ON THE CONVERGENCE AND NUMERICAL STABILITY OF THE SECOND WATERMAN SCHEME FOR APPROXIMATION OF THE ACOUSTIC FIELD SCATTERED BY A HARD OBJECT

Allan G. Dallas

Department of Mathematical Sciences
University of Delaware
Newark, DE 19716, U.S.A.

Technical Report No. 2000-7

On the Convergence and Numerical Stability of the Second Waterman Scheme For Approximation of the Acoustic Field Scattered by a Hard Obstacle*

Allan G. Dallas

Abstract. The numerical schemes of P.C. Waterman (*J. Acoust. Soc. Am.* **45** (1969), 1417–1429), frequently referred to under the name of "the T-matrix method," have formed the basis for many scattering computations in many settings. However, no successful analyses of the algorithms have been published, so the limitations on their range of applicability and numerical stability remain largely unknown; this is of particular importance because of the apparently inconsistent success achieved in numerical experiments. Here, we give an operator condition that guarantees the viability of the algorithm and mean-square convergence of the far-field patterns generated by the second Waterman scheme for the case of time-harmonic acoustic scattering by a hard obstacle; we prove further that the operator condition holds at least whenever the scattering obstacle is ellipsoidal. For the convergence proof, we also assume that the square of the wavenumber is not an interior Dirichlet eigenvalue for the negative Laplacian; in the contrary case, we show that the algorithm is at best numerically ill-conditioned. With this and previous experience in numerical applications, it appears that the performance of the algorithm is markedly shape-dependent; for certain obstacles, *e.g.*, ellipsoids, instabilities are so localized in wavenumber that they are practically numerically irrelevant, while it is not clear whether the erratic results found in applications to various other shapes arise from a failure of convergence or from numerical instability.

Contents

* This work was partially supported by the Air Force Office of Scientific Research, Air Force Materiel Command, USAF, under Grant F49620-96-1-0039. The views and conclusions contained herein are those of the author and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the Air Force Office of Scientific Research or the U.S. Government.

0. Introduction.

In 1969, P. C. WATERMAN [18] proposed certain formal computational procedures aimed at approximation of the time-harmonic acoustic fields scattered by hard and soft obstacles; *cf*., also, the earlier article [17] concerning electromagnetic scattering. Actually, for each acoustic case two procedures were motivated; evidently, one or both of these procedures have come to be known generally as "the transition-matrix method," or "the T-matrix method." Many calculations have been based on these schemes and their subsequent variants, since the same ideas were transported over—again, formally—to be applied in other sorts of scattering problems: elastic scattering, multiple scattering, scattering in and by inhomogeneous media, *etc*.

Indeed, the methods seem attractive from the computational standpoint, since they require simply the evaluation of certain surface integrals involving classical special functions, for the formation of the coefficients and righthand side of a certain linear algebraic system, followed by solution of the system. In particular, approximations of neither singular nor even weakly singular boundary operators are required.

Moreover, there seems to persist a general perception that the Waterman schemes do not suffer from the sort of numerical instabilities undermining the simplest, "unmodified," integral-equation reformulations of the exterior radiation problems when the square of the wavenumber is sufficiently near a certain type of interior eigenvalue of the negative Laplacian. In fact, the formulation of numerical procedures valid and stable at all frequencies was apparently one of the aims in [18], and, indeed, in the derivation of the *first* scheme there, by using relations usually known now as "null-field equations," Waterman obtained a moment problem for the "total" acoustic field that is uniquely solvable for all values of the wavenumber (an easily proven property recognized subsequently). The latter unique solvability is, along with various numerical results displaying no apparent anomalies, evidently the source of the perception that the Waterman algorithms are free of the interior-eigenvalue type of instability.

However, for both the hard- and soft-scattering problems, in setting up numerical schemes for approximation of the total fields through *implementation* of the moment-problem reformulations, Waterman selected sequences of trial functions (constructed from the regular spherical-wave functions) which fail to be complete at the wavenumbers corresponding to the pertinent interior eigenvalues, in the usual Hilbert space $L_2(\Gamma)$ associated with the boundary Γ of the obstacle. While the Appendix of [18] indicates that Waterman was aware of this lack of completeness, he nevertheless retained the choices, apparently because his numerical results seemed to indicate that the defect produced no instabilites. But as we show here, there are numerical instabilities present at the exceptional wavenumbers, at least for those shapes satisfying a certain operator condition (which includes the ellipsoids); the important question then concerns the widths of the surrounding intervals over which the matrix condition numbers are "too large." For nice shapes such as ellipsoids, these intervals of instability are so narrow that they are practically numerically invisible, as reported in [15]. But for other obstacles for which erratic numerical results are observed, the situation is not clear; it may be either that the algorithm is not convergent for those shapes or that the intervals of numerical instability are broader. (It is interesting to observe that, in the latter eventuality, the use of the incomplete sequences will have effectively introduced into the numerical computations for a uniquely solvable problem the same sort of shortcoming that is encountered in the use of the primitive boundary-operator reformulations for another reason, *viz*., because those problems themselves are originally not uniquely solvable at the pertinent interior eigenvalues.)

Almost all of the work published on the Waterman schemes and their modifications, including the original papers [17] and [18], is in the nature of numerical experimentation on the basis of heuristic motivation. That is, there have appeared essentially no papers establishing the needed fundamental facts about viability, convergence, and numerical stability for even the most basic schemes. These matters are of even more than the usual importance in this case, in view of the sometimes erratic and unstable numerical results appearing. That is, the schemes appear to perform very well for some obstacle shapes and frequencies but very poorly—if at all—for others, and none of the basic issues connected with understanding the range of applicability of the methods has been satisfactorily resolved. Thus, it is not known to which obstacle shapes and frequencies the methods are applicable, nor are there general results resolving the uncertainty about just which field quantities are being convergently approximated (the far-field pattern? the field outside a circumscribing sphere? the field right down to the obstacle boundary? the unknown surface field?) or the type of convergence that can be expected (pointwise? uniform? in the least-squares sense?). Remarkably, the question of the *viability* of the schemes, *i.e.*, whether the sequence of matrices figuring in the computations have the requisite property of eventual invertibility (to say nothing of their conditioning), has not even been resolved in general. In short, the schemes have remained in the status of "formalisms."

Evidently, most of the reported numerical implementations of the Waterman schemes have treated very regular and simple shapes, for which the far-field pattern has been the quantity most frequently approximated. Perhaps the strongest verification of the convergence of the far-field patterns calculated on the basis of one of the Waterman schemes is the indirect evidence provided in the examination of an inverse method by COLTON AND MONK [3]. There, to test an inverse shape-reconstruction scheme, "synthetic" far-field pattern scattering data were manufactured from a program credited to G. KRISTENSSON and implementing one of the Waterman schemes. The successful reconstruction of a number of smooth bodies of revolution shows that the data generated in the solution of the forward problems were undoubtedly correct. On the other hand, there also seem to be numerous examples of instabilities and convergence difficulties that have not appeared in published form.

As far as we know, the only collection of results on the questions of viability and convergence were given in [4]; the present note comprises a modified and amplified form of that presentation. Throughout, we restrict attention to a generalization of the *second* scheme motivated in [18] for the acoustic hard-scattering problem; the generalization admits any Neumann data belonging to $L_2(\Gamma)$ and reduces to the second Waterman algorithm in case the data comprise the negative of the normal derivative of an acoustic incident field. In all of our "positive" results we require that the squared-wavenumber not belong to the countably infinite set of interior Dirichlet eigenvalues for the negative Laplacian. Then our main development, in Theorem 5.1.*i*, shows that the operator condition which we denote by (C.2) is sufficient to ensure viability, convergence of the far-field patterns in the mean-square sense, and boundedness of the sequence of matrix condition numbers *pointwise* at each pertinent wavenumber. However, in the contrary case when the squared-wavenumber does coincide with an interior Dirichlet eigenvalue, in Theorem 5.1.*ii* we show that if the generalized second Waterman scheme is viable, then it must be numerically unstable; more precisely, we prove that, if there is a sequence of invertible matrices, then the corresponding sequence of condition numbers diverges to ∞. The operator condition (C.2) that we impose is evidently a stringent condition on the shape of the obstacle, as roughly indicated by some other facts proven in Section 5; while we do not presently know the class of shapes for which the condition obtains, we do show that it holds for ellipsoidal obstacles, by exploiting a well-known symmetry result holding in that case, which was first observed by WATERMAN [18].

In one of the other previous attempts at analysis of these methods, KRISTENSSON, RAMM, AND STRÖM [9] (*cf*., also, the reorganized version in [14]) provide a proof of convergence of a rather general set-up which would encompass the *first* Waterman scheme, but the hypotheses of their analysis are too restrictive to admit the intended application, requiring conditions on the trial- and test-functions that can be met only in the very simplest case of a spherical obstacle. Thus, the results of [9] provide no information about the procedures that are apparently usually meant when speaking of "the T-matrix method." A much more detailed explanation of this appears in [5].

This article is a sequel/companion to [5], in which basis properties of the traces and normal derivatives of the familiar collections of outgoing and regular spherical-separable solutions of the Helmholtz equation are examined and the results applied in discussions of some questions closely related to the Waterman schemes. A description of these schemes for the approximate solution of the problem of time-harmonic acoustic scattering by a hard obstacle can be found in Sections 5 and 7 of [5], so we shall not repeat here the detailed developments, but just cite the form of the second scheme proposed in [18], which is the method of present interest.

As we already indicated, WATERMAN [18] treats both the sound-hard and sound-soft cases of the acoustic-scattering problem, while we restrict attention to the former but admit more general data, *i.e.*, we examine here only the exterior Neumann/radiation problem for the Helmholtz equation. This problem is formulated in the next Section 1, where we also review some background material and notation already introduced in [5], and end with some comments on the transition matrix. We proceed in Section 2 to motivate and set up a generalization of the second Waterman scheme that is appropriate for treating the exterior Neumann/radiation problem with square-integrable boundary data. We also review and amplify there a basic result of KRASNOSEL'SKIĬ, ET AL. [8] on the use of the Galerkin-Petrov method in the construction of convergent approximations to an element of a Hilbert space by appropriately selected trial functions. Section 3 contains some further discussion of numerical instabilities inherent in the second Waterman scheme at (and near) interior Dirichlet eigenvalues. We provide in Section 4 a negative result showing that one can expect convergence to the Neumann data in $L_2(\Gamma)$ for *every* data-function chosen from $L_2(\Gamma)$ *only* if the obstacle is spherical. The main results on viability, convergence, and numerical (in)stability, which we already summarized, are presented in Section 5. Section 6 contains our proof that the operator condition (C.2) holds for ellipsoidal obstacles, which relies on Waterman's symmetry result; since the latter is of such importance in the present reasoning, we have provided an Appendix in which we recall the argument and fill in more of the details.

We close this introductory Section 0 with a few general observations about the Waterman methods and the literature concerning them.

While practically any scheme for the solution of problems of scattering by obstacles can be cast into the form of a "transition-matrix method" (*cf*. the remarks here in Section 1), the presentation of the Waterman schemes in such a form seems to be an especially convenient means for presenting them. This circumstance, coupled with the emphasis placed in [18] on the transition-matrix aspect of the algorithms, has apparently led to a common use of the term "the T-matrix method" in referring to a numerical scheme based on [18]. But this practice has led to confusion in communications and the literature, for various reasons. That is, since the algorithms are but two of many schemes that might be called "T-matrix methods," and since the latter term is sometimes used in reference to one or another class of methods that may or may not include those of Waterman, misinterpretations have resulted from the unqualified use of designations such as "*the* T-matrix method" or "*the* T-matrix approach" in reference to the Waterman schemes alone.

Moreover, as we have noted, it does not seem to be generally recognized that there are actually two numerical methods proposed in [18] for each type of scattering problem; the "transition-matrix forms" of the two algorithms are concisely summarized here in (1.11) and (1.12) of Section 1 and in [5, Section 7]. Thus, although the two methods are superficially very similar, differing "only by a matrix transposition," their analyses apparently require different approaches, and it is not so clear that the two are "equivalent" in the sense that they always either succeed or fail together. The algorithm that is implicit in the abstract of WATERMAN [18] is the second algorithm motivated in the paper; it is the one examined here and evidently the method most frequently implemented. On the other hand, the analysis of KRISTENSSON, ET AL. [9] is apparently aimed at the first scheme of [18]—*cf*. the description in [5, Section 5]—although the title, abstract, and summaries in [9] refer only to "the T-matrix approach in scattering theory." Further, even though the results of [9] do not lead to a validation for either of the Waterman schemes, because the hypotheses imposed in the analysis there are too stringent to admit the necessary choices of trial and test functions, a number of later articles have stated that "the T-matrix method" is proven to converge in [9], apparently on the strength of the unqualified assertions in the abstract and summaries of the latter work, *i.e.*, apparently without inspecting what is actually accomplished there. Thus, we find subsequent writers citing a proof of convergence of "*the* T-matrix method" in [9], unaware that there are really two methods involved, that [9] concerns the first method (while they intend to apply the second method), and that the proof of [9] is not applicable to either Waterman scheme.

In any event, a discussion of the intended meaning of the term "transition-matrix method" is moot here, since the view of either scheme of [18] as such a method does not seem to help at all in understanding its operation and analyzing its validity. We have found it much more profitable to regard the schemes as aiming to approximate quantities in the scattering process other than the transition matrix directly; accordingly, we consider the appearance of the transition matrix in a description of the algorithms as natural but nevertheless peripheral to their foundations.

Finally, it is important to point out that the original papers of Waterman, as well as many of the succeeding articles concerned with the same schemes, contain several errors and misleading statements that have also contributed to the general confusion concerning the foundations and operation of the methods. These errors arise mainly from a failure to understand some fairly basic mathematics that is involved in the formulation of practically any approximation-of-solution method. For example, there seems to be the consistent confusion of the "completeness property" and the "basis property," so that writers erroneously assert the existence of infinite-series expansions in terms of a sequence which is merely known to be complete. For that matter, there is a general failure in the literature on these methods to distinguish between an actual (convergent) infinite-series representation, or "expansion," and a finite sum intended as an "approximation." This is frequently reflected in the consistent omission of limits of summation, along with the interpretation of a summation as a finite-sum approximation at one point but as a convergent infinite-series representation at another point, according to the exigencies of the current argument. For example, these points emerge very clearly when one tries to trace in [18] the "argument" leading to the purported equality "$\mathcal{Q}\mathcal{T} = -\mathrm{Re}\,\mathcal{Q}$," claimed as connecting the infinite transition matrix $\mathcal{T}$ and a certain infinite matrix $\mathcal{Q}$, which is used in [18] and elsewhere to describe the operation of the second Waterman scheme. The steps given there constitute a completely formal symbol manipulation, so that it is indeed remarkable to find that the equality does in fact turn out to hold for some obstacles; we remark further in [5] and here at the end of Section 5 on the validity of this relation. Many of these sorts of errors and misconceptions have not been recognized and corrected by succeeding writers after appearing once (as in the example just cited), but instead were repeated and propagated, making their eventual eradication far more difficult.

1. Background; remarks on "transition-matrix methods."

In this section we formulate the exterior Neumann/radiation problem for the Helmholtz equation and briefly recall the associated analytical machinery that is needed later. We continue with the setting and notation described in [5], and rely, for the most part with little comment, on the background material and notations summarized there.

Setting. Throughout, we suppose that Ω_- is a bounded and connected regularly open subset of $\mathbb{R}^3$ for which the corresponding exterior domain $\Omega_+ := \mathbb{R}^3 \setminus \overline{\Omega}_-$ is also connected. The boundary $\Gamma := \partial\Omega_- = \partial\Omega_+$ we take to be of class $C^{2,\alpha}$, and denote by $\mathbf{n}$ the continuous unit-normal field for Γ that is oriented toward the exterior domain Ω_+. The "wavenumber" parameter κ is taken to be real and positve. By $H^0(\Gamma) \equiv \big(L_2(\Gamma), (\,\cdot\,,\,\cdot\,)_0\big)$ we denote the usual Hilbert space of equivalence classes of complex measurable functions defined a.e. and having their moduli square-integrable with respect to the Lebesgue measure λ_Γ on Γ, equipped with the inner product given by

$$\big(f,g\big)_0 := \int_\Gamma f\,\overline{g}\,d\lambda_\Gamma, \qquad \text{for} \quad f,\, g \in L_2(\Gamma),$$

an overbar throughout denoting complex conjugation.

