k_n^2 = \left(\frac{n\pi}{a}\right)^2 \tag{5.73}$$

for the x-dependent eigenvectors and eigenvalues of the Separation of Variables method. It becomes obvious that (5.72) is identical with (5.70) at the N_d discrete points $x_j = j \cdot h_x$. To check the equality of the eigenvalues (5.73) and (5.71) in the limiting case of an infinite number of discretization lines we expand the sine function in (5.71) into a Taylor series. The linear term of this expansion just provides $\lambda_i = \left(\frac{i\pi}{a}\right)^2$. All higher order contributions vanish with an increasing N_d. This confirms our result obtained only numerically in spherical coordinates. It is exactly this behaviour which forced us to make the provocative statement at the beginning of this section that the MoL turns out to be just a worsening of the Separation of Variables method, and that it provides no additional advantages compared to spectral methods.

But, in the light of the considerations performed above, we must also state that the MoL, if applied to scattering problems in open domains, offers two essential advantages compared to the conventional Finite-Difference methods. The scattering

solution requires the fulfilment of the nonlocal radiation condition (2.76) at infinity, as frequently employed in the chapters before. Even this condition is difficult to handle within the conventional Finite-Difference methods. This happens because these methods are based on an additional discretization of the radial coordinate. To accomplish this discretization the outer region Γ_+ must be necessarily restricted to a finite domain with respect to the radius. As a consequence, the nonlocal radiation condition has to be replaced by so-called "Absorbing Boundary Conditions" (ABCs) which are introduced at a certain finite (i.e., local!) distance from the scatterer. The appropriate choice of these ABCs has a major impact on the stability and accuracy of the solution. It may also happen that spurious solutions occur, as observed in several applications. This requires an additional numerical effort to filter out the correct solution by controlling energy conservation, for example. The MoL is free of this problem since solving (5.55) in agreement with the nonlocal radiation condition. Another advantage of the MoL compared to the conventional Finite-Difference methods consists in the analytical solution of (5.55). Of course, it would be also possible to solve (5.55) by a discretization procedure with respect to the r-dependence, as the conventional Finite-Difference methods will do. But, beside the problem with the radiation condition, this would result in an additional worsening of the diagonal matrices $\mathbf{U}_n^{(l)}$. Moreover, each new orientation of the scatterer in the incident field is a new scattering problem within the Finite-Difference methods thus making orientation averaging a much more cumbersome task than with T-matrix methods. In Chap. 7 of the book "Light Scattering by Nonspherical Particles" (see Sect. 10.9 for details) there is described a Finite-Difference-Time-Domain method by Yang and Liou. An intercomparison of the results obtained with this method if applied to a spherical scatterer with the results of Mie's theory is depicted in Fig. 2 on page 187 of this contribution. A maximum of 10 % difference between both phase functions can be already observed at a comparable small size parameter of $k_0 a = 15$. This difference becomes even larger if looking at the elements of the phase matrix (the quantities "phase function" and "phase matrix" are introduced in Chap. 7 of this book!). These are the reasons which cast the application of the conventional Finite-Difference methods into doubt, at least if applied to the scattering problems in open domains considered in this book, and if a more complex scatterer geometry than that of a sphere or scattering at higher size parameters is considered.

For completeness we will finally generalize the results obtained in Chaps. 3 and 4 of this book in such a way that they hold also for the MoL. This can be simply performed by employing again the "bra" and "ket" symbols already introduced in Chap. 1. $G_{\partial\Gamma}^{(N)}$, for example, may be represented in this generalized form by

$$G_{\partial\Gamma}^{(N)}(\mathbf{x},\mathbf{x}') = -\sum_{i,j=0}^{N} \left[A_{\partial\Gamma}^{(g,\varphi_0)^{-1}}\right]_{i,j} \cdot \mid \varphi_i(k_0,\mathbf{x}) >< g_j(k_0,\mathbf{x}') \mid$$
$$\mathbf{x}' \in \partial\Gamma,\ \mathbf{x} \in \Gamma_+. \tag{5.74}$$

$G^{(N)}_{\Gamma_+}$ reads correspondingly

$$G^{(N)}_{\Gamma_+}(\mathbf{x},\mathbf{x}') = G_0(\mathbf{x},\mathbf{x}') - (ik_0)\sum_{i,k=0}^{N}[T_{\partial\Gamma}]_{i,k}\cdot|\,\varphi_i(k_0,\mathbf{x})><\tilde{\varphi}^*_k(k_0,\mathbf{x}')\,| \quad \mathbf{x},\mathbf{x}'\in\Gamma_+. \tag{5.75}$$

The solution of the outer Dirichlet problem may be then written according to

$$|\,u_t(\mathbf{x})>=G_{\Gamma_+}(\mathbf{x},\mathbf{x}')\,|\,\rho(\mathbf{x}')> \tag{5.76}$$

or

$$|\,u_s(\mathbf{x})>=G_{\partial\Gamma}(\mathbf{x},\mathbf{x}')\,|\,u_{inc}(\mathbf{x}')>, \tag{5.77}$$

respectively. If the MoL is used this solution is given only at N_d discrete points along an arbitrary curvature in Γ_+. The free-space Green function in (5.75) may be discretized to fit into the MoL. $[T_{\partial\Gamma}]_{i,k}$ are still the elements of the T-matrix belonging to the outer Dirichlet and transmission problem. If they will be also calculated consequently by use of the MoL the discrete expansion vectors $|\,\tilde{x}_{l,n}>$ must be used instead of the continuously varying eigenvectors, and the scalar product (1.34) must be replaced by (1.36). Expression $<\tilde{\varphi}^*_k(k_0,\mathbf{x}')\,|\,\rho(\mathbf{x}')>$ resulting from (5.75) and (5.76) represents the volume integral

$$<\tilde{\varphi}^*_k(k_0,\mathbf{x}')\,|\,\rho(\mathbf{x}')>=\int_{\Gamma_+}\tilde{\varphi}_k(k_0,\mathbf{x}')\cdot\rho(\mathbf{x}')\,dV(\mathbf{x}') \tag{5.78}$$

performed over the source region in Γ_+. Within the MoL the integration with respect to θ has to be replaced by a corresponding summation over the discretization angles, of course.

5.4 Integral Equation Methods

Boundary integral equation methods and volume integral equation methods are two other solution techniques which are frequently applied for solving scattering problems. They are essentially based on the equivalence principle which states that a field outside a finite scattering volume Γ_- may be considered as the result of an equivalent surface current at the surface of this volume or an equivalent volume current inside this volume. These equivalent currents are the unknown quantities in the

integral equation methods which have to be determined. That is in contrast to all the methods considered so far, which take the scattered field for the unknown quantity. Once the scattered field is known the induced surface or volume currents can be calculated afterwards, of course. We will come back to this interrelation between induced currents and fields in Chap. 7 in conjunction with the physical background of electromagnetic wave scattering. Here we just want to state the different point of views underlying the methods considered so far and the integral equation methods we will discuss now. More generally speaking, regarding the Trinity of physics, "cause", "action", and "interaction", this difference represents our experience that the result of an interaction can be interpreted as a new cause (in our case an induced surface current, for example) producing the same action (the scattered field). That is exactly the physical content of Huygens' principle we expressed already in terms of Green functions.

It is not our intention here to provide a complete description of the different integral equation methods. We included several books and papers in the reference chapter dealing with these methods in much more detail. The main focus in what follows is on the problem of how one can come from the picture of Green functions and interaction operators developed so far to the integral equation methods. The boundary integral equations are discussed in conjunction with the scalar outer Dirichlet and transmission problem whereas the volume integral equations are restricted to the scalar case of the outer transmission problem. All derivations can be similarly performed for the dyadic case if using the corresponding dyadic and vector forms of Green's theorem. But in the dyadic case there appears an additional difficulty resulting from the stronger singularity of the dyadic free-space Green function—sometimes a not even simple undertaking in numerical procedures. In such cases, it may be of benefit not to take the integral equations which results in a straightforward way from the homogeneous Dirichlet condition but to use those one which are expressed in terms of the induced surface current, for example. These equations exhibit a weaker singularity, due to the operation mentioned already in (2.335). This will also be discussed in detail in Chap. 7 of this book when dealing with the scattering problem of an ideal metallic obstacle. Avoiding the confrontation with the strong singularity of the dyadic free-space Green function represents one of the advantages of the T-matrix methods which should not be underestimated.

This chapter will be finalized with deriving the so-called "Lippmann-Schwinger equations". Since these integral equations are an ideal starting point for iterative solutions of the scattering problem, they deserve a mention in this chapter. They will be derived in both scalar and dyadic form. The latter especially because of the fact that the lowest order iteration appears to be not affected by the strong singularity of the dyadic free-space Green function. Deriving the Lippmann-Schwinger equations for the dyadic Green function and the dyadic interaction operator demonstrates moreover how one can translate the scalar derivations discussed beforehand into the dyadic notation.