The trace $u\big|_\Gamma$ and normal derivative $u_{,\mathbf{n}}$ on Γ of a complex C^1-function defined in either Ω_- or Ω_+ we define in the normal-L_2 sense. If $u_{,\mathbf{n}}$ exists for such a function, then so does $u\big|_\Gamma$, and we say that u is *L_2-regular at* Γ. It is convenient to establish notations for the collections of solutions of the Helmholtz equation

$$\Delta u + \kappa^2 u = 0 \tag{1.1}$$

in the exterior domain Ω_+ that also possess L_2-regularity at Γ and satisfy the Sommerfeld radiation condition

$$\lim_{\varrho\to\infty} \varrho\big\{\hat{\mathbf{e}}\cdot \operatorname{grad} u(\varrho\,\hat{\mathbf{e}}) - \mathrm{i}\kappa u(\varrho\,\hat{\mathbf{e}})\big\} = 0 \qquad \text{uniformly for} \quad \hat{\mathbf{e}} \in \Sigma_1, \tag{1.2}$$

in which Σ_1 denotes the unit sphere (boundary of the unit ball) in $\mathbb{R}^3$. Accordingly, we set

$$W_+(\Omega_+;\kappa) := \big\{\ u \in C^2(\Omega_+) \ \big|\ (1.1) \text{ holds in } \Omega_+,\ (1.2) \text{ holds, and } u \text{ is } L_2\text{-regular at } \Gamma\ \big\}.$$

For u in $W_+(\Omega_+;\kappa)$ we refer to $u|_\Gamma$ and $u_{,\mathbf{n}}$ as, respectively, *the Dirichlet data* and *the Neumann data of* u. Integral representations of the elements of $W_+(\Omega_+;\kappa)$, and of solutions of (1.1) in Ω_- that are L_2-regular at Γ, in terms of their Neumann and Dirichlet data are well known and recorded for reference in, *e.g.*, [5], where one can also find the definitions and summaries of the simplest properties of the interior and exterior single- and double-layer potentials $V_\kappa^-\{\varphi\}$, $V_\kappa^+\{\varphi\}$, $W_\kappa^-\{\varphi\}$, and $W_\kappa^+\{\varphi\}$ for the Helmholtz operator, with density $\varphi \in H^0(\Gamma)$, as well as of the associated "direct-value" operators S_κ, D_κ, and T_κ acting in $H^0(\Gamma)$, all constructed with the help of the fundamental solution given by, for each $\mathbf{x} \in \mathbb{R}^3$,

$$E_{\mathbf{x}}^\kappa(\mathbf{y}) := -\frac{e^{\mathrm{i}\kappa|\mathbf{y}-\mathbf{x}|}}{2\pi|\mathbf{y}-\mathbf{x}|} \qquad \text{for} \quad \mathbf{y} \in \mathbb{R}^3 \setminus \{\mathbf{x}\}.$$

The exterior Neumann/radiation problem; the Neumann-to-Dirichlet-data operator $\mathbf{A}_{\boldsymbol{\kappa}}$. We formulate the exterior Neumann problem only for data in $H^0(\Gamma)$. Given $g \in H^0(\Gamma)$, the Neumann/radiation problem corresponding to Ω_-, κ, and g requires the determination of $u \in W_+(\Omega_+;\kappa)$ satisfying the Neumann condition

$$u_{,\mathbf{n}} = g. \tag{1.3}$$

This problem is well posed, *i.e.*, corresponding to each $g \in H^0(\Gamma)$ there is a unique element $\mathfrak{u}_g \in W_+(\Omega_+;\kappa)$ such that $\mathfrak{u}_{g,\mathbf{n}} = g$; the map $g \mapsto \mathfrak{u}_g$ has continuity properties in various senses. The existence and uniqueness result implies that an operator $A_\kappa : H^0(\Gamma) \to H^0(\Gamma)$ is well-defined according to

$$A_\kappa g := \mathfrak{u}_g\big|_\Gamma;$$

thus, A_κ maps the Neumann data to the corresponding Dirichlet data for each element of $W_+(\Omega_+;\kappa)$. The operator A_κ is very useful for a variety of purposes. A number of its properties are cited in [5], *e.g.*, A_κ is injective and compact in $H^0(\Gamma)$, with dense range closed under conjugation, while its adjoint coincides with its conjugate: $A_\kappa^* = \overline{A}_\kappa$, where the *conjugate* $\overline{L}$ of a linear operator defined in a space of complex functions is defined by setting $\overline{L}g := \overline{L\overline{g}}$ for $g \in \mathcal{D}(\overline{L}) := \{\ g \mid \overline{g} \in \mathcal{D}(L)\ \}$. Then A_κ^* is also injective and has range dense in $H^0(\Gamma)$. Further, A_κ has a coercivity property:

$$-\mathrm{Im}\,\big(A_\kappa g, g\big)_0 > 0 \qquad \text{whenever} \quad g \in H^0(\Gamma), \quad g \neq 0. \tag{1.4}$$

Naturally, there are relations connecting A_κ and the operators associated with the layer potentials; some of these are also given in [5].

With A_κ, the integral representation for the solution $\mathfrak{u}_g$ of the exterior Neumann/radiation problem with data g can be put into the form

$$\mathfrak{u}_g(\mathbf{x}) = \frac{1}{2}\int_\Gamma \{E^\kappa_{\mathbf{x}} g - E^\kappa_{\mathbf{x},\mathbf{n}} A_\kappa g\}\, d\lambda_\Gamma = \frac{1}{2}\int_\Gamma \{E^\kappa_{\mathbf{x}} - A_\kappa E^\kappa_{\mathbf{x},\mathbf{n}}\} g\, d\lambda_\Gamma \quad \text{for each} \quad \mathbf{x} \in \Omega_+, \tag{1.5}$$

the second equality following from the relation $A_\kappa^* = \overline{A}_\kappa$.

The operator $\mathbf{B}_\kappa$. It is very important to review the properties of a certain multiple of the "imaginary part" of A_κ, the operator B_κ defined in $H^0(\Gamma)$ by

$$B_\kappa := \frac{\mathrm{i}\kappa}{4}\big(A_\kappa - A_\kappa^*\big).$$

Clearly, B_κ is compact and self-adjoint, while (1.4) implies that it is also positive-definite, *i.e.*, that $\big(B_\kappa f, f\big)_0 > 0$ for $f \in H^0(\Gamma)$, $f \neq 0$. It follows that B_κ is injective, so $\mathcal{R}\big(B_\kappa\big)$ is dense in $H^0(\Gamma)$. From the relation $A_\kappa^* = \overline{A}_\kappa$ we find that B_κ is also self-conjugate, *i.e.*, that $\overline{B}_\kappa = B_\kappa$; this shows that $\mathcal{R}\big(B_\kappa\big)$ is closed under complex conjugation, so $g \in \mathcal{R}\big(B_\kappa\big)$ iff $\overline{g} \in \mathcal{R}\big(B_\kappa\big)$. The properties of B_κ ensure that it has a compact, self-adjoint square root $B_\kappa^{\frac{1}{2}}$, such that $B_\kappa = B_\kappa^{\frac{1}{2}} B_\kappa^{\frac{1}{2}}$. Clearly, $B_\kappa^{\frac{1}{2}}$ is also injective. Moreover, it is shown in [5] that $B_\kappa^{\frac{1}{2}}$ is self-conjugate along with B_κ, *i.e.*, that $\overline{B_\kappa^{\frac{1}{2}}} = B_\kappa^{\frac{1}{2}}$; in particular, $\mathcal{R}\big(B_\kappa^{\frac{1}{2}}\big)$ is also closed under complex conjugation. Finally, it is sometimes useful to know that $\mathcal{R}\big(B_\kappa^{\frac{1}{2}}\big) \subset \mathcal{R}\big(A_\kappa\big)$, which is also proven in [5].

Spherical-separable solutions of the Helmholtz equation. Playing the rôle of trial- and test-functions in the Waterman algorithms are certain of the traces and normal derivatives of the classical spherical-separable solutions of the Helmholtz equation. The basis properties of these functions in $H^0(\Gamma)$ and related Hilbert spaces form the major topic of [5]; we retain the notation used there. Thus, after choosing a point $\mathcal{O} \in \Omega_-$ to serve as pole, we introduce the family $\{\ V^{\kappa\mathcal{O}}_{lm} \mid m = -l, \ldots, l,\, l = 0, 1, 2, \ldots\ \}$ of outgoing spherical-separable solutions of (1.1) with singularity at the pole $\mathcal{O}$ according to

$$V^{\kappa\mathcal{O}}_{lm}(\mathbf{x}) := \sqrt{2}\, h^{(1)}_l\big(\kappa|\mathbf{x} - \mathcal{O}|\big)\widehat{Y}_{lm}\Big(\frac{\mathbf{x} - \mathcal{O}}{|\mathbf{x} - \mathcal{O}|}\Big) \qquad \text{for} \quad \mathbf{x} \in \mathbb{R}^3, \quad \mathbf{x} \neq \mathcal{O},$$

with $h_l^{(1)}$ denoting the spherical Hankel function of first kind and order l and $\{\widehat{Y}_{lm}\}$ a family of spherical-surface harmonics forming a complete and orthonormal set in the usual Hilbert space $H^0(\Sigma_1) \equiv L_2(\Sigma_1)$ associated with the Lebesgue measure on the unit sphere Σ_1. Explicitly, for $m = -l, \ldots, l$ and $l = 0, 1, 2, \ldots$, we take

$$\widehat{Y}_{lm}(\hat{\mathbf{e}}) := \left\{ \frac{2l+1}{2\pi(1+\delta_{0m})} \frac{(l-|m|)!}{(l+|m|)!} \right\}^{\frac{1}{2}} P_l^{|m|}(\cos\vartheta_{\hat{\mathbf{e}}}) \begin{cases} \sin m\varphi_{\hat{\mathbf{e}}} & \text{if } m < 0 \\ \cos m\varphi_{\hat{\mathbf{e}}} & \text{if } m \geq 0 \end{cases} \qquad \text{whenever} \quad \hat{\mathbf{e}} \in \Sigma_1,$$

with $(\vartheta_{\hat{\mathbf{e}}}, \varphi_{\hat{\mathbf{e}}})$ indicating the usual spherical coördinates of $\hat{\mathbf{e}}$ relative to a fixed coördinate system, while P_l^m denotes the associated Legendre function of order m and degree l "on the cut"; specifically, we use the definition of P_l^m given in [12] (which differs slightly from that of, *e.g.*, [1]). Since $\mathcal{O} \in \Omega_-$, (the restriction of) each $V_{lm}^{\kappa\mathcal{O}}$ gives an element of $W_+(\Omega_+;\kappa)$.

The members of the corresponding family $\{\ \mathrm{Reg}\, V_{lm}^{\kappa\mathcal{O}} \mid m = -l, \ldots, l,\ l = 0, 1, 2, \ldots\ \}$ of entire solutions of (1.1) in $\mathbb{R}^3$ are defined in a similar manner with the spherical Bessel function j_l replacing $h_l^{(1)}$ (and extended by continuity to all of $\mathbb{R}^3$). Here, $\mathrm{Reg}\, V_{lm}^{\kappa\mathcal{O}} = \mathrm{Re}\, V_{lm}^{\kappa\mathcal{O}}$, since κ is real and we are using a family of real spherical harmonics.

Since it is somewhat more convenient in the construction of a Galerkin method to work with singly indexed functions, we choose a bijection $n \mapsto \big(l^\star(n), m^\star(n)\big)$ carrying the set of positive integers onto $\{\ (l,m) \mid l = 0, 1, 2, \ldots\ , m = -l, \ldots, l\ \}$ and write, *e.g.*, $V_n^{\kappa\mathcal{O}} := V_{l^\star(n)m^\star(n)}^{\kappa\mathcal{O}}$ for $n = 1, 2, \ldots$.

The biorthonormal sequence for $\big(V_{n,\mathbf{n}}^{\kappa\mathcal{O}}\big)_{n=1}^\infty$. Closely associated with the sequence $\big(V_{n,\mathbf{n}}^{\kappa\mathcal{O}}\big)_{n=1}^\infty$ of normal derivatives is the sequence $\big(U_n^{\kappa\mathcal{O}}\big)_{n=1}^\infty$ in $H^0(\Gamma)$, with

$$U_n^{\kappa\mathcal{O}} := -\frac{\mathrm{i}\kappa}{2}\{\mathrm{Reg}\, V_n^{\kappa\mathcal{O}}|_\Gamma - A_\kappa \mathrm{Reg}\, V_{n,\mathbf{n}}^{\kappa\mathcal{O}}\}.$$

Directly from the definition it follows that $U_n^{\kappa\mathcal{O}}$ can be interpreted as the trace on Γ of the "total field" in the time-harmonic scattering of the incident acoustic field with complex amplitude $-\frac{\mathrm{i}\kappa}{2}\mathrm{Reg}\, V_n^{\kappa\mathcal{O}}$ by a hard obstacle occupying $\overline{\Omega}_-$. The functions $U_n^{\kappa\mathcal{O}}$ arise naturally in several ways. For example, $(\mathrm{i}/\kappa)U_n^{\kappa\mathcal{O}}$ is the density required to represent $\mathrm{Reg}\, V_n^{\kappa\mathcal{O}}$ in Ω_- in the form of an interior double-layer potential. That is, by using the integral representation of $\mathrm{Reg}\, V_n^{\kappa\mathcal{O}}$ in Ω_-, it is easy to check that

$$\mathrm{Reg}\, V_n^{\kappa\mathcal{O}}(\mathbf{x}) = \frac{\mathrm{i}}{\kappa} W_\kappa^-\{U_n^{\kappa\mathcal{O}}\}(\mathbf{x}) \qquad \text{for each} \quad \mathbf{x} \in \Omega_- \quad n = 1, 2, \ldots\ ,$$

with $W_\kappa^-\{\varphi\}$ denoting the interior double-layer potential with density φ. By computing the trace from this representation, we find the very useful result

$$\frac{\mathrm{i}}{\kappa}(I + D_\kappa)U_n^{\kappa\mathcal{O}} = \mathrm{Reg}\, V_n^{\kappa\mathcal{O}}|_\Gamma, \qquad \text{for} \quad n = 1, 2, 3, \ldots\ , \tag{1.6}$$

in which $D_\kappa : H^0(\Gamma) \to H^0(\Gamma)$ denotes the compact operator induced by the "direct value" of the double-layer potential, *i.e.*,

$$D_\kappa h(\mathbf{x}) := \int_\Gamma E_{\mathbf{x},\mathbf{n}}^\kappa h\, d\lambda_\Gamma \qquad \text{for} \quad \lambda_\Gamma\text{-a.a. } \mathbf{x} \in \Gamma, \qquad \text{for all} \quad h \in H^0(\Gamma).$$

Further, the sequence $\big(U_n^{\kappa\mathcal{O}}\big)_{n=1}^\infty$ figures in the construction of series expansions of outgoing solutions of the Helmholtz equation in terms of $\big(V_n^{\kappa\mathcal{O}}\big)_{n=1}^\infty$. In fact, with the help of the integral representation

(1.5) it is easy to show that the solution $\mathfrak{u}_g$ of the exterior Neumann/radiation problem with $H^0(\Gamma)$-data g has the expansion

$$\mathfrak{u}_g(\mathbf{x}) = \sum_{n=0}^{\infty} \big(g, \overline{U_n^{\kappa\mathcal{O}}}\big)_0 V_n^{\kappa\mathcal{O}}(\mathbf{x}) \qquad \text{(at least) for} \quad |\mathbf{x} - \mathcal{O}| > R_{\mathcal{O}}^{+}, \tag{1.7}$$

with $R_{\mathcal{O}}^{+}$ denoting the radius of the circumscribing ball for Ω_- that is centered at $\mathcal{O}$.

A simple computation will verify that the two sequences $\big(V_{n,\mathbf{n}}^{\kappa\mathcal{O}}\big)_{n=1}^{\infty}$ and $\big(\overline{U_n^{\kappa\mathcal{O}}}\big)_{n=1}^{\infty}$ are biorthonormal in $H^0(\Gamma)$, *i.e.*, that

$$\big(V_{m,\mathbf{n}}^{\kappa\mathcal{O}}, \overline{U_n^{\kappa\mathcal{O}}}\big)_0 = \delta_{mn}, \qquad \text{for} \quad m,\, n = 1,\, 2,\, \dots\ ,$$

and, moreover, that B_κ maps each $V_{n,\mathbf{n}}^{\kappa\mathcal{O}}$ to the corresponding $\overline{U_n^{\kappa\mathcal{O}}}$: $B_\kappa V_{n,\mathbf{n}}^{\kappa\mathcal{O}} = \overline{U_n^{\kappa\mathcal{O}}}$, for each n. Directly, it follows that the sequence $\big(B_\kappa^{\frac{1}{2}} V_{n,\mathbf{n}}^{\kappa\mathcal{O}}\big)_{n=1}^{\infty}$ is orthonormal in $H^0(\Gamma)$; since it is also easy to check its completeness in that space, it is an orthonormal basis for $H^0(\Gamma)$.

The Hilbert space associated with $\mathbf{B}_{\boldsymbol{\kappa}}^{\frac{1}{2}}$. By introducing the inner product $\big(\cdot\,,\cdot\big)_{-}^{\mathcal{N}}$ for $L_2(\Gamma)$ according to

$$\big(f, g\big)_{-}^{\mathcal{N}} := \big(B_\kappa^{\frac{1}{2}} f, B_\kappa^{\frac{1}{2}} g\big)_0, \qquad \text{for} \quad f,\, g \in L_2(\Gamma),$$

and denoting by $H_{\mathcal{N}}^{-}(\Gamma)$ the Hilbert space obtained by completing $L_2(\Gamma)$ with respect to this inner product, it is easy to see that we get a space for which $\big(V_{n,\mathbf{n}}^{\kappa\mathcal{O}}\big)_{n=1}^{\infty}$ itself is an orthonormal basis.

Connections with far-field patterns. The structure $H_{\mathcal{N}}^{-}(\Gamma)$ turns out to be intimately related to the far-field patterns of the elements of $W_+(\Omega_+;\kappa)$. To describe this, we shall denote by $u_\infty^{\mathcal{O}}$ the far-field pattern of $u \in W_+(\Omega_+;\kappa)$ and by $\Phi_{\mathcal{N}}^{\kappa\mathcal{O}} : H^0(\Gamma) \to H^0(\Sigma_1)$ the *Neumann far-field pattern operator with respect to* $\mathcal{O}$, which maps the Neumann data $g \in H^0(\Gamma)$ into the far-field pattern of $\mathfrak{u}_g$, or $\Phi_{\mathcal{N}}^{\kappa\mathcal{O}} g := \big(\mathfrak{u}_g\big)_\infty^{\mathcal{O}}$. More explicitly, from the integral representation (1.5) for $\mathfrak{u}_g$ we find that

$$\Phi_{\mathcal{N}}^{\kappa\mathcal{O}} g(\hat{\mathbf{e}}) = -\frac{1}{4\pi}\int_\Gamma \big\{ \mathrm{e}_{\hat{\mathbf{e}}}^{\kappa\mathcal{O}} g - \mathrm{e}_{\hat{\mathbf{e}},\mathbf{n}}^{\kappa\mathcal{O}} A_\kappa g \big\}\, d\lambda_\Gamma = -\frac{1}{4\pi}\int_\Gamma \big\{ \mathrm{e}_{\hat{\mathbf{e}}}^{\kappa\mathcal{O}} - A_\kappa \mathrm{e}_{\hat{\mathbf{e}},\mathbf{n}}^{\kappa\mathcal{O}} \big\} g\, d\lambda_\Gamma \qquad \text{for each} \quad \hat{\mathbf{e}} \in \Sigma_1,$$

in which $\mathrm{e}_{\hat{\mathbf{e}}}^{\kappa\mathcal{O}}$ denotes the complex amplitude of a certain plane wave propagating in the direction $-\hat{\mathbf{e}}$, $\mathrm{e}_{\hat{\mathbf{e}}}^{\kappa\mathcal{O}}(\mathbf{y}) := e^{-\mathrm{i}\kappa\hat{\mathbf{e}}\cdot(\mathbf{y}-\mathcal{O})}$ for $\mathbf{y} \in \mathbb{R}^3$, $\hat{\mathbf{e}} \in \Sigma_1$. From this, it is shown in [5] that $\Phi_{\mathcal{N}}^{\kappa\mathcal{O}}$ has the factorization

$$\Phi_{\mathcal{N}}^{\kappa\mathcal{O}} = \frac{\sqrt{2}}{\kappa}\Psi_{\mathcal{N}}^{\kappa\mathcal{O}} B_\kappa^{\frac{1}{2}}, \tag{1.8}$$

in which $\Psi_{\mathcal{N}}^{\kappa\mathcal{O}} : H^0(\Gamma) \to H^0(\Sigma_1)$ is a certain isometric isomorphism; (1.8) is recognized as the polar decomposition of $\Phi_{\mathcal{N}}^{\kappa\mathcal{O}}$.

Now we can summarize the connection between convergence of the Neumann data on Γ and convergence of the far-field patterns on Σ_1, which is very important for our later reasoning:

Proposition 1.1. *Let $u \in W_+(\Omega_+;\kappa)$ and $\big(u_n\big)_{n=1}^{\infty}$ be a sequence from $W_+(\Omega_+;\kappa)$. Then the sequence $\big((u_n)_\infty^{\mathcal{O}}\big)_{n=1}^{\infty}$ of far-field patterns converges to the far-field pattern $u_\infty^{\mathcal{O}}$ of u in the norm of $H^0(\Sigma_1)$ iff the sequence $\big(u_{n,\mathbf{n}}\big)_{n=1}^{\infty}$ of Neumann data converges to $u_{,\mathbf{n}}$ in the norm of $H_{\mathcal{N}}^{-}(\Gamma)$.*

Proof: This follows directly from the polar decomposition (1.8) of the far-field-pattern operator, which shows that $\big\|\Phi_{\mathcal{N}}^{\kappa\mathcal{O}} g\big\|_{H^0(\Sigma_1)} = \big(\sqrt{2}/\kappa\big)\big\|g\big\|_{-}^{\mathcal{N}}$ for every $g \in H^0(\Gamma)$. ☐

The transition matrix; "transition-matrix methods." We close this section with some remarks on "transition-matrix methods." In the present context of acoustic scattering by a hard obstacle and expansions in radiating spherical-separable solutions, the *transition matrix* is the infinite array $\mathcal{T}^{\kappa\mathcal{O}}$ with elements

$$\mathcal{T}^{\kappa\mathcal{O}}_{mn} := -\big(\operatorname{Reg} V^{\kappa\mathcal{O}}_{n;\mathbf{n}}, \overline{U^{\kappa\mathcal{O}}_m}\big)_, \qquad \text{for} \quad m,\, n = 1,\, 2,\, \dots\ ,$$

which acts on appropriate incident-field spherical-expansion coefficients to produce the corresponding scattered-field spherical-expansion coefficients. More precisely, let the Neumann data be given by $g = -u^{\iota}_{;\mathbf{n}}$ with u^{ι} a sufficiently regular "incident" acoustic field, *i.e.*, a solution of (1.1) in an open set Ω_{ι} containing the closure of the ball $B_{R^+_{\mathcal{O}}}(\mathcal{O})$. Then there is an expansion of the familiar form in the regular spherical-wave functions,

$$u^{\iota}(\mathbf{x}) = \sum_{n=1}^{\infty} \iota_n \operatorname{Reg} V^{\kappa\mathcal{O}}_n(\mathbf{x}), \qquad \text{for} \quad \big|\mathbf{x} - \mathcal{O}\big| < R_{\iota}, \tag{1.9}$$

for some $R_{\iota} > R^+_{\mathcal{O}}$. The convergence properties of the latter series ensure that the coefficients $\big(g, \overline{U^{\kappa\mathcal{O}}_n}\big)_0 = -\big(u^{\iota}_{;\mathbf{n}}, \overline{U^{\kappa\mathcal{O}}_n}\big)_0$ required in the expansion of the scattered field $u^{\sigma} := \mathfrak{u}_g$ appearing in (1.7) can be computed from

$$-\big(u^{\iota}_{;\mathbf{n}}, \overline{U^{\kappa\mathcal{O}}_m}\big)_0 = -\sum_{n=1}^{\infty} \big(\operatorname{Reg} V^{\kappa\mathcal{O}}_{n;\mathbf{n}}, \overline{U^{\kappa\mathcal{O}}_m}\big)_0 \iota_n = \sum_{n=1}^{\infty} \mathcal{T}^{\kappa\mathcal{O}}_{mn} \iota_n = \big(\mathcal{T}^{\kappa\mathcal{O}} \iota\big)_m, \qquad m = 1,\, 2,\, 3,\, \dots\ ,$$

as the result of the action of the array $\mathcal{T}^{\kappa\mathcal{O}}$ on the incident-field expansion coefficients $\iota := \big(\iota_n\big)_{n=1}^{\infty}$. Thus, knowledge of the elements of $\mathcal{T}^{\kappa\mathcal{O}}$ permits one to capture directly the solution of any regular scattering problem for Ω_- and κ outside the circumscribing sphere centered at $\mathcal{O}$, as

$$u^{\sigma}(\mathbf{x}) = \sum_{n=1}^{\infty} \big(\mathcal{T}^{\kappa\mathcal{O}} \iota\big)_n V^{\kappa\mathcal{O}}_n(\mathbf{x}), \qquad \text{for} \quad \big|\mathbf{x} - \mathcal{O}\big| > R^+_{\mathcal{O}}.$$

By the term "transition-matrix method" we should then understand an algorithm for constructing, for all sufficiently large N, an $N \times N$ matrix $\mathcal{T}_N$ with the property that the corresponding outgoing fields u^{σ}_N generated by the recipe

$$u^{\sigma}_N := \sum_{n=1}^{N} \big(\mathcal{T}_N \iota^N\big)_n V^{\kappa\mathcal{O}}_n, \qquad \text{with} \quad \iota^N := \big(\iota_n\big)_{n=1}^{N}, \tag{1.10}$$

converge in some reasonable sense to the scattered field u^{σ} produced by the incident field u^{ι} as in (1.9), *i.e.*, to the solution of the exterior Neumann/radiation problem $\mathfrak{u}_g$ with the data $g = -u^{\iota}_{;\mathbf{n}}$. In this broad sense, practically any method for approximate solution of the exterior Neumann/radiation problem can be recast as a "transition-matrix method." One might argue that the term should be reserved for those schemes that are based directly and decisively on approximation of the transition matrix itself, as a consequence of its characteristic property, instead of arising peripherally out of some other line of reasoning. But from that point of view, it would not be clear whether there are any "transition-matrix methods" known at all. At any rate, we already indicated that the name has become widely attached to the schemes proposed by Waterman [18], so that a reference to "*the* T-matrix method" usually indicates one or the other of those particular methods.

Using the broad terminology, the two Waterman schemes for the hard-scattering case can be summarized in "T-matrix form" as

$$\mathcal{Q}_N^{\kappa\mathcal{O}} \left(\mathcal{T}_N^{\kappa\mathcal{O}}\right)^{\mathsf{T}} = -\mathrm{Re}\, \mathcal{Q}_N^{\kappa\mathcal{O}} \tag{1.11}$$

and

$$\mathcal{Q}_N^{\kappa\mathcal{O}} \widetilde{\mathcal{T}}_N^{\kappa\mathcal{O}} = -\mathrm{Re}\, \mathcal{Q}_N^{\kappa\mathcal{O}} \tag{1.12}$$

in which the $N \times N$ matrix $\mathcal{Q}_N^{\kappa\mathcal{O}}$ has the elements

$$\mathcal{Q}_{mn}^{\kappa\mathcal{O}} := \left(\mathrm{Reg}\, V_m^{\kappa\mathcal{O}}\big|_{\Gamma}, \overline{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}}\right)_0. \tag{1.13}$$

That is, the first and second Waterman schemes propose the construction of N^{th} approximate transition-matrices $\mathcal{T}_N^{\kappa\mathcal{O}}$ and $\widetilde{\mathcal{T}}_N^{\kappa\mathcal{O}}$, for use in (1.10), satisfying (1.11) and (1.12), respectively. Some motivation for such computations is given in [18]; a summary and additional remarks can be found in [5]. In Section 7 of [5] and here at the end of Section 5, we comment on the apparently common view that (1.12) results from "truncation" in an infinite-matrix relation.

In any event, a simple comparison reveals that the method that we propose in the next Section 2 specializes to that expressed by (1.12), *i.e.*, to the second Waterman scheme.

2. Formulation of the generalized second Waterman scheme.

Before we can *analyze* one or the other of the numerical schemes proposed by WATERMAN [18], we must realize it as the outcome of applying a known approximation-of-solution apparatus to some operator problem. Such a framework is not provided in [18], so the approach that we settle on here may bear little resemblance to the heuristic arguments advanced there. While there are in fact a number of ways in which we can identify such an operator reformulation for the present case, here we shall just show how the second Waterman scheme can arise as an application of the familiar and fundamental "method of boundary-data approximation," which exploits the continuity of the solution map $g \mapsto \mathfrak{u}_g$, taking the Neumann data-function to the corresponding solution of the exterior Neumann/radiation problem.

To review the underlying idea, suppose that we can construct a sequence $\left(u_g^N\right)_{N=1}^{\infty}$ in $W_+(\Omega_+;\kappa)$ such that the corresponding sequence $\left(u_{g,\mathbf{n}}^N\right)_{N=1}^{\infty}$ of Neumann data converges in an appropriate manner to the given Neumann data $g \in H^0(\Gamma)$. Then, owing to "continuous dependence on the data," there will be a corresponding sense (or perhaps various senses) in which the sequence $\left(u_g^N\right)_{N=1}^{\infty}$ itself converges to the unique solution $\mathfrak{u}_g$ of the exterior Neumann/radiation problem with the data g. For example, if $\left(u_{g,\mathbf{n}}^N\right)_{N=1}^{\infty}$ converges to g in the norm of $H^0(\Gamma)$, then one can show easily that the sequence of traces $\left(u_g^N\big|_\Gamma\right)_{N=1}^{\infty}$ will converge to the trace $\mathfrak{u}_g\big|_\Gamma$ of the solution in $H^0(\Gamma)$, $\left(u_g^N\right)_{N=1}^{\infty}$ will converge to $\mathfrak{u}_g$ uniformly on every closed subset of Ω_+, and the sequence of approximating far-field patterns will converge to the actual far-field pattern in $H^0(\Sigma_1)$.

For the approximation of given Neumann data we choose $\left(V_{n,\mathbf{n}}^{\kappa\mathcal{O}}\right)_{n=1}^{\infty}$, since this is a sequence of normal derivatives of elements of $W_+(\Omega_+;\kappa)$ that is readily constructed (at least, when the required orders of the spherical Hankel functions are not too large) and always complete in $H^0(\Gamma)$—and also since we are reconstructing the methods of [18]. Now, a simple and obvious device for generating convergent approximations of Neumann data by linear combinations of elements of $\left(V_{n,\mathbf{n}}^{\kappa\mathcal{O}}\right)_{n=1}^{\infty}$ consists in the use of the latter sequence as *trial functions* in a projection method for the approximate solution of the (well-posed!) operator problem

$$\textit{given} \quad g \in H(\Gamma), \qquad \textit{find} \quad f \in H(\Gamma) \quad \textit{such that} \qquad Lf = Lg, \tag{2.1}$$

with $H(\Gamma)$ denoting a Hilbert space of functions on Γ in which $H^0(\Gamma)$ is densely imbedded and $L \in \mathcal{B}\big(H(\Gamma)\big)$ an isomorphism. Once $H(\Gamma)$ and L have been selected, since we have already decided on a sequence $\left(\mathcal{V}_N\right)_{N=1}^{\infty}$ of trial-function subspaces, *viz.*, by taking $\mathcal{V}_N := \operatorname{sp}\left\{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}\right\}_{n=1}^{N}$ for each N, to fix a Galerkin-Petrov projection scheme for the operator problem (2.1) it remains only to choose a sequence of test-function subspaces $\left(\mathcal{W}_N\right)_{N=1}^{\infty}$ with $\dim \mathcal{W}_N = N$ $(= \dim \mathcal{V}_N)$; supposing this done, we let $\mathcal{P}_N$ denote the orthogonal projector onto $\mathcal{W}_N$ in $H(\Gamma)$. In the formulation of the method it is useful to prepare for accommodating the introduction of a convergent approximation to the actual data-function (which will ultimately require the establishment of some continuous dependence on the data in the projection scheme). Accordingly, given $g \in H(\Gamma)$, let $\left(g_N\right)_{N=1}^{\infty}$ denote a sequence from $H(\Gamma)$ converging to g in $H(\Gamma)$.