5.4.1 Boundary Integral Equation Method Related to the Outer Dirichlet Problem

To obtain the boundary integral equation for the interaction operator related to the outer Dirichlet problem we have to perform a slight but important change in definition (4.1). We replace the quantity $G_0^>$ used in this definition by the full free-space Green function G_0, i.e., instead of (4.1) we use the definition

$$G_{\Gamma_+}(\mathbf{x},\mathbf{x}') := G_0(\mathbf{x},\mathbf{x}') + \oint_{\partial\Gamma} G_0(\mathbf{x},\bar{\mathbf{x}}) \cdot \hat{W}_{\partial\Gamma_+}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \cdot G_0(\tilde{\mathbf{x}},\mathbf{x}')\, dS(\bar{\mathbf{x}})\, dS(\tilde{\mathbf{x}}). \tag{5.79}$$

To distinguish the interaction operators introduced by the different definitions we will mark the new interaction operator in (5.79) with a "hat". The Green function G_{Γ_+} defined according to (5.79) is also a solution of the inhomogeneous Helmholtz equation subject to the radiation condition with respect to $\mathbf{x}$. We can then use the additionally required homogeneous Dirichlet condition at the scatterer surface to determine the interaction operator $\hat{W}_{\partial\Gamma_+}$, as already done in Chap. 4. For this, we have to move $\mathbf{x}$ toward the scatterer surface. But this procedure forces us now to take the singularity of $G_0(\mathbf{x},\bar{\mathbf{x}})$ at the surface point $\mathbf{x} = \bar{\mathbf{x}}$ seriously into account. Please, remember: In contrast to $G_0(\mathbf{x},\bar{\mathbf{x}})$ used in (5.79) the quantity $G_0^>(\mathbf{x},\bar{\mathbf{x}})$ used in (4.1) was assumed to obey generally the homogeneous Helmholtz equation also if $\mathbf{x} \in \partial\Gamma$. The integral expression

$$\oint_{\partial\Gamma} G_0(\mathbf{x},\bar{\mathbf{x}}) \cdot f(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}); \quad \mathbf{x},\bar{\mathbf{x}} \in \partial\Gamma \tag{5.80}$$

represents therefore an improper integral, due to the singularity of $G_0(\mathbf{x},\bar{\mathbf{x}})$ at the surface point $\mathbf{x} = \bar{\mathbf{x}}$. To calculate the boundary integral (5.80) we exclude at first a small surface element $\partial\Gamma_\delta$ which encloses the singular point. The improper integral is convergent if there exists a finite value of the sum of the integrals

$$\int_{\partial\Gamma - \partial\Gamma_\delta} G_0(\mathbf{x},\bar{\mathbf{x}}) \cdot f(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}) + \int_{\partial\Gamma_\delta} G_0(\mathbf{x},\bar{\mathbf{x}}) \cdot f(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}) \tag{5.81}$$

in the limiting case $\lim \partial\Gamma_\delta \to 0$. Even if it is not quite exact from a mathematical point of view it is common practice to denote the limiting value of the first integral of expression (5.81) as "principal value",

$$p.v. \oint_{\partial\Gamma} G_0(\mathbf{x},\bar{\mathbf{x}}) \cdot f(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}) := \lim_{\partial\Gamma_\delta \to 0} \int_{\partial\Gamma - \partial\Gamma_\delta} G_0(\mathbf{x},\bar{\mathbf{x}}) \cdot f(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}), \tag{5.82}$$

and that is the way we will use it, too. It can be moreover shown that for any sufficiently smooth function $f(\bar{\mathbf{x}})$ with no singularities along $\partial\Gamma$

$$\lim_{\partial\Gamma_\delta \to 0} \int_{\partial\Gamma_\delta} G_0(\mathbf{x}, \bar{\mathbf{x}}) \cdot f(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}) \to 0 \tag{5.83}$$

holds. Thus we have

$$\oint_{\partial\Gamma} G_0(\mathbf{x}, \bar{\mathbf{x}}) \cdot f(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}) = p.v. \oint_{\partial\Gamma} G_0(\mathbf{x}, \bar{\mathbf{x}}) \cdot f(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}) \tag{5.84}$$

if $\mathbf{x}, \bar{\mathbf{x}} \in \partial\Gamma$. To prove (5.83), let us consider the boundary integral

$$\int_{\partial\Gamma_\delta} G_0(\mathbf{x}, \bar{\mathbf{x}}) \cdot f(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}) \tag{5.85}$$

with $\partial\Gamma_\delta$ being a very small but finite surface patch enclosing the singular point. Correspondingly, we can replace the analytical expression (2.261) of the free-space Green function $G_0(\mathbf{x}, \bar{\mathbf{x}})$ by its static approximation

$$G_0(\mathbf{x}, \bar{\mathbf{x}}) \approx \frac{1}{4\pi|\mathbf{x} - \bar{\mathbf{x}}|}. \tag{5.86}$$

$\partial\Gamma_\delta$ can be assumed w.l.o.g. to be a surface patch with a circular boundary, and with the z-axis of the coordinate system running through the centre of the boundary circle. This holds even if the scatterer surface is a nonspherical ones (compare Fig. 5.5). The observation point $\mathbf{x}$ is placed into the centre of the circle in distance a from the origin of the coordinate system. $|\mathbf{x}| = |\bar{\mathbf{x}}| = a$ is assumed to be constant across the small

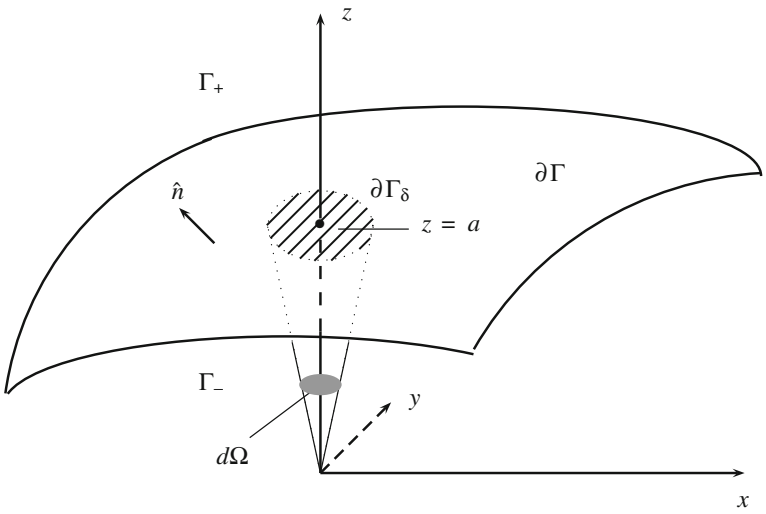

Fig. 5.5 Geometrical configuration to calculate the boundary integrals (5.85) and (5.107)

surface patch $\partial\Gamma_\delta$. In conjunction with (2.51), because of approximation

$$|\mathbf{x} - \bar{\mathbf{x}}| \;\approx\; a \cdot \sin\bar{\theta} \tag{5.87}$$

for every $\bar{\mathbf{x}} \in \partial\Gamma_\delta$, and due to the factor 2π which results from the $\bar{\phi}$-integration we obtain in spherical coordinates

$$\int_{\partial\Gamma_\delta} \frac{f(\bar{\mathbf{x}})}{4\pi|\mathbf{x} - \bar{\mathbf{x}}|}\, dS(\bar{\mathbf{x}}) \approx \frac{f(a)}{2} \cdot a \cdot \int_0^{\bar{\theta}_\delta} d\bar{\theta}. \tag{5.88}$$

In deriving (5.88) it was moreover assumed that the sufficiently smooth function $f(\bar{\mathbf{x}})$ can be replaced by its value in point $(r = a, \theta = 0°, \phi = 0°)$ everywhere across the small surface patch. Thus we have finally

$$\int_{\partial\Gamma_\delta} \frac{f(\bar{\mathbf{x}})}{4\pi|\mathbf{x} - \bar{\mathbf{x}}|}\, dS(\bar{\mathbf{x}}) \approx \frac{f(a)}{2} \cdot a \cdot \bar{\theta}_\delta. \tag{5.89}$$

If $\bar{\theta}_\delta$ tends to zero this expression vanishes indeed. But in the numerical realization of the boundary integral equation method it may be of some benefit to take the contribution from the second integral term in (5.81) into account. It is reported in several papers (see the paper of Fikioris and Magoulas cited in Sect. 10.6, for example) that this may lead to an improved stability and accuracy of the numerical procedure. Otherwise, one has to cover the scatterer surface with a very fine surface mesh to obtain accurate results which may increase the numerical effort drastically.

Now, we are prepared to move the observation point in expression (5.79) towards the surface. Applying the homogeneous Dirichlet condition we get the integral equation

$$\begin{aligned} -G_0(\mathbf{x}, \mathbf{x}') = p.v. \oint_{\partial\Gamma} & G_0(\mathbf{x}, \bar{\mathbf{x}}) \cdot \hat{W}_{\partial\Gamma_+}(\bar{\mathbf{x}}, \tilde{\mathbf{x}}) \cdot G_0(\tilde{\mathbf{x}}, \mathbf{x}')\, dS(\bar{\mathbf{x}})\, dS(\tilde{\mathbf{x}}); \\ & \mathbf{x} \in \partial\Gamma \end{aligned} \tag{5.90}$$

to calculate the interaction operator $\hat{W}_{\partial\Gamma_+}(\bar{\mathbf{x}}, \tilde{\mathbf{x}})$. The principal value symbol therein corresponds to the integration with respect to the variable $\bar{\mathbf{x}}$. Let us now consider one possible way to calculate $\hat{W}_{\partial\Gamma_+}(\bar{\mathbf{x}}, \tilde{\mathbf{x}})$ in more detail. The interaction operator may be approximated by the bilinear expansion

$$\hat{W}_{\partial\Gamma_+}(\bar{\mathbf{x}}, \tilde{\mathbf{x}}) = -\sum_{k,l=0}^{N} \left[\hat{W}_{\partial\Gamma_+}\right]_{k,l} \cdot \varphi_k(k_0, \bar{\mathbf{x}}) \cdot \varphi_l(k_0, \tilde{\mathbf{x}}); \quad \bar{\mathbf{x}}, \tilde{\mathbf{x}} \in \partial\Gamma \tag{5.91}$$

in terms of the radiating eigensolutions of Helmholtz's equation. Both the free-space Green functions $G_0(\mathbf{x}, \mathbf{x}')$ and $G_0(\tilde{\mathbf{x}}, \mathbf{x}')$ in (5.90) can be replaced without any problems by the series expansion (2.278) since the source point $\mathbf{x}'$ is still located

outside the smallest sphere circumscribing the scatterer. This results into the equation

$$\sum_{j=0}^{N} \psi_j(k_0, \mathbf{x}) \cdot \tilde{\varphi}_j(k_0, \mathbf{x}') = \sum_{j,k,l=0}^{N} p.v. \oint_{\partial\Gamma} G_0(\mathbf{x}, \bar{\mathbf{x}}) \cdot \left[\hat{W}_{\partial\Gamma_+}\right]_{k,l} \cdot \varphi_k(k_0, \bar{\mathbf{x}}) \cdot \varphi_l(k_0, \tilde{\mathbf{x}}) \cdot \psi_j(k_0, \tilde{\mathbf{x}}) \cdot \tilde{\varphi}_j(k_0, \mathbf{x}')\, dS(\bar{\mathbf{x}})\, dS(\tilde{\mathbf{x}}); \quad \mathbf{x} \in \partial\Gamma. \tag{5.92}$$