With all of the components in place, the N^{th} subsidiary problem of the corresponding Galerkin-Petrov procedure for the problem (2.1) appears as

$$\textit{given} \quad g \in H(\Gamma), \qquad \textit{find} \quad f_N \in \mathcal{V}_N \quad \textit{such that} \qquad \mathcal{P}_N L f_N = \mathcal{P}_N L g_N. \tag{2.2}$$

Observe that the operator figuring in the problem (2.2) is the restriction $\mathcal{P}_N L \,\big|\, \mathcal{V}_N : \mathcal{V}_N \to \mathcal{W}_N$, acting between finite-dimensional spaces of the same dimension. Of course, the conditions $f_N \in \mathcal{V}_N$

and $\mathcal{P}_N L f_N = \mathcal{P}_N L g_N$ can be realized as an equivalent system of linear algebraic equations by making the obvious choice of basis for each trial-subspace $\mathcal{V}_N$ and selecting bases for the test-subspaces $\mathcal{W}_N$. The entire point here is that the elements of the scheme that have been left free are to be chosen to produce the approximants given in (2.3), *infra*, with the coefficients obtained from the linear systems appearing in (2.4), since this yields a generalization of the second scheme of WATERMAN [18], as we shall show.

Indeed, there are a number of choices of the components fixing the Galerkin-Petrov procedure that *all* lead directly to the same systems in (2.4) (and the same approximants in (2.3)). It is important to maintain this flexibility, not only because different choices in the set-up lead to various useful conclusions (*cf.*, *e.g.*, Sections 4 and 5 here) but also because the analysis of the Waterman scheme is still underway, since we have not found a "definitive" operator reformulation. We should also point out that, in any positive result yielded by our analysis, the convergence of approximations to the given Neumann data will take place in whatever Hilbert space we have identified as $H(\Gamma)$, and that mode of convergence may not be as strong as, say, convergence in the norm of $H^0(\Gamma)$. Of course, if we manage to assert only a relatively weak sort of convergence and cannot eventually strengthen the conclusion, we may never be sure whether that state of affairs is actually "in the nature of things" or arises merely out of our own limitations in analysis. In fact, we have little numerical-experimental evidence on the manner in which the Waterman schemes converge, when they appear to converge at all. More precisely, while there is ample numerical evidence that convergence of the far-field patterns obtains in some sense for some obstacles, there are but few indications concerning the convergent approximation of other parts of the scattered field.

To complete the initial motivation, we shall indicate for now just one selection of $H(\Gamma)$, L, and $\mathcal{W}_N$ in the projection scheme that leads to (2.3) and (2.4); by inserting requirements of numerical stability and the convergence of the radiating fields of ultimate interest, we produce what we call the "generalized second Waterman scheme." If we can establish the viability and convergence properties of the projection method, so that we know when and how the approximating Neumann data converge to the given data g, then we expect that we will be be able to make a corresponding assertion about the sense in which the constructed sequence $\left(u_g^N\right)_{N=N_0}^{\infty}$ of approximants converges to the desired solution $\mathfrak{u}_g$. Subsequently, we shall show that this scheme is really a generalization, *i.e.*, that it does subsume the second algorithm proposed in [18] when the data have the special form $-u^\iota_{;\mathbf{n}}$ for a sufficiently regular incident field u^ι, in the problem of time-harmonic acoustic scattering by a hard obstacle occupying the closure of Ω_-. In this way, an analysis of the proposed Galerkin-Petrov method(s) for the problem (2.1) will enable us to draw conclusions about the second Waterman scheme.

Specifically, let us here identify $H(\Gamma)$ as $H^0(\Gamma)$, L as the identity operator, and the test-function subspace $\mathcal{W}_N$ as $\mathrm{sp}\left\{\mathrm{Reg}\, V_n^{\kappa\mathcal{O}}\big|_\Gamma\right\}_{n=1}^N$, for $N = 1, 2, \ldots$; then $\mathcal{P}_N$ is the orthoprojector onto $\mathcal{W}_N$ in $H^0(\Gamma)$.

(The sequence $\left(\mathrm{sp}\left\{\mathrm{Reg}\, V_n^{\kappa\mathcal{O}}\big|_\Gamma\right\}_{n=1}^N\right)_{N=1}^{\infty}$ is chosen as test-subspaces even though it is not ultimately dense in $H^0(\Gamma)$ when κ^2 is a Dirichlet eigenvalue for $-\Delta$ in Ω_-, since $\left(\mathrm{Reg}\, V_n^{\kappa\mathcal{O}}\big|_\Gamma\right)_{n=1}^{\infty}$ then fails to be complete in $H^0(\Gamma)$; again, we are constrained here to make choices leading to a re-derivation of the second scheme of [18], on which the majority of numerical computations have evidently been based. This lack of completeness intrudes—in one guise or another—in the later reasoning, where it has a decisive effect, at least on the numerical-stability question.)

It is easy to check that these choices in the projection method (2.2) lead to (2.3) and (2.4) for the determination of the N^{th} approximant, so that we have motivated the formulation of

(gW.II.) The generalized second Waterman scheme:

(1.) Establish viability: *Show that there exists* N_0 *such that* $\{(V^{\kappa\mathcal{O}}_{n,\mathbf{n}}, \operatorname{Reg} V^{\kappa\mathcal{O}}_m|_\Gamma)_0\}_{N\times N}$ *is a nonsingular matrix for* $N \geq N_0$.

Assuming that the scheme is viable, let $g \in H^0(\Gamma)$ and suppose that $(g_N)_{N=1}^{\infty}$ is a sequence from $H^0(\Gamma)$ converging in a given sense to g; construct the sequence $(u_g^N)_{N=N_0}^{\infty}$ of outgoing solutions of (1.1) as

$$u_g^N := \sum_{n=1}^{N} \alpha_n^N V_n^{\kappa\mathcal{O}}, \qquad \text{for} \quad N \geq N_0, \tag{2.3}$$

in which the collections of coefficients $(\alpha_n^N)_{n=1}^{N}$ are determined by (*cf*. (2.2))

$$\sum_{n=1}^{N} (V^{\kappa\mathcal{O}}_{n,\mathbf{n}}, \operatorname{Reg} V^{\kappa\mathcal{O}}_m|_\Gamma)_0 \alpha_n^N = (g_N, \operatorname{Reg} V^{\kappa\mathcal{O}}_m|_\Gamma)_0, \qquad \text{for} \quad m = 1, \ldots, N, \quad \text{for} \quad N \geq N_0. \tag{2.4}$$

(2.) Establish convergence: *Show that the sequence* $(u_g^N)_{N=N_0}^{\infty}$ *converges in some sense to the solution* $\mathfrak{u}_g$ *of the Neumann/radiation problem in* Ω_+ *with data* g.

(3.) Establish numerical stability: *Show that the condition numbers* $(\operatorname{cond}(\mathcal{Q}_N^{\kappa\mathcal{O}}))_{N=N_0}^{\infty}$ *of the matrix operators in the systems* (2.4) *have a "sufficiently small" upper bound.*

Remarks. (1.) The manner in which the sequence $(g_N)_{N=1}^{\infty}$ is *required* to converge to g and the manner in which the sequence $(u_g^N)_{N=N_0}^{\infty}$ *can be shown* to converge to $\mathfrak{u}_g$ must be specified without ambiguity in any statement describing the success of the generalized second Waterman scheme.

(2.) We regard the operator underlying the N^{th} finite-dimensional problem in (2.4) as acting in N-dimensional complex unitary space ℓ_2^N. That is, the $N \times N$ matrix with elements $\mathcal{Q}^{\kappa\mathcal{O}}_{mn} := (V^{\kappa\mathcal{O}}_{n,\mathbf{n}}, \operatorname{Reg} V^{\kappa\mathcal{O}}_m|_\Gamma)_0$, as in (1.13), induces an operator $\mathcal{Q}_N^{\kappa\mathcal{O}} : \ell_2^N \to \ell_2^N$ with respect to the canonical basis for ℓ_2^N (no confusion will arise from the use of the same symbol to denote the operator and its generating matrix); explicitly, the components of $\mathcal{Q}_N^{\kappa\mathcal{O}}\beta^N$ are given by

$$(\mathcal{Q}_N^{\kappa\mathcal{O}}\beta^N)_m = \sum_{n=1}^{N} (V^{\kappa\mathcal{O}}_{n,\mathbf{n}}, \operatorname{Reg} V^{\kappa\mathcal{O}}_m|_\Gamma)_0 \beta_n^N, \qquad m = 1, \ldots, N, \qquad \text{for} \quad \beta^N \equiv (\beta_1^N, \ldots, \beta_N^N) \in \ell_2^N, \tag{2.5}$$

so that the equalities in (2.4) can be written as $\mathcal{Q}_N^{\kappa\mathcal{O}}\alpha^N = \gamma^N$. Then, recalling that the ℓ_2^N-condition number of the operator $\mathcal{Q}_N^{\kappa\mathcal{O}}$ is

$$\operatorname{cond}(\mathcal{Q}_N^{\kappa\mathcal{O}}) := \|\mathcal{Q}_N^{\kappa\mathcal{O}}\| \, \|\mathcal{Q}_N^{\kappa\mathcal{O}^{-1}}\|, \qquad \text{for} \quad N \geq N_0, \tag{2.6}$$

requirement (gW.II.3) demands that the sequence $(\operatorname{cond}(\mathcal{Q}_N^{\kappa\mathcal{O}}))_{N=N_0}^{\infty}$ have an upper bound that is "not too large." Recall that $\operatorname{cond}(\mathcal{Q}_N^{\kappa\mathcal{O}})$ measures the maximum possible ratio of the relative ℓ_2^N-error in the solution of $\mathcal{Q}_N^{\kappa\mathcal{O}}\alpha^N = \gamma^N$ to the relative ℓ_2^N-error in the computed righthand side and matrix elements, so that satisfaction of the third requirement will ensure that the numerical computations can be accomplished with an acceptable error. In fact, since there are always errors in the data, if the condition numbers grow too large, then the computed solutions of the systems (2.4) can be rendered so inaccurate as to be worthless.

To see that the scheme (gW.II) does indeed reduce to the second proposal of [18] under an appropriate choice of the g_N, consider the problem of time-harmonic scattering of acoustic waves by a hard obstacle occupying the closure $\overline{\Omega}_-$, in which the Neumann-data function is $g = -u^\iota_{,\mathbf{n}}$, with u^ι denoting a regular incident field, *i.e.*, a solution of (1.1) in a ball $B_{R_\iota}(\mathcal{O})$ containing $\overline{\Omega}_-$ and centered at $\mathcal{O}$. Then u^ι has an expansion as in (1.9), converging absolutely and uniformly on closed subsets of $B_{R_\iota}(\mathcal{O})$; the series can be differentiated term-by-term any number of times, with each resultant series retaining the same convergence properties (*cf.*, *e.g.*, VEKUA [16]). Then we can take g_N to be the partial sum $-\sum_{n=1}^{N} \iota_n \mathrm{Reg}\, V_{n,\mathbf{n}}^{\kappa\mathcal{O}}$ for $N \geq 1$, giving $g_N \to g$ uniformly on Γ, and so also in $H^0(\Gamma)$. With this choice, the linear system in (2.4) becomes

$$\sum_{n=1}^{N} \big(V_{n,\mathbf{n}}^{\kappa\mathcal{O}}, \mathrm{Reg}\, V_m^{\kappa\mathcal{O}}|_\Gamma\big)_0 \alpha_n^N = -\sum_{n=1}^{N} \big(\mathrm{Reg}\, V_{n,\mathbf{n}}^{\kappa\mathcal{O}}, \mathrm{Reg}\, V_m^{\kappa\mathcal{O}}|_\Gamma\big)_0 \iota_n, \qquad \text{for} \quad m = 1, \ldots, N. \tag{2.7}$$

Clearly, the prospective N^{th} approximate transition matrix $\widetilde{\mathcal{T}}_N^{\kappa\mathcal{O}}$ deriving from (2.7) would satisfy (1.12), which, as we pointed out in Section 1, is precisely the second scheme proposed by WATERMAN [18]; *cf*., also, [5, Section 7].

Our results on the viability, convergence, and numerical stability of the Galerkin-Petrov method represented by (2.2) will derive from application of the following Theorem 2.1. To understand its implications, let L_N denote the operator $\mathcal{P}_N L$ in (2.2) and $\widetilde{L}_N$ indicate its restriction $L_N \,|\, \mathcal{V}_N = (\mathcal{P}_N L) \,|\, \mathcal{V}_N : \mathcal{V}_N \to \mathcal{W}_N$. Then, when $\widetilde{L}_N$ is bijective, the unique solution of the problem in (2.2) is given by $\widetilde{L}_N^{-1} L_N g_N$. Therefore, to establish the viability and convergence of the Galerkin-Petrov scheme we must verify the bijectivity of the $\widetilde{L}_N$ for all sufficiently large N and the convergence of the sequence $\big(\widetilde{L}_N^{-1} L_N g_N\big)_{N=N_0}^{\infty}$ to g for every $g \in H(\Gamma)$. Theorem 2.1 gives sufficient conditions and necessary and sufficient conditions for this viability and convergence, in a slightly more general setting that need not involve orthoprojectors. The theorem is obtained by an appropriate modification of the statement and proof of Theorem 15.1 of KRASNOSEL'SKIĬ, ET AL. [8]. In the statement, the finite-dimensional range $\mathcal{R}(L_N)$ of the operator L_N plays the rôle of the test subspace $\mathcal{W}_N$.

We continue to denote by $\mathcal{B}(H)$ the collection of all bounded linear operators mapping the Hilbert space H into itself; the norm of $L \in \mathcal{B}(H)$ is indicated by $\|L\|_{\mathcal{B}(H)}$. The norm of a bounded linear operator $L : H_1 \to H_2$ between Hilbert spaces H_1 and H_2 we may denote by $\|L; H_1, H_2\|$. Recall that a sequence $(V_N)_{N=1}^{\infty}$ of subspaces of the Hilbert space H is said to be *ultimately dense in* H iff $\lim_{N\to\infty} \operatorname{dist}(h, V_N) = 0$ for every $h \in H$, *i.e.*, iff the sequence of orthoprojectors onto the V_N converges strongly to the identity operator in $\mathcal{B}(H)$.

Theorem 2.1. *Let H be a Hilbert space and $(V_N)_{N=1}^{\infty}$ an ultimately dense sequence of finite-dimensional subspaces of H; denote by Π_N the orthoprojector in H onto V_N. Suppose that $(L_N)_{N=1}^{\infty}$ is a sequence of finite-rank operators bounded in $\mathcal{B}(H)$, with $\|L_N\|_{\mathcal{B}(H)} \leq c'$ for $N \geq 1$, and such that $\dim \mathcal{R}(L_N) \leq \dim V_N$ for each N. Let $\widetilde{L}_N$ denote the restriction of L_N to V_N, regarded as $\widetilde{L}_N := L_N \,|\, V_N : V_N \to \mathcal{R}(L_N)$.*

(*i.*) *If the $\widetilde{L}_N$ are eventually injective and uniformly invertible, i.e., if there exist N_0 and $c > 0$ such that*

$$\|L_N v_N\|_H \geq c\,\|v_N\|_H \qquad \textit{for each} \quad v_N \in V_N, \qquad \textit{for each} \quad N \geq N_0, \tag{2.8}$$

then whenever $g \in H$ and $(g_N)_{N=1}^{\infty}$ is a sequence from H converging to g in the norm of H we have

$$\|\Pi_N g - g\|_H \leq \|\widetilde{L}_N^{-1} L_N g_N - g\|_H \leq \frac{c'}{c}\|g_N - g\|_H + \Big(1 + \frac{c'}{c}\Big)\|\Pi_N g - g\|_H \quad \textit{for} \quad N \geq N_0; \tag{2.9}$$

in particular, the sequence $\left(\widetilde{L}_N^{-1} L_N g_N\right)_{N=N_0}^{\infty}$ *then converges to* g *in the norm of* H.