Since the functions $\tilde{\varphi}_j(k_0, \mathbf{x}')$ form a linearly independent system in Γ_+ we get the equation

$$\psi_j(k_0, \mathbf{x}) = \sum_{k,l=0}^{N} p.v. \oint_{\partial\Gamma} G_0(\mathbf{x}, \bar{\mathbf{x}}) \cdot \left[\hat{W}_{\partial\Gamma_+}\right]_{k,l} \cdot \varphi_k(k_0, \bar{\mathbf{x}}) \cdot \varphi_l(k_0, \tilde{\mathbf{x}}) \cdot \psi_j(k_0, \tilde{\mathbf{x}})\, dS(\bar{\mathbf{x}})\, dS(\tilde{\mathbf{x}}); \quad \mathbf{x} \in \partial\Gamma; \ j = 0, \cdots, N \tag{5.93}$$

to determine the unknown elements $\left[\hat{W}_{\partial\Gamma_+}\right]_{k,l}$ in the bilinear expansion (5.91). For this we integrate both sides of this equation according to

$$\oint_{\partial\Gamma} g_i^*(\mathbf{x}) \cdots\, dS(\mathbf{x}); \quad i = 0, \cdots, N \tag{5.94}$$

with respect to $\mathbf{x}$. $g_i(\mathbf{x})$ therein are again yet not specified weighting functions. In doing so, we obtain the matrix equation

$$\mathbf{A}_{\partial\Gamma}^{(g,\psi_0)} = \mathbf{B}_{\partial\Gamma}^{(g,G_0\,\varphi_0)} \cdot \hat{\mathbf{W}}_{\partial\Gamma_+} \cdot \mathbf{C}_{\partial\Gamma}^{(\varphi_0^*,\psi_0)} \tag{5.95}$$

with matrix elements defined by the integral expressions

$$\left[A_{\partial\Gamma}^{(g,\psi_0)}\right]_{i,j} := \oint_{\partial\Gamma} g_i^*(\mathbf{x}) \cdot \psi_j(k_0, \mathbf{x})\, dS(\mathbf{x}) \tag{5.96}$$

$$\left[B_{\partial\Gamma}^{(g,G_0\,\varphi_0)}\right]_{i,j} := p.v. \oint_{\partial\Gamma} g_i^*(\mathbf{x}) \cdot G_0(\mathbf{x}, \bar{\mathbf{x}}) \cdot \varphi_j(k_0, \bar{\mathbf{x}})\, dS(\mathbf{x})\, dS(\bar{\mathbf{x}}) \tag{5.97}$$

$$\left[C_{\partial\Gamma}^{(\varphi_0^*,\psi_0)}\right]_{i,j} := \oint_{\partial\Gamma} \varphi_i(k_0, \tilde{\mathbf{x}}) \cdot \psi_j(k_0, \tilde{\mathbf{x}})\, dS(\tilde{\mathbf{x}}). \tag{5.98}$$

Thus we have finally

$$\hat{\mathbf{W}}_{\partial\Gamma_+} = \mathbf{B}_{\partial\Gamma}^{(g,G_0\,\varphi_0)^{-1}} \cdot \mathbf{A}_{\partial\Gamma}^{(g,\psi_0)} \cdot \mathbf{C}_{\partial\Gamma}^{(\varphi_0^*,\psi_0)^{-1}} \tag{5.99}$$

to calculate the elements $\left[\hat{W}_{\partial\Gamma_+}\right]_{k,l}$. This expression becomes especially simple if $g_i(\mathbf{x}) = \varphi_i^*(k_0, \mathbf{x})$ are chosen as weighting functions. Then

$$\mathbf{A}_{\partial\Gamma}^{(\varphi_0^*,\psi_0)} \cdot \mathbf{C}_{\partial\Gamma}^{(\varphi_0^*,\psi_0)^{-1}} = \mathbf{E} \tag{5.100}$$

holds and we have

$$\hat{\mathbf{W}}_{\partial\Gamma_+} = \mathbf{B}_{\partial\Gamma}^{(\varphi_0^*,G_0\,\varphi_0)^{-1}}. \tag{5.101}$$

If we now insert the elements $\left[\hat{W}_{\partial\Gamma_+}\right]_{k,l}$ into the bilinear expansion (5.91), and, moreover, this expansion into equation (5.79) we are able to calculate the Green function related to the outer Dirichlet problem at any observation point $\mathbf{x} \in \Gamma_+$. This raises the following question: What is the interrelation between the approximation of this Green function derived in Chaps. 3 and 4, respectively, in conjunction with the T-matrix and the approximation derived just now? Since, this question is strongly related to Rayleigh's hypothesis, we will shift it to the next chapter.

The way described above to derive the boundary integral equation related to the outer Dirichlet problem is not the usual way one can find in the relevant literature. It is more customary not to introduce an interaction operator but to employ the induced surface current as the unknown quantity. However, this at first glance not very important aspect has the consequence that the boundary integral equation methods are considered to be inappropriate if a certain scattering problem requires orientation averaging. This is because each new orientation of the scatterer in the primary incident field produces a new induced surface current, i.e., the induced surface current exhibits a crucial link to the primary incident field. This situation can be avoided if choosing the interaction operator as the unknown quantity in the boundary integral equation, as described above. To see this, we have to reveal the relation between the interaction operator and the induced surface current. Inserting (5.79) into (2.286) provides

$$u_t(\mathbf{x}) = u_{inc}(\mathbf{x}) + \oint_{\partial\Gamma} G_0(\mathbf{x}, \bar{\mathbf{x}}) \cdot \hat{W}_{\partial\Gamma_+}(\bar{\mathbf{x}}, \tilde{\mathbf{x}}) \cdot u_{inc}(\tilde{\mathbf{x}})\, dS(\bar{\mathbf{x}})\, dS(\tilde{\mathbf{x}}) \tag{5.102}$$

for the total field in the outer region Γ_+ if taking (2.271) into account (u_0 in (2.271) is just the primary incident field!). If defining the induced surface current $J_{\partial\Gamma}$ according to

$$J_{\partial\Gamma}(\bar{\mathbf{x}}) := \oint_{\partial\Gamma} \hat{W}_{\partial\Gamma_+}(\bar{\mathbf{x}}, \tilde{\mathbf{x}}) \cdot u_{inc}(\tilde{\mathbf{x}})\, dS(\tilde{\mathbf{x}}) \tag{5.103}$$

(5.102) may be rewritten into

$$u_t(\mathbf{x}) = u_{inc}(\mathbf{x}) + \oint_{\partial\Gamma} G_0(\mathbf{x}, \bar{\mathbf{x}}) \cdot J_{\partial\Gamma}(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}). \tag{5.104}$$

Now, we can move again $\mathbf{x}$ in this equation toward the scatterer surface by taking the homogeneous Dirichlet condition into account. In this way we end up with the

known boundary integral equation

$$-u_{inc}(\mathbf{x}) = p.v. \oint_{\partial\Gamma} G_0(\mathbf{x}, \bar{\mathbf{x}}) \cdot J_{\partial\Gamma}(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}); \quad \mathbf{x} \in \partial\Gamma \tag{5.105}$$

which allows us to calculate the unknown surface current related to the outer Dirichlet problem. It may be expanded, for example, in terms of the radiating solutions at the scatterer surface (but for the surface current we use a single expansion, and not a bilinear expansion, of course). The unknown expansion coefficients can be determined in the way described just now for the interaction operator. As it becomes obvious from definition (5.103) each new direction of incidence of the primary field results in a new surface current although the interaction operator is still the same. The decoupling of the primary incident field and the interaction operator is therefore an advantage of the latter quantity, and its practical implications should not be underestimated.

5.4.2 *Boundary Integral Equation Method Related to the Outer Transmission Problem*

To derive the corresponding boundary integral equations related to the outer transmission problem we have to deal first with the improper integral

$$\oint_{\partial\Gamma} \frac{\partial G_0(\mathbf{x}, \bar{\mathbf{x}})}{\partial \hat{n}_-} \cdot f(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}); \quad \mathbf{x}, \bar{\mathbf{x}} \in \partial\Gamma. \tag{5.106}$$

This expression appears if $\mathbf{x}$ approaches point ($z = a$, $\theta = 0°$, $\phi = 0°$) of the surface patch $\partial\Gamma_\delta$. We have moreover to distinguish whether $\mathbf{x}$ approaches this point from the outer region Γ_+ or from the inner region Γ_- (see again Fig. 5.5). Equation (5.106) is a consequence of the transmission condition (2.282). As already done in the former subsection we replace the free-space Green function G_0 by the static approximation (5.86), and the function $f(\bar{\mathbf{x}})$ by its value $f(a)$ across the small surface patch $\partial\Gamma_\delta$. In this way, we obtain the approximate expression

$$\int_{\partial\Gamma_\delta} \frac{\partial G_0(\mathbf{x}, \bar{\mathbf{x}})}{\partial \hat{n}_-} \cdot f(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}) \approx \frac{f(a)}{4\pi} \cdot \int_{\partial\Gamma_\delta} \frac{1}{\partial \hat{n}_-} \frac{1}{|\mathbf{x} - \bar{\mathbf{x}}|}\, dS(\bar{\mathbf{x}}). \tag{5.107}$$

The remaining integral on the right-hand side is nothing but the solid angle subtended by the surface element $dS(\bar{\mathbf{x}})$ (which is an infinitesimal part of $\partial\Gamma_\delta$) as seen from points $a \pm \epsilon$, respectively. Then, if we let $\epsilon \to 0$, this integral becomes simply $\pm 2\pi$. This value is independent of the form of $\partial\Gamma_\delta$. The positive sign applies if approaching point $r = a$ from region Γ_+, and the negative sign applies if coming from inside the scatterer. The improper integral (5.106) may be therefore represented by

$$\oint_{\partial\Gamma} \frac{\partial G_0(\mathbf{x},\bar{\mathbf{x}})}{\partial \hat{n}_-} \cdot f(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}) = \pm\frac{f(\mathbf{x})}{2} + p.v. \oint_{\partial\Gamma} \frac{\partial G_0(\mathbf{x},\bar{\mathbf{x}})}{\partial \hat{n}_-} \cdot f(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}) \tag{5.108}$$

with the principal value according to (5.82), and $\mathbf{x}$ located at the outer side (this corresponds to the positive sign!) or inner side (this corresponds to the negative sign!) of the scatterer surface. Now, we can derive the relevant boundary integral equations related to the outer transmission problem.

In close analogy to (5.79) of the outer Dirichlet problem we first introduce the two interaction operators $\hat{W}^{(d)}_{\partial\Gamma_+}$ and $\hat{W}^{(d)}_{\partial\Gamma_-}$ needed for the outer transmission problem by the definitions

$$G^{(d)}_{\Gamma_+}(\mathbf{x},\mathbf{x}') := G_0(\mathbf{x},\mathbf{x}') + \oint_{\partial\Gamma} G_0(\mathbf{x},\bar{\mathbf{x}})\, \hat{W}^{(d)}_{\partial\Gamma_+}(\bar{\mathbf{x}},\tilde{\mathbf{x}})\, G_0(\tilde{\mathbf{x}},\mathbf{x}')\, dS(\bar{\mathbf{x}})\, dS(\tilde{\mathbf{x}}) \tag{5.109}$$

and

$$G^{(-/+)}(\mathbf{x},\mathbf{x}') := \oint_{\partial\Gamma} G_{0_s}(\mathbf{x},\bar{\mathbf{x}})\, \hat{W}^{(d)}_{\partial\Gamma_-}(\bar{\mathbf{x}},\tilde{\mathbf{x}})\, G_0(\tilde{\mathbf{x}},\mathbf{x}')\, dS(\bar{\mathbf{x}})\, dS(\tilde{\mathbf{x}}). \tag{5.110}$$

These definitions differ again from the definitions (4.12) and (4.13) in using $G_0(\mathbf{x},\bar{\mathbf{x}})$ and $G_{0_s}(\mathbf{x},\bar{\mathbf{x}})$ instead of $G_0^{>}(\mathbf{x},\bar{\mathbf{x}})$ and $G_{0_s}^{<}(\mathbf{x},\bar{\mathbf{x}})$. If the observation point $\mathbf{x}$ approaches the scatterer surface $\partial\Gamma$ then the transmission conditions (2.281) and (2.282) as well as relations (5.84) and (5.108) result in the two boundary integral equations

$$\begin{aligned} G_0(\mathbf{x},\mathbf{x}') + p.v. \oint_{\partial\Gamma} G_0(\mathbf{x},\bar{\mathbf{x}})\, \hat{W}^{(d)}_{\partial\Gamma_+}(\bar{\mathbf{x}},\tilde{\mathbf{x}})\, G_0(\tilde{\mathbf{x}},\mathbf{x}')\, dS(\bar{\mathbf{x}})\, dS(\tilde{\mathbf{x}}) \\ = p.v. \oint_{\partial\Gamma} G_{0_s}(\mathbf{x},\bar{\mathbf{x}})\, \hat{W}^{(d)}_{\partial\Gamma_-}(\bar{\mathbf{x}},\tilde{\mathbf{x}})\, G_0(\tilde{\mathbf{x}},\mathbf{x}')\, dS(\bar{\mathbf{x}})\, dS(\tilde{\mathbf{x}}) \end{aligned} \tag{5.111}$$

and

$$\begin{aligned} \partial_{\hat{n}_-} G_0(\mathbf{x},\mathbf{x}') + \frac{1}{2}\cdot \oint_{\partial\Gamma} \hat{W}^{(d)}_{\partial\Gamma_+}(\mathbf{x},\tilde{\mathbf{x}})\, G_0(\tilde{\mathbf{x}},\mathbf{x}')\, dS(\tilde{\mathbf{x}}) \\ + p.v. \oint_{\partial\Gamma} \partial_{\hat{n}_-} G_0(\mathbf{x},\bar{\mathbf{x}})\, \hat{W}^{(d)}_{\partial\Gamma_+}(\bar{\mathbf{x}},\tilde{\mathbf{x}})\, G_0(\tilde{\mathbf{x}},\mathbf{x}')\, dS(\bar{\mathbf{x}})\, dS(\tilde{\mathbf{x}}) \\ = -\frac{1}{2}\cdot \oint_{\partial\Gamma} \hat{W}^{(d)}_{\partial\Gamma_-}(\mathbf{x},\tilde{\mathbf{x}})\, G_0(\tilde{\mathbf{x}},\mathbf{x}')\, dS(\tilde{\mathbf{x}}) \\ + p.v. \oint_{\partial\Gamma} \partial_{\hat{n}_-} G_{0_s}(\mathbf{x},\bar{\mathbf{x}})\, \hat{W}^{(d)}_{\partial\Gamma_-}(\bar{\mathbf{x}},\tilde{\mathbf{x}})\, G_0(\tilde{\mathbf{x}},\mathbf{x}')\, dS(\bar{\mathbf{x}})\, dS(\tilde{\mathbf{x}}). \end{aligned} \tag{5.112}$$

Here, we used the abbreviation

$$\partial_{\hat{n}_-} G(\mathbf{x},\mathbf{x}') := \hat{n}_- \cdot \nabla_{\mathbf{x}} G(\mathbf{x},\mathbf{x}'). \tag{5.113}$$

If employing again a bilinear expansion for both interaction operators $\hat{W}^{(d)}_{\partial\Gamma_+}$ and $\hat{W}^{(d)}_{\partial\Gamma_-}$ we can proceed exactly in the same way as already done in the case of the outer Dirichlet problem. But now we have two equations from which we can determine $\hat{W}^{(d)}_{\partial\Gamma_+}$ needed to calculate $G^{(d)}_{\Gamma_+}$. Once we know $G^{(d)}_{\Gamma_+}$ we can calculate the total field outside the scatterer. Moreover, with the definitions

$$J^{(+)}_{\partial\Gamma}(\bar{\mathbf{x}}) := \oint_{\partial\Gamma} \hat{W}^{(d)}_{\partial\Gamma_+}(\bar{\mathbf{x}}, \tilde{\mathbf{x}}) \cdot u_{inc}(\tilde{\mathbf{x}})\, dS(\tilde{\mathbf{x}}) \tag{5.114}$$

and

$$J^{(-)}_{\partial\Gamma}(\bar{\mathbf{x}}) := \oint_{\partial\Gamma} \hat{W}^{(d)}_{\partial\Gamma_-}(\bar{\mathbf{x}}, \tilde{\mathbf{x}}) \cdot u_{inc}(\tilde{\mathbf{x}})\, dS(\tilde{\mathbf{x}}) \tag{5.115}$$

we are again able to derive the conventional boundary integral equations of the outer transmission problem. For this we have to multiply (5.111) and (5.112) with the source distribution $\rho(\mathbf{x}')$ (where it is again assumed that $\rho(\mathbf{x}')$ is located somewhere outside the smallest sphere circumscribing the scatterer) and have to integrate over Γ_+. Thus, we get the boundary integral equations

$$\begin{aligned} u_{inc}(\mathbf{x}) + p.v. \oint_{\partial\Gamma} G_0(\mathbf{x}, \bar{\mathbf{x}})\, J^{(+)}_{\partial\Gamma}(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}) \\ = p.v. \oint_{\partial\Gamma} G_{0_s}(\mathbf{x}, \bar{\mathbf{x}})\, J^{(-)}_{\partial\Gamma}(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}) \end{aligned} \tag{5.116}$$

and

$$\begin{aligned} \partial_{\hat{n}_-} u_{inc}(\mathbf{x}) + \frac{1}{2} \cdot J^{(+)}_{\partial\Gamma}(\mathbf{x}) + p.v. \oint_{\partial\Gamma} \partial_{\hat{n}_-} G_0(\mathbf{x}, \bar{\mathbf{x}})\, J^{(+)}_{\partial\Gamma}(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}) \\ = -\frac{1}{2} \cdot J^{(-)}_{\partial\Gamma}(\mathbf{x}) + p.v. \oint_{\partial\Gamma} \partial_{\hat{n}_-} G_{0_s}(\mathbf{x}, \bar{\mathbf{x}})\, J^{(-)}_{\partial\Gamma}(\bar{\mathbf{x}})\, dS(\bar{\mathbf{x}}), \end{aligned} \tag{5.117}$$

from which we can calculate the two induced surface currents $J^{(+)}_{\partial\Gamma}$ and $J^{(-)}_{\partial\Gamma}$. But for the scattered field u_s in Γ_+ we need only the surface current $J^{(+)}_{\partial\Gamma}$.