Now suppose also that each L_N *has the special form* $L_N = Q_N L$ *for each* N, *in which* $L \in \mathcal{B}(H)$ *and* $(Q_N)_{N=1}^{\infty}$ *is a sequence of finite-rank projectors in* $\mathcal{B}(H)$.

($ii.$) *If* L *is bijective and* $\widetilde{L}_N$ *is injective for* $N \geq$ *some* N_0, *then* (2.8) *is necessary for the sequence* $\left(\widetilde{L}_N^{-1} L_N\right)_{N=N_0}^{\infty}$ *to converge strongly to the identity operator in* $\mathcal{B}(H)$.

($iii.$) *If* L *is not injective, then either* (a) $\widetilde{L}_N$ *fails to be injective for all sufficiently large* N *or* (b) *the subsequence* $\left(\widetilde{L}_{N_k}\right)_{k=1}^{\infty}$ *of injective operators satisfies* $\lim_{k\to\infty} \left\| \widetilde{L}_{N_k}^{-1}; \mathcal{R}(L_{N_k}), V_{N_k} \right\| = \infty$.

Proof: Since $\dim \mathcal{R}(L_N) \leq \dim V_N = \dim \mathcal{R}(\widetilde{L}_N) + \dim \mathcal{N}(\widetilde{L}_N) \leq \dim \mathcal{R}(L_N) + \dim \mathcal{N}(\widetilde{L}_N)$, it is clear that we have $\dim \mathcal{R}(L_N) = \dim V_N = \dim \mathcal{R}(\widetilde{L}_N)$ whenever we know that $\widetilde{L}_N : V_N \to \mathcal{R}(L_N)$ is injective, for any N. We shall use this in the remainder of the proof without comment.

(i). Because of (2.8), for $N \geq N_0$ the restriction $\widetilde{L}_N$ is injective and therefore also bijective. Moreover, the family $\left\{\widetilde{L}_N^{-1} L_N : H \to V_N\right\}_{N=N_0}^{\infty}$ is norm-bounded:

$$\left\|\widetilde{L}_N^{-1} L_N\right\|_{\mathcal{B}(H)} \leq \left\|\widetilde{L}_N^{-1}; \mathcal{R}(L_N), V_N\right\| \left\|L_N\right\|_{\mathcal{B}(H)} \leq \frac{1}{c} c' \qquad \text{for} \quad N \geq N_0.$$

Now let $g \in H$ and $(g_N)_{N=1}^{\infty}$ be a sequence from H. For $N \geq N_0$ we can write, upon noting that $\widetilde{L}_N^{-1} L_N \Pi_N = \widetilde{L}_N^{-1} \widetilde{L}_N \Pi_N = \Pi_N$,

$$\begin{aligned} \left\|\widetilde{L}_N^{-1} L_N g_N - g\right\|_H &\leq \left\|\widetilde{L}_N^{-1} L_N (g_N - g)\right\|_H + \left\|\widetilde{L}_N^{-1} L_N (\Pi_N g - g)\right\|_H + \left\|\Pi_N g - g\right\|_H \\ &\leq \frac{c'}{c} \left\|g_N - g\right\|_H + \left(1 + \frac{c'}{c}\right) \left\|\Pi_N g - g\right\|_H. \end{aligned}$$

This establishes the second inequality in (2.9), while the first inequality there is obviously true, since $\widetilde{L}_N^{-1} L_N g_N$ belongs to V_N. Now the final assertion of (i) follows when $(g_N)_{N=1}^{\infty}$ converges to g in H, in view of the ultimate denseness of $(V_N)_{N=1}^{\infty}$ in H.

(ii). Under the special form $L_N = Q_N L$, with L bijective and $\widetilde{L}_N$ injective for $N \geq N_0$, suppose that $\left(\widetilde{L}_N^{-1} L_N\right)_{N=N_0}^{\infty}$ converges strongly in $\mathcal{B}(H)$ to the identity operator, *i.e.*, that $\left(\widetilde{L}_N^{-1} L_N g\right)_{N=N_0}^{\infty}$ converges to g in the norm of H for every $g \in H$. In particular, the sequence of operators is pointwise bounded, so the Banach-Steinhaus Theorem says that it is also norm-bounded; let $\left\|\widetilde{L}_N^{-1} L_N\right\|_{\mathcal{B}(H)} \leq c''$ for $N \geq N_0$. Let $N \geq N_0$ and $u_N \in \mathcal{R}(L_N) = \mathcal{R}(Q_N)$: since Q_N is a projector, we have $u_N = Q_N u_N = Q_N L L^{-1} u_N = L_N L^{-1} u_N$, so

$$\left\|\widetilde{L}_N^{-1} u_N\right\|_H = \left\|\widetilde{L}_N^{-1} L_N L^{-1} u_N\right\|_H \leq c'' \left\|L^{-1}\right\|_{\mathcal{B}(H)} \left\|u_N\right\|_H.$$

This implies (2.8).

(iii). Suppose that alternative (a) of the statement does not hold; then it makes sense to speak of the subsequence of injective operators, which we denote by $\left(\widetilde{L}_{N_k}\right)_{k=1}^{\infty}$. We shall show that every subsequence of $\left(\left\|\widetilde{L}_{N_k}^{-1}; \mathcal{R}(L_{N_k}), V_{N_k}\right\|\right)_{k=1}^{\infty}$ possesses a subsequence diverging to ∞, from which it will follow that $\lim_{k\to\infty} \left\|\widetilde{L}_{N_k}^{-1}; \mathcal{R}(L_{N_k}), V_{N_k}\right\| = \infty$, as claimed. Accordingly, we choose any subsequence of $\left(\widetilde{L}_{N_k}\right)_{k=1}^{\infty}$ and denote it again by $\left(\widetilde{L}_{N_k}\right)_{k=1}^{\infty}$. Assume that the counterpart of (2.8) holds for this subsequence, *i.e.*, that there exist K_0 and $c_0 > 0$ such that

$$\left\|L_{N_k} v_{N_k}\right\|_H \geq c_0 \left\|v_{N_k}\right\|_H \qquad \text{for each} \quad v_{N_k} \in V_{N_k}, \qquad \text{for each} \quad k \geq K_0. \tag{2.8$'$}$$

Then, by recalling the boundedness of the sequence $\left(\|L_N\|_{\mathcal{B}(H)}\right)_{N=1}^{\infty}$, for each $f \in H$ we get

$$\left\|Q_{N_k}Lf\right\|_H = \left\|L_{N_k}\Pi_{N_k}f + L_{N_k}(I-\Pi_{N_k})f\right\|_H \geq c_0\left\|\Pi_{N_k}f\right\|_H - c'\left\|(I-\Pi_{N_k})f\right\|_H \quad \text{for} \quad k \geq K_0.$$

Since it is clear that any subsequence of $\left(V_N\right)_{N=1}^{\infty}$ is also ultimately dense in H, from the latter inequality it follows that $\liminf_{k\to\infty}\|Q_{N_k}Lf\|_H \geq c_0\|f\|_H$ for each $f \in H$, which implies, in particular, that L must be injective. Since this contradicts the hypothesis, we are forced to conclude that there are no K_0 and c_0 for which $(2.8)'$ holds. In turn, this clearly implies that there is a subsequence of $\left(\|\widetilde{L}_{N_k}^{-1};\mathcal{R}(L_{N_k}),V_{N_k}\|\right)_{k=1}^{\infty}$ diverging to ∞. We have already indicated how this suffices for the proof of (iii). $\square$

In our applications of Theorem 2.1, we always arrange matters so that we have $L_N = Q_N L$ with $L \in \mathcal{B}(H)$ and Q_N an *orthogonal* projector in H with $\dim\mathcal{R}(Q_N) = \dim V_N$ for every N. Then the hypothesis $\dim\mathcal{R}(L_N) \leq \dim V_N$ will clearly be fulfilled in every case.

Supposing that the hypotheses of Theorem 2.1.i obtain, let us display the finite systems that must be solved to compute the elements of the sequence $\left(\widetilde{L}_N^{-1}L_N g_N\right)_{N=N_0}^{\infty}$ converging to $g \in H$, for the case in which $L_N = Q_N L$, with Q_N as described in the preceding paragraph and $L \in \mathcal{B}(H)$ bijective. Obviously, we have then $\mathcal{R}(L_N) = \mathcal{R}(Q_N)$; let $d_N := \dim V_N = \dim\mathcal{R}(L_N)$, and let $\{v_n^N\}_{n=1}^{d_N}$ and $\{w_n^N\}_{n=1}^{d_N}$ denote bases for V_N and $\mathcal{R}(L_N)$, respectively. Then, for $N \geq N_0$, $\widetilde{L}_N^{-1}L_N g_N$ is the unique solution of the problem

$$\textit{find} \quad v \in V_N \quad \textit{such that} \qquad Q_N L v = Q_N L g_N,$$

and so is given by

$$\widetilde{L}_N^{-1}L_N g_N = \sum_{n=1}^{d_N}\alpha_n^N v_n^N, \tag{2.10}$$

in which the coefficients $\{\alpha_n^N\}_{n=1}^{d_N}$ are uniquely determined by

$$\sum_{n=1}^{d_N}\left(Lv_n^N, w_m^N\right)_H\alpha_n^N = \left(Lg_N, w_m^N\right)_H, \qquad \text{for} \quad m = 1, \ldots, d_N. \tag{2.11}$$

In fact, it is easy to see from (2.8) and the linear independence of the set $\{v_n^N\}_{n=1}^{d_N}$ that the matrix of the system (2.11) is nonsingular for $N \geq N_0$.

Our strategy for establishing results about the generalized second Waterman scheme on the basis of Theorem 2.1 should now be apparent: choosing $V_N = \mathcal{V}_N := \mathrm{sp}\left\{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}\right\}_{n=1}^{N}$ for all N (and then, of course, $v_n^N = V_{n,\mathbf{n}}^{\kappa\mathcal{O}}$, $n = 1, \ldots, N$), we want to identify a Hilbert space H associated with Γ, an operator L, and orthogonal projectors Q_N in H in just such a way that the system (2.11) has exactly the form (2.4). Once such a set-up is found, we must decide which hypotheses of Theorem 2.1 are fulfilled. For example, if the conditions of Theorem 2.1.i are met, we get from (2.10) with coefficients determined by (2.11), *i.e.*, from the Neumann data of the u_g^N in (2.3) with the coefficients generated by (2.4), a sequence $\left(u_{g,\mathbf{n}}^N\right)_{N=N_0}^{\infty}$ of normal derivatives of outgoing solutions of (1.1), which will then be known to converge to the Neumann-data-function g in the norm of the space H; finally, an appropriate continuity statement about the solution-map $g \mapsto \mathfrak{u}_g$ will then allow us to establish a certain type of convergence for the approximations $\left(u_g^N\right)_{N=N_0}^{\infty}$ in (2.3) to $\mathfrak{u}_g$.

In the discussion motivating the formulation of (gW.II), we essentially already cited one example of identifications for which (2.11) coincides with (2.4), *viz.*, with $V_N = \mathcal{V}_N$ (and $v_n^N = V_{n,\mathbf{n}}^{\kappa\mathcal{O}}$), take

H to be $H^0(\Gamma)$, L to be the identity operator, Q_N to be the orthogonal projector in $H^0(\Gamma)$ onto $\mathcal{W}_N := \text{sp}\,\{\text{Reg}\, V_n^{\kappa\mathcal{O}}\big|_\Gamma\}_{n=1}^N$, and L_N to be $Q_N L = Q_N$. Then (2.11) becomes (2.4), with (2.10) giving the normal derivative of u_g^N in (2.3). We shall not pursue the latter set-up, since it turns out that condition (2.8) cannot hold in that setting for any but the spherical obstacles (and when κ^2 is not an interior Dirichlet eigenvalue). Two other sets of identifications of the desired sort are given in Section 4 and in Section 5; in each of those cases, we show that Theorem 2.1 can be used to draw some useful conclusions about (gW.II). In particular, the reasoning of Section 4 concerns convergence in $H^0(\Gamma)$, and we use it to verify the negative assertion just made.

To prepare for the later developments concerning numerical stability and requirement (gW.II.3), it is important to expose the connection between the "abstract" operator $\widetilde{L}_N = Q_N L \,\big|\, V_N : V_N \to \mathcal{R}(L_N)$ and the "numerical" operator $\widetilde{\mathcal{L}}_N : \ell_2^{d_N} \to \ell_2^{d_N}$ induced by the $d_N \times d_N$ matrix figuring in (2.11) with respect to the canonical basis of the d_N-dimensional complex unitary space $\ell_2^{d_N}$; explicitly, we have

$$\big(\widetilde{\mathcal{L}}_N \beta^N\big)_m = \sum_{n=1}^{d_N} \big(L v_n^N, w_m^N\big)_H \beta_n^N, \qquad m = 1, \ldots, d_N, \qquad \text{for each} \quad \beta^N \equiv \big(\beta_1^N, \ldots, \beta_{d_N}^N\big) \in \ell_2^{d_N}. \tag{2.12}$$

(Of course, in our later applications of Theorem 2.1, the $\widetilde{\mathcal{L}}_N$ will coincide with the $\mathcal{Q}_N^{\kappa\mathcal{O}}$ defined by (2.5).) Now, while the viability and convergence of the Galerkin-Petrov scheme can be examined by studying the $\widetilde{L}_N$ alone, the numerical stability of the scheme depends upon the behavior of the $\widetilde{\mathcal{L}}_N$, in particular, upon the growth of the sequence of $\ell_2^{d_N}$-condition numbers $\big(\text{cond}\,(\widetilde{\mathcal{L}}_N)\big)_{N=N_0}^\infty$. Let the operators $\mathcal{F}_N : \ell_2^{d_N} \to V_N$ and $\mathcal{G}_N : \ell_2^{d_N} \to \mathcal{R}(L_N)$ be defined by

$$\left.\begin{aligned} \mathcal{F}_N \beta^N &:= \sum_{n=1}^{d_N} \beta_n^N v_n^N \\ \mathcal{G}_N \beta^N &:= \sum_{n=1}^{d_N} \beta_n^N w_n^N \end{aligned}\right\} \qquad \text{for each} \quad \beta^N \equiv \big(\beta_1^N, \ldots, \beta_{d_N}^N\big) \in \ell_2^{d_N}. \tag{2.13}$$

Then it is easy to check that the adjoint operator $\mathcal{G}_N^* : \mathcal{R}(L_N) \to \ell_2^{d_N}$ is given by

$$\mathcal{G}_N^* w = \big((w, w_n^N)_H\big)_{n=1}^{d_N} \qquad \text{for each} \quad w \in \mathcal{R}(L_N),$$

and so verify the relation

$$\widetilde{\mathcal{L}}_N = \mathcal{G}_N^* \widetilde{L}_N \mathcal{F}_N, \qquad \text{for each} \quad N. \tag{2.14}$$

Relation (2.14) permits us to draw conclusions about numerical stability from information about the "abstract" operator $\widetilde{L}_N$ (*i.e.*, from information about "potential stability") and the properties of the bases chosen for V_N and $\mathcal{R}(L_N)$, which determine the respective properties of the $\mathcal{F}_N$ and $\mathcal{G}_N$.

3. Numerical instabilities at interior Dirichlet eigenvalues.

One of the curious features of the Waterman schemes for the acoustic hard-scattering problem is their use of the sequence $\left(\operatorname{Reg} V_n^{\kappa\mathcal{O}}\big|_\Gamma\right)_{n=1}^\infty$ of traces, which fails to be complete in $H^0(\Gamma)$ when κ^2 is a Dirichlet eigenvalue for $-\Delta$ in Ω_- (and, for the soft-scattering problem, their use of the sequence $\left(\operatorname{Reg} V_{n,\mathbf{n}}^{\kappa\mathcal{O}}\right)_{n=1}^\infty$ of normal derivatives, which fails to be complete in $H^0(\Gamma)$ when κ^2 is a Neumann eigenvalue for $-\Delta$ in Ω_-); *cf.*, *e.g.*, [13], and the review in [5]. Experience with projection methods for the approximate solution of operator problems suggests that this may be the source of some defect in the schemes which can have an important effect on their performance. We have included this brief section to emphasize that it should therefore not be surprising to discover at least a numerical instability in the Waterman schemes at the pertinent wavenumbers.

The most striking example of such behavior shows up in the simplest case, when Ω_- is a ball $B_R(\mathcal{O})$ of radius R centered at $\mathcal{O}$. There, the finite matrices figuring in the Waterman scheme, *i.e.*, the matrices of the systems displayed in (2.4), are eventually singular whenever κR coincides with a zero of one of the spherical Bessel functions j_l, $l = 0, 1, 2, \ldots$; for such wavenumbers the method is not viable, and the requisite computations cannot be effected. The corresponding set of κ^2-values comprise the Dirichlet eigenvalues for $-\Delta$ in $B_R(\mathcal{O})$.

In fact, in our "positive" viability and convergence result of Theorem 5.1.*i*, along with the operator condition (C.2) described in Section 5 we find it at least convenient to require that κ be a "regular" value, *i.e.*, that

$$\kappa^2 \textit{ is not a Dirichlet eigenvalue for } -\Delta \textit{ in } \Omega_-. \tag{C.1}$$

For each such regular κ, we also prove that the condition numbers of the operators $\mathcal{Q}_N^{\kappa\mathcal{O}}$ of (2.5) form a bounded sequence. However, in the contrary case when (C.1) fails (but still under the same operator hypothesis (C.2)), in Theorem 5.1.*ii* we show that either the operators $\mathcal{Q}_N^{\kappa\mathcal{O}}$ fail to be invertible for all sufficiently large N or the sequence of condition numbers of the invertible operators diverges to ∞, so that there is a numerical breakdown in either case. This result leads one to suspect a similarity to the situation which is well known in numerical methods based on the most primitive integral-equation reformulations of the exterior radiation problems, *viz.*, that there will be an interval of κ-values surrounding each exceptional value in which the condition numbers, while remaining bounded at each κ, grow so large that the computations cannot be performed accurately (although we do not prove this).

Apropos of the stability question, we should also point out that the surface integrals appearing in the matrix elements needed to set up the Waterman schemes can be exceedingly difficult to approximate with acceptable accuracy, *e.g.*, when values of the spherical Hankel functions of the larger orders at "small" arguments are required and/or when the integrands are highly oscillatory. In such cases, the occurrence of large condition numbers in the matrices themselves can seriously degrade the accuracy of computed solutions of the linear systems (2.4).

Since instabilities strictly confined to discrete values of κ would be of no numerical consequence at all, the question of central importance actually concerns the widths of any intervals of "effective numerical instability." For example, in the simple integral-equation set-ups, these intervals overlap when the wavenumbers are sufficiently large, undermining the computations at every such κ. In the case of the Waterman schemes, however, it is reasonable to conjecture that the widths are strongly dependent on the shape and/or smoothness of Ω_-. For example, when Γ is an ellipsoid, computations reported in [15] indicate that the instabilities, while present, are so remarkably localized near the square roots of the interior eigenvalues that they are practically invisible. In fact, it was found for ellipsoidal boundaries that the use of double-precision arithmetic is completely inadequate to reveal the regions of instability, which appear only with the help of quadruple-precision computations. But it is very likely that this fortunate behavior arises out of some special property of ellipsoids and cannot be expected in general. In numerical experiments with other shapes, especially those with less smoothness, erratic behavior seems to be commonly encountered. In such cases, it is not clear whether the numerical difficulties arise from the failure of the scheme to converge or from overlapping of the regions of instability.

Since, in contrast to the motivation described in [18], the present study of the second Waterman scheme does not *directly* employ the traces $\operatorname{Reg} V_n^{\kappa\mathcal{O}}\big|_\Gamma$, it may be helpful to explain how condition (C.1) naturally arises here. In examining the matrices $\mathcal{Q}_N^{\kappa\mathcal{O}}$ with elements given in (1.13), we exploit the relations

$$(I+\overline{D}_\kappa)B_\kappa V_{n,\mathbf{n}}^{\kappa\mathcal{O}} = \mathrm{i}\kappa \operatorname{Reg} V_n^{\kappa\mathcal{O}}\big|_\Gamma, \qquad \text{for} \quad n=1,\,2,\,\dots\,,$$

which follow from (1.6) and the equality $B_\kappa V_{n,\mathbf{n}}^{\kappa\mathcal{O}} = \overline{U_n^{\kappa\mathcal{O}}}$. Thus, in our applications of Theorem 2.1 to draw conclusions about the second generalized Waterman scheme, we have been led to identify the operator L figuring in that statement as either $I+\overline{D_\kappa^*}$ acting in $H^0(\Gamma)$ or an extension of this operator acting in the larger Hilbert space $H_N^-(\Gamma)$ with preservation of the null space $\mathcal{N}\big(I+\overline{D_\kappa^*}\big)$; by appropriate selection of the remaining elements, it turns out that the systems (2.11) will then take on the form (2.4). Now, it is well known that $\mathcal{N}\big(I+\overline{D_\kappa^*}\big)$ is nontrivial iff condition (C.1) holds; *cf.*, *e.g.*, [2, Theorem 3.22] (with due regard for the notation used there). Therefore, to ensure the bijectivity hypothesis on L that is needed when we wish to apply statements (*i*) and (*ii*) of Theorem 2.1, we must require the condition (C.1). On the other hand, when κ^2 is an interior Dirichlet eigenvalue, so L $(=I+\overline{D_\kappa^*})$ fails to be injective, we will be able to rely on Theorem 2.1.*iii* and the preparations made following the proof of that theorem to assert the existence of the numerical instability already described, at least in those (nice) circumstances in which condition (C.2) of Section 5 is fulfilled. In any event, this provides some indications on the rôle of condition (C.1) and the appearance of the traces $\operatorname{Reg} V_n^{\kappa\mathcal{O}}\big|_\Gamma$ in the formulation examined here, as an outcome of our “reverse-engineering” an analytical origin for the second Waterman algorithm.

4. An observation about viability and convergence to the data in $H^0(\Gamma)$.

It is reasonable to attempt first to identify those obstacles Ω_-, wave-numbers κ, and Neumann-data functions g for which the second generalized Waterman scheme succeeds in producing a sequence $\left(u^N_{g,\mathbf{n}}\right)_{N=N_0}^{\infty}$ converging to g in the norm of $H^0(\Gamma)$. In this section, we consider instead an easier question, by asking when the following statement is true:

$$\left.\begin{array}{l}\textit{The scheme (gW.II) is viable and the sequence } \left(u^N_{g,\mathbf{n}}\right)_{N=N_0}^{\infty} \textit{ of normal derivatives} \\ \textit{constructed from (2.3) converges to } g \textit{ in the norm of } H^0(\Gamma) \textit{ whenever } g \in H^0(\Gamma) \\ \textit{and the sequence } \left(g_N\right)_{N=1}^{\infty} \textit{ converges to } g \textit{ in } H^0(\Gamma).\end{array}\right\} \qquad (\mathrm{S})_0$$

Perhaps surprisingly, we find the following negative result: when the scheme is viable one cannot expect that *every* $g \in H^0(\Gamma)$ will be convergently approximated in $H^0(\Gamma)$ unless the geometry is very special.

Theorem 4.1. *Let condition* (C.1) *hold. Then statement* $(\mathrm{S})_0$ *obtains iff* Ω_- *is a ball centered at* $\mathcal{O}$.

Proof: In the statement of Theorem 2.1 we take $H = H^0(\Gamma)$, $V_N = \mathcal{V}_N := \mathrm{sp}\,\{V^{\kappa\mathcal{O}}_{n,\mathbf{n}}\}_{n=1}^N$, $Q_N = R_N :=$ the orthogonal projector in $H^0(\Gamma)$ onto the subspace $\mathfrak{U}^\star_N := \mathrm{sp}\,\{\overline{U^{\kappa\mathcal{O}}_n}\}_{n=1}^N$, $L = \left(I + \overline{D^*_\kappa}\right)$, and then $L_N = Q_N L = R_N\left(I + \overline{D^*_\kappa}\right)$. Naturally, we also take $v^N_m = V^{\kappa\mathcal{O}}_{m,\mathbf{n}}$ and $w^N_m = \overline{U^{\kappa\mathcal{O}}_m}$ here. Under these identifications, it is easy to check that the system in (2.11) coincides with that of the scheme (gW.II) in (2.4). In fact, for any $h \in H^0(\Gamma)$ and any m, by recalling (1.6) and noting that each $\mathrm{Reg}\, V^{\kappa\mathcal{O}}_m$ is real, we find

$$\left(Lh, w^N_m\right)_H = \left((I + \overline{D^*_\kappa})h, \overline{U^{\kappa\mathcal{O}}_m}\right)_0 = \left(h, (I + \overline{D}_\kappa)\overline{U^{\kappa\mathcal{O}}_m}\right)_0 = -\mathrm{i}\kappa\left(h, \mathrm{Reg}\, V^{\kappa\mathcal{O}}_m|_\Gamma\right)_0,$$

whence it is clear that (2.11) does now take on the form (2.4).

Clearly, $I + \overline{D^*_\kappa}$ is a bijection of $H^0(\Gamma)$ onto itself, since (C.1) implies that the operator is injective and $\overline{D^*_\kappa}$ is compact in $H^0(\Gamma)$. Thus, $\dim \mathcal{R}\left(L_N\right) = \dim \mathcal{R}\left(R_N(I + \overline{D^*_\kappa})\right) = N = \dim \mathcal{V}_N = \dim V_N$ for each N. Statement (i) of Theorem 2.1 now implies that $(\mathrm{S})_0$ holds if there exist N_0 and $c > 0$ such that (2.8) holds, *i.e.*, such that

$$\left\|R_N(I + \overline{D^*_\kappa})v_N\right\|_0 \geq c\left\|v_N\right\|_0 \qquad \text{for each} \quad v_N \in \mathcal{V}_N, \qquad \text{for each} \quad N \geq N_0. \tag{4.1}$$

On the other hand, since (gW.II) is viable precisely when the operators $\widetilde{L}_N := L_N \,\big|\, V_N : V_N \to \mathcal{R}\left(L_N\right)$ are injective for all sufficiently large N, Theorem 2.1.*ii* shows that (4.1) is also necessary for $(\mathrm{S})_0$, so that the two statements are equivalent.

Now, we claim that (4.1) holds, in turn, iff $\left(V^{\kappa\mathcal{O}}_{n,\mathbf{n}}\right)_{n=1}^{\infty}$ is a basis for $H^0(\Gamma)$; since it is shown in [5] that the latter basis-property obtains iff Ω_- is a ball centered at $\mathcal{O}$, the proof of the theorem will be effectively complete once we establish the equivalence claimed. For this, we require some auxiliary results. First, we recall a well-known basis-criterion:

Lemma 4.1. (M. M. Grinblyum) *A complete sequence* $\left(v_n\right)_{n=1}^{\infty}$ *in a Banach space* B *is a basis for* B *iff there is an* $\alpha > 0$ *such that*

$$\mathrm{dist}\left(\widehat{V}_N, V'_N\right) \geq \alpha \qquad \textit{for all} \quad N,$$

in which $\widehat{V}_N := \left\{\ v \in \mathrm{sp}\,\{v_n\}_{n=1}^N \;\middle|\; \|v\|_B = 1\ \right\}$ *and* $V'_N := \overline{\mathrm{sp}}\,\{v_n\}_{n=N+1}^{\infty}$.

Proof: A proof is given in [11]. ◻

Lemma 4.2. *Let H be a Hilbert space and $\left(V_N\right)_{N=1}^{\infty}$ and $\left(U_N\right)_{N=1}^{\infty}$ sequences of subspaces of H, with $\left(U_N\right)_{N=1}^{\infty}$ ultimately dense. Let P_N denote the orthoprojector onto U_N. Suppose that $K \in \mathcal{B}(H)$ is compact and that $I+K$ is injective. Then there exist N_1 and $c_1 > 0$ such that*

$$\left\|P_N v_N\right\|_H \geq c_1 \left\|v_N\right\|_H \qquad \text{for each} \quad v_N \in V_N \quad \text{and} \quad N \geq N_1 \tag{4.2}$$

iff there exist N_2 and $c_2 > 0$ such that

$$\left\|P_N (I+K) v_N\right\|_H \geq c_2 \left\|v_N\right\|_H \qquad \text{for each} \quad v_N \in V_N \quad \text{and} \quad N \geq N_2. \tag{4.3}$$

Proof: Suppose that (4.2) holds while (4.3) fails. Then there exists a sequence $\left(v_{N_k}\right)_{k=1}^{\infty}$ with $v_{N_k} \in V_{N_k}$, $\|v_{N_k}\|_H = 1$, and $\|P_{N_k}(I+K)v_{N_k}\|_H < \frac{1}{k}$ for each k; we may suppose that $\left(v_{N_k}\right)_{k=1}^{\infty}$ converges weakly in H to some v, which we indicate, as usual, by $v_{N_k} \rightharpoonup v$, for $k \to \infty$. Thus, on the one hand, $P_{N_k}(I+K)v_{N_k} \to 0$ in the norm of H, while, on the other, it is easy to check that $P_{N_k}(I+K)v_{N_k} \rightharpoonup (I+K)v$, as $k \to \infty$; we used here the ultimate denseness of $\left(U_{N_k}\right)_{k=1}^{\infty}$ in H, which follows from that of $\left(U_N\right)_{N=1}^{\infty}$. Therefore, we must have $(I+K)v = 0$, and so also $v = 0$. Now, the compactness of K gives $Kv_{N_k} \to Kv = 0$ in norm, and this clearly implies in turn that $P_{N_k}Kv_{N_k} \to 0$, whence the convergence $P_{N_k}(I+K)v_{N_k} \to 0$ gives $P_{N_k}v_{N_k} \to 0$ in norm, as $k \to \infty$. But this is impossible, since it contradicts (4.2), which requires that $\|P_{N_k}v_{N_k}\|_H \geq c_1 > 0$ for all sufficiently large k. Therefore, (4.3) is implied by (4.2).