5.4.3 *Volume Integral Equation Method Related to the Outer Transmission Problem*

Alternatively, we can solve the outer transmission problem by appropriate volume integral equations. To derive these equations we have to juggle again with Green's theorem (2.239). We apply it with the two quantities

$$\Psi(\mathbf{x}) = G^{(d)}_{\Gamma_+}(\mathbf{x}, \mathbf{x}'); \quad \mathbf{x}, \mathbf{x}' \in \Gamma_+ \tag{5.118}$$

$$\Phi(\mathbf{x}) = G_0(\mathbf{x}, \mathbf{x}''); \quad \mathbf{x} \in \Gamma_+. \tag{5.119}$$

Concerning the location of the source point $\mathbf{x}''$ we have to distinguish two cases. The source point may be located either in the outer region Γ_+ (case 1a) or somewhere inside Γ_- (case 1b). In the former case, the free-space Green function G_0 solves the inhomogeneous Helmholtz equation (2.241) in Γ_+. But in the latter case, it is a solution of the homogeneous Helmholtz equation within Γ_+. From Green's theorem it follows for each of these cases:

case 1a:

$$G^{(d)}_{\Gamma_+}(\mathbf{x}'', \mathbf{x}') = G_0(\mathbf{x}', \mathbf{x}'') + \oint_{\partial\Gamma} \left[G_0(\mathbf{x}, \mathbf{x}'') \cdot \frac{\partial G^{(d)}_{\Gamma_+}(\mathbf{x}, \mathbf{x}')}{\partial \hat{n}_-} - G^{(d)}_{\Gamma_+}(\mathbf{x}, \mathbf{x}') \cdot \frac{\partial G_0(\mathbf{x}, \mathbf{x}'')}{\partial \hat{n}_-} \right] dS(\mathbf{x}). \tag{5.120}$$

case 1b:

$$G_0(\mathbf{x}'', \mathbf{x}') = -\oint_{\partial\Gamma} \left[G_0(\mathbf{x}'', \mathbf{x}) \cdot \frac{\partial G^{(d)}_{\Gamma_+}(\mathbf{x}, \mathbf{x}')}{\partial \hat{n}_-} - G^{(d)}_{\Gamma_+}(\mathbf{x}, \mathbf{x}') \cdot \frac{\partial G_0(\mathbf{x}'', \mathbf{x})}{\partial \hat{n}_-} \right] dS(\mathbf{x}). \tag{5.121}$$

In the next step we apply Green's theorem with the two quantities

$$\Psi(\mathbf{x}) = G^{(-/+)}(\mathbf{x}, \mathbf{x}'); \quad \mathbf{x} \in \Gamma_-; \ \mathbf{x}' \in \Gamma_+ \tag{5.122}$$

$$\Phi(\mathbf{x}) = G_0(\mathbf{x}, \mathbf{x}''); \quad \mathbf{x} \in \Gamma_- \tag{5.123}$$

inside the scatterer. Here we have again to distinguish the two cases $\mathbf{x}'' \in \Gamma_+$ (case 2a) and $\mathbf{x}'' \in \Gamma_-$ (case 2b). $G^{(-/+)}$ solves the homogeneous Helmholtz equation (2.283) in both cases. This results into

case 2a:

$$\kappa_d^2 \int_{\Gamma_-} G_0(\mathbf{x}, \mathbf{x}'') \cdot G^{(-/+)}(\mathbf{x}, \mathbf{x}')\, dV(\mathbf{x}) = \oint_{\partial\Gamma} \left[G_0(\mathbf{x}, \mathbf{x}'') \cdot \frac{\partial G^{(-/+)}(\mathbf{x}, \mathbf{x}')}{\partial \hat{n}_-} - G^{(-/+)}(\mathbf{x}, \mathbf{x}') \cdot \frac{\partial G_0(\mathbf{x}, \mathbf{x}'')}{\partial \hat{n}_-} \right] dS(\mathbf{x}). \tag{5.124}$$

case 2b:

$$-G^{(-/+)}(\mathbf{x}'',\mathbf{x}')+\kappa_d^2\int_{\Gamma_-}G_0(\mathbf{x},\mathbf{x}'')\cdot G^{(-/+)}(\mathbf{x},\mathbf{x}')\,dV(\mathbf{x})$$
$$=\oint_{\partial\Gamma}\left[G_0(\mathbf{x},\mathbf{x}'')\cdot\frac{\partial G^{(-/+)}(\mathbf{x},\mathbf{x}')}{\partial\hat{n}_-}-G^{(-/+)}(\mathbf{x},\mathbf{x}')\cdot\frac{\partial G_0(\mathbf{x},\mathbf{x}'')}{\partial\hat{n}_-}\right]dS(\mathbf{x}). \tag{5.125}$$

κ_d^2 therein is given by

$$\kappa_d^2=k^2-k_0^2. \tag{5.126}$$

Next, we combine the two cases 1a and 2a as well as 1b and 2b. The results are

$$G_{\Gamma_+}^{(d)}(\mathbf{x},\mathbf{x}')=G_0(\mathbf{x},\mathbf{x}')+\kappa_d^2\int_{\Gamma_-}G_0(\mathbf{x},\bar{\mathbf{x}})\cdot G^{(-/+)}(\bar{\mathbf{x}},\mathbf{x}')\,dV(\bar{\mathbf{x}})$$
$$\mathbf{x},\mathbf{x}'\in\Gamma_+ \tag{5.127}$$

and

$$G^{(-/+)}(\mathbf{x},\mathbf{x}')=G_0(\mathbf{x},\mathbf{x}')+\kappa_d^2\int_{\Gamma_-}G_0(\mathbf{x},\bar{\mathbf{x}})\cdot G^{(-/+)}(\bar{\mathbf{x}},\mathbf{x}')\,dV(\bar{\mathbf{x}})$$
$$\mathbf{x}'\in\Gamma_+,\mathbf{x}\in\Gamma_-. \tag{5.128}$$

In deriving these two equations we have to take the transmission conditions (2.281)/(2.282) into account, to rename $\mathbf{x}$ as $\bar{\mathbf{x}}$ and $\mathbf{x}''$ as $\mathbf{x}$, and to consider the symmetry relation (2.245) of G_0. These are the relevant volume integral equations we were looking for. Once we have calculated $G^{(-/+)}(\mathbf{x},\mathbf{x}')$ from (5.128) (if using again a bilinear expansion for this Green function, for example) we are then able to calculate $G_{\Gamma_+}^{(d)}(\mathbf{x},\mathbf{x}')$ from (5.127). In the process of solving (5.128) the singularity of G_0 at point $\mathbf{x}=\bar{\mathbf{x}}$ inside the scatterer deserves some attention. But due to the weak singularity of the scalar free-space Green function this is not too difficult. The integration may be performed in the sense of the principal value discussed in the context of the boundary integral equations. We just have to exclude a small volume element Γ_δ enclosing the singular point from the integration,

$$G^{(-/+)}(\mathbf{x},\mathbf{x}')=G_0(\mathbf{x},\mathbf{x}')$$
$$+\lim_{\Gamma_\delta\to 0}\kappa_d^2\int_{\Gamma_--\Gamma_\delta}G_0(\mathbf{x},\bar{\mathbf{x}})\cdot G^{(-/+)}(\bar{\mathbf{x}},\mathbf{x}')\,dV(\bar{\mathbf{x}});$$
$$\mathbf{x}'\in\Gamma_+\ ,\ \mathbf{x}\in\Gamma_-. \tag{5.129}$$

with the definition

$$G^{(d)}_{\Gamma_+}(\mathbf{x},\mathbf{x}') := G_0(\mathbf{x},\mathbf{x}') + \int_{\Gamma_-} G_0(\mathbf{x},\bar{\mathbf{x}})\, \hat{W}^{(d)}_{\Gamma_-}(\bar{\mathbf{x}},\tilde{\mathbf{x}})\, G_0(\tilde{\mathbf{x}},\mathbf{x}')\, dV(\bar{\mathbf{x}})\, dV(\tilde{\mathbf{x}}) \tag{5.130}$$

of the corresponding interaction operator $\hat{W}^{(d)}_{\Gamma_-}$ (which describes now the interaction of the primary incident field with the whole scattering volume!) we obtain after intercomparison with (5.127) the relation

$$\kappa_d^2\, G^{(-/+)}(\bar{\mathbf{x}},\mathbf{x}') = \int_{\Gamma_-} \hat{W}^{(d)}_{\Gamma_-}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \cdot G_0(\tilde{\mathbf{x}},\mathbf{x}')\, dV(\tilde{\mathbf{x}}). \tag{5.131}$$