The proof of the reversed implication is constructed in a similar argument. Let (4.3) hold but suppose that (4.2) is false. Then there is a sequence $\left(v_{N_k}\right)_{k=1}^{\infty}$ with $v_{N_k} \in V_{N_k}$, $\|v_{N_k}\|_H = 1$, and $\|P_{N_k}v_{N_k}\|_H < \frac{1}{k}$ for each k, while $v_{N_k} \rightharpoonup v$ as $k \to \infty$, for some $v \in H$. Thus, $P_{N_k}v_{N_k} \to 0$ in the norm of H and $P_{N_k}v_{N_k} \rightharpoonup v$, so again we must have $v = 0$. Since the compactness of K again shows that $P_{N_k}Kv_{N_k} \to Kv = 0$ in norm, we get $P_{N_k}(I+K)v_{N_k} = P_{N_k}v_{N_k} + P_{N_k}Kv_{N_k} \to 0$; this contradicts (4.3), which says that $\|P_{N_k}(I+K)v_{N_k}\|_H \geq c_2 > 0$ for all sufficiently large k. Therefore, (4.2) is also implied by (4.3), and the proof is complete. □

Returning to the proof of Theorem 4.1, from Lemma 4.2 we see that there exist N_0 and $c > 0$ such that (4.1) holds iff there exist N_1 and $c_1 > 0$ such that $\|R_N v_N\|_0 \geq c_1 \|v_N\|_0$ for each $v_N \in \mathcal{V}_N$ and $N \geq N_1$. In the present case, the latter is in fact equivalent to the existence of $c_2 > 0$ such that

$$\left\|R_N v_N\right\|_0 \geq c_2 \left\|v_N\right\|_0 \qquad \text{for each} \quad v_N \in \mathcal{V}_N, \qquad \text{for all} \quad N \geq 1, \tag{4.4}$$

for, recalling that $\left(V_{n,\mathbf{n}}^{\kappa\mathcal{O}}\right)_{n=1}^{\infty}$ and $\left(\overline{U_n^{\kappa\mathcal{O}}}\right)_{n=1}^{\infty}$ are biorthonormal, we see that the restriction $R_N|\mathcal{V}_N$ maps $\mathcal{V}_N$ bijectively to $\mathcal{U}_N^{\star}$ for each N. Now, it is easy to use the completeness of $\left(V_{n,\mathbf{n}}^{\kappa\mathcal{O}}\right)_{n=1}^{\infty}$ in $H^0(\Gamma)$ to check that the closed span $\mathcal{V}_N' := \overline{\mathrm{sp}}\left\{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}\right\}_{n=N+1}^{\infty}$ in $H^0(\Gamma)$ is, for each N, just the orthogonal complement $H^0(\Gamma) \ominus \mathcal{U}_N^{\star}$, so that also $H^0(\Gamma) \ominus \mathcal{V}_N' = \mathcal{U}_N^{\star}$. From this we find that $R_N = I - P_N$, with P_N denoting the orthogonal projector onto $\mathcal{V}_N'$, so it follows that the $H^0(\Gamma)$-distance between $\mathcal{V}_N'$ and the unit sphere $\widehat{\mathcal{V}}_N$ within the span $\mathcal{V}_N$ is just

$$\operatorname{dist}\left(\widehat{\mathcal{V}}_N, \mathcal{V}_N'\right) = \inf_{v_N \in \mathcal{V}_N, \|v_N\|_0 = 1} \left\|(I - P_N)v_N\right\|_0 = \inf_{v_N \in \mathcal{V}_N, \|v_N\|_0 = 1} \left\|R_N v_N\right\|_0.$$

Consequently, Lemma 4.1 implies that there exists $c_2 > 0$ such that (4.4) holds iff $\left(V_{n,\mathbf{n}}^{\kappa\mathcal{O}}\right)_{n=1}^{\infty}$ is a basis for $H^0(\Gamma)$. But we have already pointed out that this happens iff Ω_- is a ball centered at $\mathcal{O}$. □

5. Viability and convergence of the far-field patterns in $H^0(\Sigma_1)$.

In this section, we investigate the viability of the generalized second Waterman scheme and the convergence in $H^0(\Sigma_1)$ of the far-field patterns of the approximants constructed as in (2.3); we also establish some results about the numerical stability of the algorithm. In particular, we shall identify some conditions under which the following statement holds:

$$\left.\begin{array}{l}\textit{The scheme (gW.II) is viable and the sequence } \left(u^N_{g,\mathbf{n}}\right)_{N=N_0}^{\infty} \textit{ of normal derivatives}\\ \textit{constructed from (2.3) converges to } g \textit{ in the norm of } H^-_{\mathcal{N}}(\Gamma) \textit{ whenever } g\in H^0(\Gamma)\\ \textit{and the sequence } \left(g_N\right)_{N=1}^{\infty} \textit{ from } H^0(\Gamma) \textit{ converges to } g \textit{ in } H^-_{\mathcal{N}}(\Gamma).\end{array}\right\} \qquad (\mathrm{S})^{\mathcal{N}}_{-}$$

In turn, $(\mathrm{S})^{\mathcal{N}}_{-}$ implies viability and a weak sort of convergence for the generalized second Waterman scheme itself, merely in the sense of far-field-pattern convergence in $H^0(\Sigma_1)$, by Proposition 1.1. As one might anticipate, we must here investigate the behavior of one or another of the familiar boundary operators in the Hilbert space $H^-_{\mathcal{N}}(\Gamma)$. It is convenient to introduce some notation for working in this setting: let $\left[\overline{D^*_\kappa}\right]^-_{\mathcal{N}} : \{L_2(\Gamma)\subset H^-_{\mathcal{N}}(\Gamma)\}\to H^-_{\mathcal{N}}(\Gamma)$ denote the operator $\overline{D^*_\kappa}$ regarded as densely defined and acting in $H^-_{\mathcal{N}}(\Gamma)$, *i.e.*, such that $\left[\overline{D^*_\kappa}\right]^-_{\mathcal{N}} f := \overline{D^*_\kappa} f$ for each $f\in L_2(\Gamma)$. In this notation, we shall show that (C.1) along with the following condition gives us enough to establish $(\mathrm{S})^{\mathcal{N}}_{-}$:

$$\left[\overline{D^*_\kappa}\right]^-_{\mathcal{N}} : \left\{L_2(\Gamma)\subset H^-_{\mathcal{N}}(\Gamma)\right\}\to H^-_{\mathcal{N}}(\Gamma) \quad \textit{is compact.} \qquad \text{(C.2)}$$

Lemma 5.1. *The conditions* (C.1) *and* (C.2) *are sufficient to ensure* $(\mathrm{S})^{\mathcal{N}}_{-}$.

Proof: Let (C.1) and (C.2) hold. Let the compact extension of $\left[\overline{D^*_\kappa}\right]^-_{\mathcal{N}}$ to all of $H^-_{\mathcal{N}}(\Gamma)$ be denoted again by $\left[\overline{D^*_\kappa}\right]^-_{\mathcal{N}}$. We show first that $I+\left[\overline{D^*_\kappa}\right]^-_{\mathcal{N}}$ is a bijection of $H^-_{\mathcal{N}}(\Gamma)$ onto itself, for which we need only check that the operator is injective. Since (C.1) implies that $I+\overline{D^*_\kappa}$ is injective, this operator maps $L_2(\Gamma)$ onto itself. This shows that the range of $I+\left[\overline{D^*_\kappa}\right]^-_{\mathcal{N}}$ contains $L_2(\Gamma)$ and is therefore dense in $H^-_{\mathcal{N}}(\Gamma)$. From the compactness of $\left[\overline{D^*_\kappa}\right]^-_{\mathcal{N}}$ we know the range of $I+\left[\overline{D^*_\kappa}\right]^-_{\mathcal{N}}$ also to be closed in $H^-_{\mathcal{N}}(\Gamma)$, so that it must be all of $H^-_{\mathcal{N}}(\Gamma)$. This implies that the ($H^-_{\mathcal{N}}(\Gamma)$-) adjoint of $I+\left[\overline{D^*_\kappa}\right]^-_{\mathcal{N}}$ is injective, allowing us to assert the same for $I+\left[\overline{D^*_\kappa}\right]^-_{\mathcal{N}}$ itself, in this case. (In fact, one can apply THEOREM IV of LAX [10] to show here that the null spaces of $I+\overline{D^*_\kappa}$ in $H^0(\Gamma)$ and $I+\left[\overline{D^*_\kappa}\right]^-_{\mathcal{N}}$ in $H^-_{\mathcal{N}}(\Gamma)$ coincide, from which the desired result also follows.)

In the statement of Theorem 2.1 we take $H=H^-_{\mathcal{N}}(\Gamma)$, $V_N=\mathcal{V}_N := \mathrm{sp}\,\{V^{\kappa\mathcal{O}}_{n,\mathbf{n}}\}_{n=1}^{N}$, $Q_N=\mathcal{P}_N :=$ the orthogonal projector in $H^-_{\mathcal{N}}(\Gamma)$ onto $\mathcal{V}_N$, $L=I+\left[\overline{D^*_\kappa}\right]^-_{\mathcal{N}}$, and $L_N=Q_N L=\mathcal{P}_N\left(I+\left[\overline{D^*_\kappa}\right]^-_{\mathcal{N}}\right)$; clearly, $\mathcal{V}_N$ then coincides with $\mathcal{R}(L_N)=\mathcal{R}\left(\mathcal{P}_N\left(I+\left[\overline{D^*_\kappa}\right]^-_{\mathcal{N}}\right)\right)$ for each N. We shall verify that, under these identifications, the system in (2.11) coincides with that of the scheme (gW.II) in (2.4) when we take $v^N_n=w^N_n=V^{\kappa\mathcal{O}}_{n,\mathbf{n}}$ for $n=1,\ldots,N$ and all N. In fact, for any $h\in L_2(\Gamma)$ and any m, by recalling (1.6) we find

$$\left(Lh, V^{\kappa\mathcal{O}}_{m,\mathbf{n}}\right)^{\mathcal{N}}_{-} = \left(B_\kappa(I+\overline{D^*_\kappa})h, V^{\kappa\mathcal{O}}_{m,\mathbf{n}}\right)_0 = \left(h,(I+\overline{D}_\kappa)\overline{U^{\kappa\mathcal{O}}_m}\right)_0 = -\mathrm{i}\kappa\left(h,\mathrm{Reg}\,V^{\kappa\mathcal{O}}_m\big|_\Gamma\right)_0.$$

It follows that (2.11) does now take on the form (2.4) when the g_N belong to $H^0(\Gamma)$.

Let us check that the hypothesis of Theorem 2.1.*i* is fulfilled with the indicated choices. For each N and $v_N\in\mathcal{V}_N$ we have

$$\begin{aligned}\left\|\mathcal{P}_N\left(I+\left[\overline{D^*_\kappa}\right]^-_{\mathcal{N}}\right)v_N\right\|^{\mathcal{N}}_{-} &= \left\|\left(I+\left[\overline{D^*_\kappa}\right]^-_{\mathcal{N}}\right)v_N-\left(I-\mathcal{P}_N\right)\left[\overline{D^*_\kappa}\right]^-_{\mathcal{N}}v_N\right\|^{\mathcal{N}}_{-}\\ &\geq c_0\left\|v_N\right\|^{\mathcal{N}}_{-} - \left\|\left(I-\mathcal{P}_N\right)\left[\overline{D^*_\kappa}\right]^-_{\mathcal{N}}\right\|_{\mathcal{B}(H^-_{\mathcal{N}}(\Gamma))}\left\|v_N\right\|^{\mathcal{N}}_{-},\end{aligned}$$

with $c_0 := \|(I + [\overline{D^*_\kappa}]^-_{\mathcal{N}})^{-1}\|^{-1}_{\mathcal{B}(H^-_{\mathcal{N}}(\Gamma))}$. The completeness of the sequence $(V^{\kappa\mathcal{O}}_{n,\mathbf{n}})^\infty_{n=1}$ in $H^-_{\mathcal{N}}(\Gamma)$ follows from its completeness in $H^0(\Gamma)$, whence $(I - \mathcal{P}_N)^\infty_{N=1}$ converges strongly, *i.e.*, pointwise, to the zero operator on $H^-_{\mathcal{N}}(\Gamma)$; this convergence is therefore uniform on any compact subset of $H^-_{\mathcal{N}}(\Gamma)$. Since $[\overline{D^*_\kappa}]^-_{\mathcal{N}}$ is compact, it follows that $\|(I - \mathcal{P}_N)[\overline{D^*_\kappa}]^-_{\mathcal{N}}\|_{\mathcal{B}(H^-_{\mathcal{N}}(\Gamma))} \to 0$ as $N \to \infty$. Thus, the preceding estimate shows that there exist N_0 and $c > 0$ such that (2.8) holds in the present case. Now statement $(\mathrm{S})^{\mathcal{N}}_-$ follows from the conclusions of Theorem 2.1.*i*. □

We can now establish our basic result on viability, convergence, and numerical stability (or instability):

Theorem 5.1. Let condition (C.2) hold.

(*i*.) *If* (C.1) *is also true, then the generalized second Waterman scheme is viable and, for every* $g \in H^0(\Gamma)$ *and any sequence* $(g_N)^\infty_{N=1}$ *from* $H^0(\Gamma)$ *converging to* g *in the norm of* $H^-_{\mathcal{N}}(\Gamma)$, *the sequence* $((u^N_g)^{\mathcal{O}}_\infty)^\infty_{N=N_0}$ *of far-field patterns constructed from* (2.3) *and* (2.4) *converges to the far-field pattern* $(\mathfrak{u}_g)^{\mathcal{O}}_\infty$ *of the solution* $\mathfrak{u}_g$ *in the norm of* $H^0(\Sigma_1)$;

moreover, the sequence $(\mathrm{cond}\,(\mathcal{Q}^{\kappa\mathcal{O}}_N))^\infty_{N=N_0}$ *of* ℓ^N_2*-condition numbers of the numerical operators defined in* (2.5) *is bounded.*

(*ii*.) *Suppose that* (C.1) *does not hold, so that* κ^2 *is a Dirichlet eigenvalue for* $-\Delta$ *in* Ω_-. *Then, either (a) the operator* $\mathcal{Q}^{\kappa\mathcal{O}}_N : \ell^N_2 \to \ell^N_2$ *defined in* (2.5) *fails to be injective for all sufficiently large* N *or (b) the subsequence* $(\mathcal{Q}^{\kappa\mathcal{O}}_{N_k})^\infty_{k=1}$ *of injective operators satisfies* $\lim_{k\to\infty} \mathrm{cond}\,(\mathcal{Q}^{\kappa\mathcal{O}}_{N_k}) = \infty$, *so that the scheme is at best numerically ill-conditioned.*

Proof: (*i*). By Lemma 5.1, (C.1) and (C.2) imply that $(\mathrm{S})^{\mathcal{N}}_-$ is true. Therefore, if $g \in H^0(\Gamma)$, the sequence $(u^N_g)^\infty_{N=N_0}$ *can* be constructed from (2.3) with (2.4) and the derived sequence $(u^N_{g,\mathbf{n}})^\infty_{N=N_0}$ of Neumann data converges to the given Neumann data g in the norm of $H^-_{\mathcal{N}}(\Gamma)$. Now the convergence assertion follows directly from Proposition 1.1, which establishes the equivalence between convergence of Neumann data in $H^-_{\mathcal{N}}(\Gamma)$ and convergence of the corresponding far-field patterns in $H^0(\Sigma_1)$.

To see that the sequence $(\mathrm{cond}\,(\mathcal{Q}^{\kappa\mathcal{O}}_N))^\infty_{N=N_0}$ of ℓ^N_2-condition numbers is bounded, with $\mathcal{Q}^{\kappa\mathcal{O}}_N$ defined in (2.5), let us make here (and in the coming proof of (*ii*)) the same identifications in the statement of Theorem 2.1 that we used in the proof of Lemma 5.1; then the operator $\mathcal{Q}^{\kappa\mathcal{O}}_N$ coincides with $\widetilde{\mathcal{L}}_N$, introduced in (2.12), for all N. We recall that $(V^{\kappa\mathcal{O}}_{n,\mathbf{n}})^\infty_{n=1}$ is an orthonormal basis for $H^-_{\mathcal{N}}(\Gamma)$, while we shall agree to regard the $\mathcal{V}_N$ here as subspaces of $H^-_{\mathcal{N}}(\Gamma)$. Therefore, the operators $\mathcal{F}_N : \ell^N_2 \to \mathcal{V}_N$ and $\mathcal{G}_N : \ell^N_2 \to \mathcal{R}(L_N)$, defined in (2.13) and coinciding now because $\mathcal{R}(L_N) = \mathcal{V}_N$ and we naturally choose $w^N_n = v^N_n$ for $n = 1, \ldots, N$ and all N, are clearly isometric isomorphisms. Thus, the relation (2.14) implies that $\|\mathcal{Q}^{\kappa\mathcal{O}}_N\|_{\mathcal{B}(\ell^N_2)} = \|\widetilde{L}_N\|_{\mathcal{B}(\mathcal{V}_N)}$ for all N and $\|\mathcal{Q}^{\kappa\mathcal{O}^{-1}}_N\|_{\mathcal{B}(\ell^N_2)} = \|\widetilde{L}^{-1}_N\|_{\mathcal{B}(\mathcal{V}_N)}$ for $N \geq N_0$, and we get $\mathrm{cond}\,(\mathcal{Q}^{\kappa\mathcal{O}}_N) = \mathrm{cond}\,(\widetilde{L}_N)$ for all sufficiently large N. But it is obvious that the sequence $(\|\widetilde{L}_N\|_{\mathcal{B}(\mathcal{V}_N)})^\infty_{N=1}$ of norms is bounded, while the boundedness of $(\|\widetilde{L}^{-1}_N\|_{\mathcal{B}(\mathcal{V}_N)})^\infty_{N=N_0}$ follows from (2.8), which is shown in the proof of Lemma 5.1 to hold in the present setting. The boundedness of $(\mathrm{cond}\,(\mathcal{Q}^{\kappa\mathcal{O}}_N))^\infty_{N=N_0}$ follows.