The following statement seems to be appropriate at this point: It seems as if the difference of definition (5.130) compared to the definition (4.12) used in Sect. 4.2.2 to solve the outer transmission problem consists not only in the replacement of $G_0^>$ by the full free-space Green function G_0 but also by performing a volume integration over the scatterer volume instead of the boundary integration over its surface. However, the usage of the definitions

$$G^{(d)}_{\Gamma_+}(\mathbf{x},\mathbf{x}') := G_0(\mathbf{x},\mathbf{x}') + \int_{\Gamma_-} G_0^>(\mathbf{x},\bar{\mathbf{x}}) \cdot W^{(d)}_{\Gamma_+}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \cdot G_0(\tilde{\mathbf{x}},\mathbf{x}')\, dV(\bar{\mathbf{x}})\, dV(\tilde{\mathbf{x}}) \tag{5.132}$$

and

$$G^{(-/+)}(\mathbf{x},\mathbf{x}') := \int_{\Gamma_-} G_{0_s}^<(\mathbf{x},\bar{\mathbf{x}})\, W^{(d)}_{\Gamma_-}(\bar{\mathbf{x}},\tilde{\mathbf{x}})\, G_0(\tilde{\mathbf{x}},\mathbf{x}')\, dV(\bar{\mathbf{x}})\, dV(\tilde{\mathbf{x}}) \tag{5.133}$$

instead of definitions (4.12) and (4.13) would not change the result obtained in Sect. 4.2.2. That is because the change of the definitions affects only the corresponding definitions (4.17) and (4.18) of the matrix elements of the relevant interaction operators. This change would therefore result into

$$\left[W^{(d)}_{\Gamma_+}\right]_{i,k} := (ik_0) \int_{\Gamma_-} \tilde{\psi}_i(k_0,\bar{\mathbf{x}})\, W^{(d)}_{\Gamma_+}(\bar{\mathbf{x}},\tilde{\mathbf{x}})\, \psi_k(k_0,\tilde{\mathbf{x}})\, dV(\bar{\mathbf{x}})\, dV(\tilde{\mathbf{x}}) \tag{5.134}$$

and

$$\left[W^{(d)}_{\Gamma_-}\right]_{i,k} := (ik) \int_{\Gamma_-} \tilde{\varphi}_i(k_0,\bar{\mathbf{x}})\, W^{(d)}_{\Gamma_-}(\bar{\mathbf{x}},\tilde{\mathbf{x}})\, \psi_k(k_0,\tilde{\mathbf{x}})\, dV(\bar{\mathbf{x}})\, dV(\tilde{\mathbf{x}}). \tag{5.135}$$

It is then not difficult to convince oneself that expression (4.22) derived in Sect. 4.2.2 holds also for the new matrix elements $\left[W^{(d)}_{\Gamma_+}\right]_{i,k}$.

If we now replace $G^{(-/+)}$ on the left-hand side of Eq. (5.131) by expression (5.128) and apply again (5.131) afterwards we end up with the volume integral equation

$$\hat{W}^{(d)}_{\Gamma_-}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) = \kappa_d^2 \cdot \left[\delta(\bar{\mathbf{x}}-\tilde{\mathbf{x}}) + \int_{\Gamma_-} G_0(\bar{\mathbf{x}},\hat{\mathbf{x}}) \cdot \hat{W}^{(d)}_{\Gamma_-}(\hat{\mathbf{x}},\tilde{\mathbf{x}})\, dV(\hat{\mathbf{x}})\right] \tag{5.136}$$

of the interaction operator $\hat{W}^{(d)}_{\Gamma_-}$ which is equivalent to (5.128). This type of equation is called a "Lippmann-Schwinger" equation. They are of our interest in the next section. But we can also define the equivalent volume current inside the scatterer via the definition

$$J_{\Gamma_-}(\mathbf{x}) := \int_{\Gamma_-} \hat{W}^{(d)}_{\Gamma_-}(\mathbf{x},\tilde{\mathbf{x}}) \cdot u_{inc}(\tilde{\mathbf{x}})\, dV(\tilde{\mathbf{x}}). \tag{5.137}$$

Then, the total field outside the scatterer reads because of (2.286) and (5.130)

$$u_t(\mathbf{x}) = u_{inc}(\mathbf{x}) + \int_{\Gamma_-} G_0(\mathbf{x},\bar{\mathbf{x}}) \cdot J_{\Gamma_-}(\bar{\mathbf{x}})\, dV(\bar{\mathbf{x}}). \tag{5.138}$$

If we multiply (5.136) with the primary incident field u_{inc} and integrate the resulting equation over the volume of the scatterer subsequently we get the known volume integral equation

$$J_{\Gamma_-}(\mathbf{x}) = \kappa_d^2 \cdot \left[u_{inc}(\mathbf{x}) + \int_{\Gamma_-} G_0(\mathbf{x},\bar{\mathbf{x}}) \cdot J_{\Gamma_-}(\bar{\mathbf{x}})\, dV(\bar{\mathbf{x}})\right] \tag{5.139}$$

from which we can calculate the equivalent volume current inside the scatterer.

5.5 Lippmann-Schwinger Equations

5.5.1 The Scalar Problem

Equation (5.130) provides already an appropriate starting point to solve the outer transmission problem iteratively. Its lowest order iteration is of course given by

$$\left[G^{(d)}_{\Gamma_+}(\mathbf{x},\mathbf{x}')\right]^{(0)} = G_0(\mathbf{x},\mathbf{x}') \tag{5.140}$$

and represents nothing but the unperturbed problem, i.e., the Green function in the absence of any scatterer. The first iteration which takes the existence of a scatterer into account can then be calculated from the lowest order iteration

$$\left[\hat{W}^{(d)}_{\Gamma_-}(\bar{\mathbf{x}},\tilde{\mathbf{x}})\right]^{(1)} = \kappa_d^2\, \delta(\bar{\mathbf{x}}-\tilde{\mathbf{x}}) \tag{5.141}$$

of the Lippmann-Schwinger equation (5.136) of the related interaction operator. The result is

$$\left[G_{\Gamma_+}^{(d)}(\mathbf{x},\mathbf{x}')\right]^{(1)} = G_0(\mathbf{x},\mathbf{x}') + \kappa_d^2 \cdot \int_{\Gamma_-} G_0(\mathbf{x},\bar{\mathbf{x}}) \cdot G_0(\bar{\mathbf{x}},\mathbf{x}')\, dV(\bar{\mathbf{x}}). \quad (5.142)$$

The corresponding iteration of the Green function $G^{(-/+)}$ becomes

$$\left[G^{(-/+)}(\mathbf{x},\mathbf{x}')\right]^{(1)} = G_0(\mathbf{x},\mathbf{x}') \quad (5.143)$$

because of (5.131). This iteration procedure can be continued indefinitely. At all higher iterations we have to consider carefully the singularity of the free-space Green function in the integral terms. But then it becomes questionable whether higher order iterations are of benefit compared with the non-iterative solution of (5.136). In most of its applications the iteration procedure is therefore restricted to the first iteration (5.142), or at most to the second one. The required transmission conditions are obviously not fulfilled in these cases. Therefore, using the iterative solutions makes only sense if the scatterer affects only slightly the unperturbed problem. What exactly do we mean by "slightly" depends "strongly" on the problem under consideration and cannot be defined in advance.

We are now interested to derive the Lippmann-Schwinger equations of the Green function and the interaction operator related to the outer Dirichlet problem. For this we have to go back to (3.27) which reads in more detail

$$G_{\Gamma_+}(\mathbf{x},\mathbf{x}') = G_0(\mathbf{x},\mathbf{x}') + \oint_{\partial\Gamma} G_0(\mathbf{x},\bar{\mathbf{x}}) \cdot \hat{\bar{n}}_- \cdot \nabla_{\bar{x}}\, G_{\Gamma_+}(\bar{\mathbf{x}},\mathbf{x}')\, dS(\bar{\mathbf{x}}), \quad (5.144)$$

if making use of the symmetry relation (2.245) and the definition (3.22) of the surface Green function related to G_{Γ_+}. It should be emphasized that the homogeneous Dirichlet condition (2.280) at the scatterer surface was already incorporated in deriving (3.27). Now, if employing the scalar delta distribution at the scatterer surface defined in (3.6), we can "inflate" (5.144) identical into

$$G_{\Gamma_+}(\mathbf{x},\mathbf{x}') = G_0(\mathbf{x},\mathbf{x}') + \oint_{\partial\Gamma} G_0(\mathbf{x},\bar{\mathbf{x}}) \cdot \delta_{\partial\Gamma}(\tilde{\mathbf{x}}-\bar{\mathbf{x}}) \cdot \hat{\tilde{n}}_- \cdot \nabla_{\tilde{x}}\, G_{\Gamma_+}(\tilde{\mathbf{x}},\mathbf{x}')\, dS(\tilde{\mathbf{x}})\, dS(\bar{\mathbf{x}}). \quad (5.145)$$

with the definition of the operator

$$U_{\partial\Gamma}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) := \delta_{\partial\Gamma}(\tilde{\mathbf{x}}-\bar{\mathbf{x}}) \cdot \hat{\tilde{n}}_- \cdot \nabla_{\tilde{x}} \quad (5.146)$$

we can thus write

$$G_{\Gamma_+}(\mathbf{x},\mathbf{x}') = G_0(\mathbf{x},\mathbf{x}') + \oint_{\partial\Gamma} G_0(\mathbf{x},\bar{\mathbf{x}}) \cdot U_{\partial\Gamma}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \cdot G_{\Gamma_+}(\tilde{\mathbf{x}},\mathbf{x}')\, dS(\tilde{\mathbf{x}})\, dS(\bar{\mathbf{x}}) \tag{5.147}$$

instead of (3.27). Please, note that the product $U_{\partial\Gamma} \cdot G_{\Gamma_+}$ on the right-hand side of this equation does not mean the conventional product of two functions but the application of the operator $U_{\partial\Gamma}$ to the function which follows this operator (G_{Γ_+} in our case). As a consequence, we can not change its position under the integral sign. The shortened operator notation of (5.147) reads

$$G_{\Gamma_+}(\mathbf{x},\mathbf{x}') = G_0(\mathbf{x},\mathbf{x}') + G_0(\mathbf{x},\bar{\mathbf{x}}) \circ U_{\partial\Gamma}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \circ G_{\Gamma_+}(\tilde{\mathbf{x}},\mathbf{x}') \tag{5.148}$$

where we have to integrate according to $\oint_{\partial\Gamma} \cdots dS$ over variables which appear twice. Equation (5.147) or (5.148) represents the Lippmann-Schwinger equation of the Green function G_{Γ_+} related to the outer Dirichlet problem. Its lowest order iteration (the unperturbed problem) is again given by

$$G^{(0)}_{\Gamma_+}(\mathbf{x},\mathbf{x}') = G_0(\mathbf{x},\mathbf{x}'). \tag{5.149}$$

Its next iteration

$$G^{(1)}_{\Gamma_+}(\mathbf{x},\mathbf{x}') = G_0(\mathbf{x},\mathbf{x}') + G_0(\mathbf{x},\bar{\mathbf{x}}) \circ U_{\partial\Gamma}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \circ G_0(\tilde{\mathbf{x}},\mathbf{x}') \tag{5.150}$$

or, more precisely,

$$\begin{aligned} G^{(1)}_{\Gamma_+}(\mathbf{x},\mathbf{x}') &= G_0(\mathbf{x},\mathbf{x}') \\ &\quad + \oint_{\partial\Gamma} G_0(\mathbf{x},\bar{\mathbf{x}}) \cdot U_{\partial\Gamma}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \cdot G_0(\tilde{\mathbf{x}},\mathbf{x}')\, dS(\tilde{\mathbf{x}})\, dS(\bar{\mathbf{x}}) \\ &= G_0(\mathbf{x},\mathbf{x}') + \oint_{\partial\Gamma} G_0(\mathbf{x},\bar{\mathbf{x}}) \cdot \hat{\bar{n}}_- \cdot \nabla_{\bar{x}}\, G_0(\bar{\mathbf{x}},\mathbf{x}')\, dS(\bar{\mathbf{x}}) \end{aligned} \tag{5.151}$$

considers already the existence of the scatterer. Here it holds also that all higher iterations become affected by the singularity of the free-space Green function. This can be easily seen if replacing G_{Γ_+} on the right-hand side of (5.148) by its iteration (5.150)/(5.151).

To derive the equivalent Lippmann-Schwinger equation of the interaction operator we remember the definition (5.79) which reads in operator notation

$$G_{\Gamma_+}(\mathbf{x},\mathbf{x}') := G_0(\mathbf{x},\mathbf{x}') + G_0(\mathbf{x},\bar{\mathbf{x}}) \circ \hat{W}_{\partial\Gamma_+}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \circ G_0(\tilde{\mathbf{x}},\mathbf{x}'). \tag{5.152}$$

Comparing this with expression (5.148) provides

$$G_0(\mathbf{x},\bar{\mathbf{x}})\circ U_{\partial\Gamma}(\bar{\mathbf{x}},\tilde{\mathbf{x}})\circ G_{\Gamma_+}(\tilde{\mathbf{x}},\mathbf{x}') = G_0(\mathbf{x},\bar{\mathbf{x}})\circ \hat{W}_{\partial\Gamma_+}(\bar{\mathbf{x}},\tilde{\mathbf{x}})\circ G_0(\tilde{\mathbf{x}},\mathbf{x}'). \quad (5.153)$$

Replacing G_{Γ_+} on the left-hand side again by its definition (5.152) provides the Lippmann-Schwinger equation

$$\hat{W}_{\partial\Gamma_+}(\mathbf{x},\mathbf{x}') = U_{\partial\Gamma}(\mathbf{x},\mathbf{x}') + U_{\partial\Gamma}(\mathbf{x},\bar{\mathbf{x}})\circ G_0(\bar{\mathbf{x}},\tilde{\mathbf{x}})\circ \hat{W}_{\partial\Gamma_+}(\tilde{\mathbf{x}},\mathbf{x}') \quad (5.154)$$

of the interaction operator related to the outer Dirichlet problem we were looking for. If its lowest order iteration

$$\hat{W}^{(1)}_{\partial\Gamma_+}(\mathbf{x},\mathbf{x}') = U_{\partial\Gamma}(\mathbf{x},\mathbf{x}'). \quad (5.155)$$

is inserted into (5.152) we obtain again the first iteration (5.151) of the Green function.

5.5.2 The Dyadic Problem

We proceed in close analogy to the scalar case but with the difference that we have to apply now the dyadic-dyadic Green theorem (2.319) in the respective regions. Let us start with the outer transmission problem. From the application of (2.319) in Γ_+ with the two dyadics

$$\mathbf{Q}(\mathbf{x},\mathbf{x}'') = \mathbf{G_0}(\mathbf{x},\mathbf{x}''); \quad \mathbf{x}\in\Gamma_+ \quad (5.156)$$

$$\mathbf{P}(\mathbf{x},\mathbf{x}') = \mathbf{G}^{(\mathbf{d})}_{\mathbf{\Gamma}_+}(\mathbf{x},\mathbf{x}'); \quad \mathbf{x},\mathbf{x}'\in\Gamma_+ \quad (5.157)$$

where we have again to distinguish between the two cases $\mathbf{x}''\in\Gamma_+$ (case 1a) and $\mathbf{x}''\in\Gamma_-$ (case 1b), and, on the other hand, from the application in Γ_- with the two dyadics

$$\mathbf{Q}(\mathbf{x},\mathbf{x}'') = \mathbf{G_0}(\mathbf{x},\mathbf{x}''); \quad \mathbf{x}\in\Gamma_+ \quad (5.158)$$

$$\mathbf{P}(\mathbf{x},\mathbf{x}') = \mathbf{G}^{(-/+)}(\mathbf{x},\mathbf{x}'); \quad \mathbf{x}\in\Gamma_-\,,\ \mathbf{x}'\in\Gamma_+ \quad (5.159)$$

and $\mathbf{x}''\in\Gamma_+$ (case 2a) or $\mathbf{x}''\in\Gamma_-$ (case 2b) we obtain from the transmission conditions (2.343) and (2.344) the two equations

$$\mathbf{G}^{(\mathbf{d})}_{\mathbf{\Gamma}_+}(\mathbf{x},\mathbf{x}') = \mathbf{G_0}(\mathbf{x},\mathbf{x}') + \kappa_d^2\int_{\mathbf{\Gamma}_-}\mathbf{G_0}(\mathbf{x},\bar{\mathbf{x}})\cdot\mathbf{G}^{(-/+)}(\bar{\mathbf{x}},\mathbf{x}')\,dV(\bar{\mathbf{x}})$$
$$\mathbf{x},\mathbf{x}'\in\Gamma_+ \quad (5.160)$$

and

$$\mathbf{G}^{(-/+)}(\mathbf{x},\mathbf{x}') = \mathbf{G_0}(\mathbf{x},\mathbf{x}') + \kappa_d^2 \int_{\mathbf{\Gamma}_-} \mathbf{G_0}(\mathbf{x},\bar{\mathbf{x}}) \cdot \mathbf{G}^{(-/+)}(\bar{\mathbf{x}},\mathbf{x}')\, dV(\bar{\mathbf{x}})$$
$$\mathbf{x}' \in \Gamma_+, \mathbf{x} \in \Gamma_-. \tag{5.161}$$

This is the dyadic analogue to the scalar case. The interim results are omitted here because the derivation runs along the same track as in the scalar case. With the definition

$$\mathbf{G}^{(\mathbf{d})}_{\mathbf{\Gamma}_+}(\mathbf{x},\mathbf{x}') := \mathbf{G_0}(\mathbf{x},\mathbf{x}') + \int_{\mathbf{\Gamma}_-} \mathbf{G_0}(\mathbf{x},\bar{\mathbf{x}})\, \hat{\mathbf{W}}^{(d)}_{\mathbf{\Gamma}_-}(\bar{\mathbf{x}},\tilde{\mathbf{x}})\, \mathbf{G_0}(\tilde{\mathbf{x}},\mathbf{x}')\, dV(\bar{\mathbf{x}})\, dV(\tilde{\mathbf{x}}) \tag{5.162}$$

we thus obtain

$$\hat{\mathbf{W}}^{(d)}_{\mathbf{\Gamma}_-}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) = \kappa_d^2 \cdot \left[\mathbf{I}\delta(\bar{\mathbf{x}}-\tilde{\mathbf{x}}) + \int_{\mathbf{\Gamma}_-} \mathbf{G_0}(\bar{\mathbf{x}},\hat{\mathbf{x}}) \cdot \hat{\mathbf{W}}^{(d)}_{\mathbf{\Gamma}_-}(\hat{\mathbf{x}},\tilde{\mathbf{x}})\, dV(\hat{\mathbf{x}}) \right] \tag{5.163}$$

as the Lippmann-Schwinger equation of the dyadic interaction operator of the outer transmission problem. It is the analogue of the scalar equation (5.136). Its lowest order iteration, if inserted into (5.162), provides again the first iteration of $\mathbf{G}_{\mathbf{\Gamma}_+}(\mathbf{x},\mathbf{x}')$ which takes the existence of the scatterer into account. All higher iterations have to consider carefully the (now strong!) singularity of $\mathbf{G_0}$ inside the scatterer.

The treatment of the outer Dirichlet problem in the dyadic case is also quite similar to the scalar case. By use of (2.329) and identity (2.312) we can rewrite (3.80) into

$$\mathbf{G}_{\mathbf{\Gamma}_+}(\mathbf{x},\mathbf{x}') = \mathbf{G_0}(\mathbf{x},\mathbf{x}') - \oint_{\partial\Gamma} \mathbf{G_0}(\mathbf{x},\bar{\mathbf{x}}) \cdot \left[\hat{\bar{n}}_- \times \nabla_{\bar{\mathbf{x}}} \times \mathbf{G}_{\mathbf{\Gamma}_+}(\bar{\mathbf{x}},\mathbf{x}') \right] dS(\bar{\mathbf{x}}). \tag{5.164}$$

The dyadic delta distribution at the scatterer surface introduced in (3.58) allows us to define the operator

$$\mathbf{U}^{(\hat{\tilde{\mathbf{n}}})}_{\partial\mathbf{\Gamma}}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) := -\mathbf{D}^{(\hat{\tilde{\mathbf{n}}})}_{\partial\mathbf{\Gamma}}(\tilde{\mathbf{x}}-\bar{\mathbf{x}}) \cdot \left[\hat{\tilde{n}} \times \nabla_{\tilde{x}} \times \right] \mathbf{I}, \tag{5.165}$$

so that

$$\oint_{\partial\Gamma} \mathbf{U}^{(\hat{\tilde{\mathbf{n}}}_-)}_{\partial\mathbf{\Gamma}}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \cdot \mathbf{G}_{\mathbf{\Gamma}_+}(\tilde{\mathbf{x}},\mathbf{x}')\, dS(\tilde{\mathbf{x}}) = -\hat{\bar{n}}_- \times \nabla_{\bar{\mathbf{x}}} \times \mathbf{G}_{\mathbf{\Gamma}_+}(\bar{\mathbf{x}},\mathbf{x}') \tag{5.166}$$

holds. Thus, we can rewrite (5.164) into

$$\mathbf{G}_{\mathbf{\Gamma}_+}(\mathbf{x},\mathbf{x}') = \mathbf{G}_{\mathbf{0}}(\mathbf{x},\mathbf{x}') + \oint_{\partial\Gamma} \mathbf{G}_{\mathbf{0}}(\mathbf{x},\bar{\mathbf{x}}) \cdot \mathbf{U}_{\partial\mathbf{\Gamma}}^{(\hat{\bar{\mathbf{n}}}_-)}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \cdot \mathbf{G}_{\mathbf{\Gamma}_+}(\tilde{\mathbf{x}},\mathbf{x}')\, dS(\tilde{\mathbf{x}})\, dS(\bar{\mathbf{x}}), \quad (5.167)$$

or, if employing the more simple operator notation,

$$\mathbf{G}_{\mathbf{\Gamma}_+}(\mathbf{x},\mathbf{x}') = \mathbf{G}_{\mathbf{0}}(\mathbf{x},\mathbf{x}') + \mathbf{G}_{\mathbf{0}}(\mathbf{x},\bar{\mathbf{x}}) \circ \mathbf{U}_{\partial\mathbf{\Gamma}}^{(\hat{\bar{\mathbf{n}}}_-)}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \circ \mathbf{G}_{\mathbf{\Gamma}_+}(\tilde{\mathbf{x}},\mathbf{x}'). \quad (5.168)$$

This represents already the Lippmann-Schwinger equation of the outer Dirichlet problem in the dyadic case. The first two iterations are given by

$$\mathbf{G}_{\mathbf{\Gamma}_+}^{(\mathbf{0})}(\mathbf{x},\mathbf{x}') = \mathbf{G}_{\mathbf{0}}(\mathbf{x},\mathbf{x}') \quad (5.169)$$

(this is the unperturbed problem) and

$$\mathbf{G}_{\mathbf{\Gamma}_+}^{(\mathbf{1})}(\mathbf{x},\mathbf{x}') = \mathbf{G}_{\mathbf{0}}(\mathbf{x},\mathbf{x}') + \mathbf{G}_{\mathbf{0}}(\mathbf{x},\bar{\mathbf{x}}) \circ \mathbf{U}_{\partial\mathbf{\Gamma}}^{(\hat{\bar{\mathbf{n}}}_-)}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \circ \mathbf{G}_{\mathbf{0}}(\tilde{\mathbf{x}},\mathbf{x}') \quad (5.170)$$

or, in more detail,

$$\begin{aligned}\mathbf{G}_{\mathbf{\Gamma}_+}^{(1)}(\mathbf{x},\mathbf{x}') &= \mathbf{G}_{\mathbf{0}}(\mathbf{x},\mathbf{x}') \\ &\quad + \oint_{\partial\Gamma} \mathbf{G}_{\mathbf{0}}(\mathbf{x},\bar{\mathbf{x}}) \cdot \mathbf{U}_{\partial\mathbf{\Gamma}}^{(\hat{\bar{\mathbf{n}}}_-)}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \cdot \mathbf{G}_{\mathbf{0}}(\tilde{\mathbf{x}},\mathbf{x}')\, dS(\tilde{\mathbf{x}})\, dS(\bar{\mathbf{x}}) \\ &= \mathbf{G}_{\mathbf{0}}(\mathbf{x},\mathbf{x}') - \oint_{\partial\Gamma} \mathbf{G}_{\mathbf{0}}(\mathbf{x},\bar{\mathbf{x}}) \cdot \left[\hat{\bar{n}}_- \times \nabla_{\bar{\mathbf{x}}} \times \mathbf{G}_{\mathbf{0}}(\bar{\mathbf{x}},\mathbf{x}')\right] dS(\bar{\mathbf{x}}) \quad (5.171)\end{aligned}$$

(this is the first deviation from the unperturbed problem). These two iterations avoid the strong singularity of $\mathbf{G}_{\mathbf{0}}$. The equivalent Lippmann-Schwinger equation of the dyadic interaction operator can be obtained from the defining equation

$$\mathbf{G}_{\mathbf{\Gamma}_+}(\mathbf{x},\mathbf{x}') := \mathbf{G}_{\mathbf{0}}(\mathbf{x},\mathbf{x}') + \oint_{\partial\Gamma} \mathbf{G}_{\mathbf{0}}(\mathbf{x},\bar{\mathbf{x}}) \cdot \hat{\mathbf{W}}_{\partial\Gamma_+}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \cdot \mathbf{G}_{\mathbf{0}}(\tilde{\mathbf{x}},\mathbf{x}')\, dS(\bar{\mathbf{x}})\, dS(\tilde{\mathbf{x}}), \quad (5.172)$$

the dyadic analogue of (4.23). This reads in operator notation

$$\mathbf{G}_{\mathbf{\Gamma}_+}(\mathbf{x},\mathbf{x}') := \mathbf{G}_{\mathbf{0}}(\mathbf{x},\mathbf{x}') + \mathbf{G}_{\mathbf{0}}(\mathbf{x},\bar{\mathbf{x}}) \circ \hat{\mathbf{W}}_{\partial\Gamma_+}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \circ \mathbf{G}_{\mathbf{0}}(\tilde{\mathbf{x}},\mathbf{x}'). \quad (5.173)$$

From this equation and after intercomparison with (5.168) we get finally the Lippmann-Schwinger equation

$$\hat{\mathbf{W}}_{\partial\mathbf{\Gamma}_+}(\mathbf{x},\mathbf{x}') = \mathbf{U}_{\partial\mathbf{\Gamma}}^{(\hat{\bar{\mathbf{n}}}_-)}(\mathbf{x},\mathbf{x}') + \mathbf{U}_{\partial\mathbf{\Gamma}}^{(\hat{\bar{\mathbf{n}}}_-)}(\mathbf{x},\bar{\mathbf{x}}) \circ \mathbf{G}_{\mathbf{0}}(\bar{\mathbf{x}},\tilde{\mathbf{x}}) \circ \hat{\mathbf{W}}_{\partial\mathbf{\Gamma}_+}(\tilde{\mathbf{x}},\mathbf{x}') \quad (5.174)$$

of the dyadic interaction operator related to the outer Dirichlet problem. Its lowest order iteration, if inserted into (5.171), just provides the first iteration (5.171) of the corresponding dyadic Green function.

At the end of this chapter, we will once again emphasize the difference between the integral equation methods discussed above and the approach considered in Chap. 4 which results into the T-matrix methods. Both classes of methods can be obtained by starting from the representation of the Green functions related to the scattering problems by appropriate interaction operators. The defining equations of the interaction operators can be considered to be expressions of Huygens' principle. To derive the T-matrices the auxiliary functions $G_0^>$ or $\mathbf{G}_\mathbf{t}^>$, depending on whether the scalar or dyadic case is considered, must be employed in the respective defining equations. These functions are solutions of the homogeneous Helmholtz or vector-wave equation. The Green functions represented in this way solve the corresponding inhomogeneous Helmholtz or vector-wave equation subject to the radiation condition with respect to the observation point. From the additional conditions the Green functions have to fulfil at the scatterer surface we are then able to derive explicit expressions for the T-matrices. Thereby, it is of no importance whether the interaction operators are introduced via a boundary or volume integral. This affects only the definition of the corresponding matrix elements, as demonstrated above for the outer transmission problem. On the other hand, to derive the boundary or volume integral equations we have to replace the auxiliary functions $G_0^>$ or $\mathbf{G}_\mathbf{t}^>$ in the defining equations of the interaction operators by the full free-space Green functions G_0 or $\mathbf{G_0}$. But these functions are singular at the boundary surface or inside the scatterer thus resulting in singular boundary or volume integral equations for the interaction operators itself as well as for the strongly related induced surface or volume currents. These singularities must be considered seriously in every numerical procedure. One essential advantage of the T-matrices is the fact that these are not affected by such singularities. But in contrast to the singular boundary or volume integral equation methods the T-matrix methods are faced with the problem of Rayleigh's hypothesis.