(*ii*). Now we suppose that (C.1) does not hold. Assume further that alternative (*a*) is not the case, so it makes sense to denote by $(\mathcal{Q}^{\kappa\mathcal{O}}_{N_k})^\infty_{k=1}$ the subsequence of invertible operators of the sequence defined from (2.5). Of course, just as in the proof of (*i*), $\mathcal{F}_N$ and $\mathcal{G}_N$ are isometric isomorphisms, so the equalities $\|\mathcal{Q}^{\kappa\mathcal{O}}_N\|_{\mathcal{B}(\ell^N_2)} = \|\widetilde{L}_N\|_{\mathcal{B}(\mathcal{V}_N)}$ (for all N), $\|\mathcal{Q}^{\kappa\mathcal{O}^{-1}}_{N_k}\|_{\mathcal{B}(\ell^{N_k}_2)} = \|\widetilde{L}^{-1}_{N_k}\|_{\mathcal{B}(\mathcal{V}_{N_k})}$, and $\mathrm{cond}\,(\mathcal{Q}^{\kappa\mathcal{O}}_{N_k}) =$

$\text{cond}\,(\widetilde{L}_{N_k})$ (for all k) remain valid. Since the operator $L = I + [\overline{D^*_\kappa}]^-_{\mathcal{N}}$ here is not injective, we can apply Theorem 2.1.*iii* to assert that $\lim_{k\to\infty} \|\widetilde{L}^{-1}_{N_k}\|_{\mathcal{B}(\mathcal{V}_{N_k})} = \infty$. Now, since $\widetilde{L}_N = L_N \mid \mathcal{V}_N = \mathcal{P}_N(I + [\overline{D^*_\kappa}]^-_{\mathcal{N}}) \mid \mathcal{V}_N$, it is easy to check that the sequence $(\widetilde{L}_N \mathcal{P}_N)_{N=1}^\infty$ converges strongly to $I + [\overline{D^*_\kappa}]^-_{\mathcal{N}}$ in $H^-_{\mathcal{N}}(\Gamma)$, so that

$$\liminf_{N\to\infty} \|\widetilde{L}_N\|_{\mathcal{B}(\mathcal{V}_N)} = \liminf_{N\to\infty} \|\widetilde{L}_N \mathcal{P}_N\|_{\mathcal{B}(H^-_{\mathcal{N}}(\Gamma))} \geq \|I + [\overline{D^*_\kappa}]^-_{\mathcal{N}}\|_{\mathcal{B}(H^-_{\mathcal{N}}(\Gamma))} > 0,$$

(the first equality holding here since $\|\widetilde{L}_N\|_{\mathcal{B}(\mathcal{V}_N)} = \|\widetilde{L}_N \mathcal{P}_N\|_{\mathcal{B}(H^-_{\mathcal{N}}(\Gamma))}$); this implies that the sequence $(\|\widetilde{L}_{N_k}\|_{\mathcal{B}(\mathcal{V}_{N_k})})_{k=1}^\infty$ has a positive lower bound. Thus, we can conclude that $\lim_{k\to\infty} \text{cond}\,(\mathcal{Q}^{\kappa\mathcal{O}}_{N_k}) = \lim_{k\to\infty} \text{cond}\,(\widetilde{L}_{N_k}) = \infty$. This completes the proof. $\square$

Naturally, the goal now is the determination of all domains Ω_- for which (C.2) is true. Presently, while we have no geometric characterization of this class of domains, we can show that it is nonvoid. In fact, in the next section we give an operator condition sufficient to guarantee that (C.2) holds and show that this sufficient condition obtains whenever Γ is ellipsoidal. In the remainder of this section, we supply some related results giving additional information about (C.2) which may be useful in developing more definitive conditions for its validity.

There are conditions equivalent to (C.2) and phrased in terms of more familiar objects, one of which we give in Proposition 5.1, *infra*. To understand the latter statement, it is helpful to consider first just the boundedness relations given in

Lemma 5.2. *The following four statements are pairwise equivalent*:

(*i.*) *The densely defined operator* $[\overline{D^*_\kappa}]^-_{\mathcal{N}} : \{L_2(\Gamma) \subset H^-_{\mathcal{N}}(\Gamma)\} \to H^-_{\mathcal{N}}(\Gamma)$ *is bounded.*

(*ii.*) *The densely defined operator* $B_\kappa^{\frac{1}{2}} \overline{D^*_\kappa} B_\kappa^{-\frac{1}{2}} : \{\mathcal{R}(B_\kappa^{\frac{1}{2}}) \subset H^0(\Gamma)\} \to H^0(\Gamma)$, *acting in* $H^0(\Gamma)$, *is bounded.*

(*iii.*) $\mathcal{R}(B_\kappa^{\frac{1}{2}})$ *is invariant under* D_κ.

(*iv.*) *The operator* $B_\kappa^{-\frac{1}{2}} D_\kappa B_\kappa^{\frac{1}{2}}$ *belongs to* $\mathcal{B}(H^0(\Gamma))$.

Proof: *Equivalence of* (*i*) *and* (*ii*): It is easy to see, directly from the definitions, that the densely defined operator $[\overline{D^*_\kappa}]^-_{\mathcal{N}}$, acting in $H^-_{\mathcal{N}}(\Gamma)$, is bounded iff there exists a positive M such that $\|B_\kappa^{\frac{1}{2}} \overline{D^*_\kappa} f\|_0 \leq M \|B_\kappa^{\frac{1}{2}} f\|_0$ for all $f \in L_2(\Gamma)$, *i.e.*, such that $\|B_\kappa^{\frac{1}{2}} \overline{D^*_\kappa} B_\kappa^{-\frac{1}{2}} h\|_0 \leq M \|h\|_0$ for all $h \in \mathcal{R}(B_\kappa^{\frac{1}{2}})$, which is precisely the condition for the boundedness of the densely defined operator $B_\kappa^{\frac{1}{2}} \overline{D^*_\kappa} B_\kappa^{-\frac{1}{2}} : \{\mathcal{R}(B_\kappa^{\frac{1}{2}}) \subset H^0(\Gamma)\} \to H^0(\Gamma)$, acting in $H^0(\Gamma)$.

Equivalence of (*ii*) *and* (*iii*): Suppose first that $\mathcal{R}(B_\kappa^{\frac{1}{2}})$ is invariant under D_κ. Then $B_\kappa^{-\frac{1}{2}} D_\kappa B_\kappa^{\frac{1}{2}}$ is defined on all of $H^0(\Gamma)$; since it is easy to check that the operator is also closed, the Closed Graph Theorem says that it must be bounded. Therefore, the $H^0(\Gamma)$-adjoint $(B_\kappa^{-\frac{1}{2}} D_\kappa B_\kappa^{\frac{1}{2}})^*$ is also in $\mathcal{B}(H^0(\Gamma))$. Explicitly, for $h \in \mathcal{R}(B_\kappa^{\frac{1}{2}})$ it is clear that $(B_\kappa^{-\frac{1}{2}} D_\kappa B_\kappa^{\frac{1}{2}})^* h = B_\kappa^{\frac{1}{2}} D^*_\kappa B_\kappa^{-\frac{1}{2}} h$, which shows that the densely defined operator $B_\kappa^{\frac{1}{2}} D^*_\kappa B_\kappa^{-\frac{1}{2}} : \{\mathcal{R}(B_\kappa^{\frac{1}{2}}) \subset H^0(\Gamma)\} \to H^0(\Gamma)$ is bounded; the same is then true of its conjugate, which is just $B_\kappa^{\frac{1}{2}} \overline{D^*_\kappa} B_\kappa^{-\frac{1}{2}} : \{\mathcal{R}(B_\kappa^{\frac{1}{2}}) \subset H^0(\Gamma)\} \to H^0(\Gamma)$, since $B_\kappa^{\frac{1}{2}}$ is self-conjugate. Conversely, suppose that the latter operator is bounded: then its adjoint $(B_\kappa^{\frac{1}{2}} \overline{D^*_\kappa} B_\kappa^{-\frac{1}{2}})^*$ coincides with the adjoint of its bounded extension in $\mathcal{B}(H^0(\Gamma))$, and so is, in particular, defined on all of $H^0(\Gamma)$; *cf*. [19, Theorem 5.3(c)]. Moreover, according to [19, Theorem 4.19(b)], we have

$\big(B_\kappa^{\frac12}\overline{D_\kappa^*}B_\kappa^{-\frac12}\big)^* = B_\kappa^{-\frac12}\big(B_\kappa^{\frac12}\overline{D_\kappa^*}\big)^* = B_\kappa^{-\frac12}\overline{D}_\kappa B_\kappa^{\frac12}$; the domain $\{\ f \in H^0(\Gamma)\ \big|\ \overline{D}_\kappa B_\kappa^{\frac12} f \in \mathcal{R}\big(B_\kappa^{\frac12}\big)\ \}$ of the latter operator must then be all of $H^0(\Gamma)$, *i.e.*, $\mathcal{R}\big(B_\kappa^{\frac12}\big)$ is invariant under $\overline{D}_\kappa$. The same is then true for D_κ.

Equivalence of (iii) and (iv): This equivalence was essentially already established in the second part of the proof. In fact, the implication $(iii) \Longrightarrow (iv)$ was verified there directly, while, conversely, the inclusion $B_\kappa^{-\frac12} D_\kappa B_\kappa^{\frac12} \in \mathcal{B}\big(H^0(\Gamma)\big)$ implies that the domain $\{\ f \in H^0(\Gamma)\ \big|\ D_\kappa B_\kappa^{\frac12} f \in \mathcal{R}\big(B_\kappa^{\frac12}\big)\ \}$ of $B_\kappa^{-\frac12} D_\kappa B_\kappa^{\frac12}$ is all of $H^0(\Gamma)$, which says precisely that $\mathcal{R}\big(B_\kappa^{\frac12}\big)$ is invariant under $\overline{D}_\kappa$. ∎

Now the condition (C.2)′ given in the following statement has been clarified.

Proposition 5.1. *The condition* (C.2) *holds iff*

$$\mathcal{R}\big(B_\kappa^{\frac12}\big) \text{ is invariant under } D_\kappa \quad \text{and} \quad B_\kappa^{-\frac12} D_\kappa B_\kappa^{\frac12} \in \mathcal{B}\big(H^0(\Gamma)\big) \text{ is compact.} \qquad \text{(C.2)}'$$

Proof: Suppose first that (C.2) holds. Then, in particular, $\big[\overline{D_\kappa^*}\big]_{\mathcal{N}}^-$ is bounded, so Lemma 5.2 says that $\mathcal{R}\big(B_\kappa^{\frac12}\big)$ is invariant under D_κ, while $B_\kappa^{\frac12}\overline{D_\kappa^*}B_\kappa^{-\frac12} : \{\mathcal{R}\big(B_\kappa^{\frac12}\big) \subset H^0(\Gamma)\} \to H^0(\Gamma)$ is bounded and $B_\kappa^{-\frac12} D_\kappa B_\kappa^{\frac12} \in \mathcal{B}\big(H^0(\Gamma)\big)$. Of course, as we have noted, $B_\kappa^{\frac12}\overline{D_\kappa^*}B_\kappa^{-\frac12}$ is the restriction to $\mathcal{R}\big(B_\kappa^{\frac12}\big)$ of the adjoint $\big(B_\kappa^{-\frac12}\overline{D}_\kappa B_\kappa^{\frac12}\big)^*$, so that the compactness of $B_\kappa^{-\frac12}\overline{D}_\kappa B_\kappa^{\frac12}$, and then also that of $B_\kappa^{-\frac12} D_\kappa B_\kappa^{\frac12}$, will follow if we show that $B_\kappa^{\frac12}\overline{D_\kappa^*}B_\kappa^{-\frac12}$ is compact; we shall prove the latter. Thus, letting $\big(f_n\big)_{n=1}^\infty$ be a sequence from $\mathcal{R}\big(B_\kappa^{\frac12}\big)$ that is bounded in $H^0(\Gamma)$, we must produce a subsequence $\big(f_{n_k}\big)_{k=1}^\infty$ for which $\big(B_\kappa^{\frac12}\overline{D_\kappa^*}B_\kappa^{-\frac12} f_{n_k}\big)_{k=1}^\infty$ is a Cauchy sequence in $H^0(\Gamma)$. With $\widetilde{f}_n \in H^0(\Gamma)$ such that $f_n = B_\kappa^{\frac12}\widetilde{f}_n$ for each n, it follows readily that $\big(\widetilde{f}_n\big)_{n=1}^\infty$ is bounded in $H_{\mathcal{N}}^-(\Gamma)$. By the compactness of $\big[\overline{D_\kappa^*}\big]_{\mathcal{N}}^-$, there is a subsequence such that $\big(\overline{D_\kappa^*}\widetilde{f}_{n_k}\big)_{k=1}^\infty$ is Cauchy in $H_{\mathcal{N}}^-(\Gamma)$, whence it is clear that $\big(B_\kappa^{\frac12}\overline{D_\kappa^*}\widetilde{f}_{n_k}\big)_{k=1}^\infty$, *i.e.*, the subsequence $\big(B_\kappa^{\frac12}\overline{D_\kappa^*}B_\kappa^{-\frac12} f_{n_k}\big)_{k=1}^\infty$, is Cauchy in $H^0(\Gamma)$, as required, completing the first half of the proof.

Now assume that (C.2)′ is true. Since $B_\kappa^{\frac12}$ is self-conjugate, it clearly follows that $B_\kappa^{-\frac12}\overline{D}_\kappa B_\kappa^{\frac12}$ is also compact, so its adjoint $\big(B_\kappa^{-\frac12}\overline{D}_\kappa B_\kappa^{\frac12}\big)^*$ has the same property. To prove that (C.2) holds, let $\big(f_n\big)_{n=1}^\infty$ be a sequence from $L_2(\Gamma)$ that is bounded in $H_{\mathcal{N}}^-(\Gamma)$, so that $\big(B_\kappa^{\frac12} f_n\big)_{n=1}^\infty$ is bounded in $H^0(\Gamma)$. Therefore, there is a subsequence such that $\big(\big(B_\kappa^{-\frac12}\overline{D}_\kappa B_\kappa^{\frac12}\big)^* B_\kappa^{\frac12} f_{n_k}\big)_{k=1}^\infty$ is a Cauchy sequence in $H^0(\Gamma)$. But we have $\big(B_\kappa^{-\frac12}\overline{D}_\kappa B_\kappa^{\frac12}\big)^* B_\kappa^{\frac12} f_{n_k} = B_\kappa^{\frac12}\overline{D_\kappa^*} f_{n_k}$ for each k, so $\big(B_\kappa^{\frac12}\overline{D_\kappa^*} f_{n_k}\big)_{k=1}^\infty$ is Cauchy in $H^0(\Gamma)$, from which it is clear that $\big(\overline{D_\kappa^*} f_{n_k}\big)_{k=1}^\infty$ is Cauchy in $H_{\mathcal{N}}^-(\Gamma)$. This shows that $\big[\overline{D_\kappa^*}\big]_{\mathcal{N}}^-$ is compact in $H_{\mathcal{N}}^-(\Gamma)$ and completes the proof. ∎

Obviously, it is of interest to accumulate information about the range $\mathcal{R}\big(B_\kappa^{\frac12}\big)$; alternate characterizations of $\mathcal{R}\big(B_\kappa^{\frac12}\big)$ are of particular importance. In this direction, we have

Proposition 5.2. *(i.)* $\mathcal{R}\big(B_\kappa^{\frac12}\big) = \Big\{\ f \in H^0(\Gamma)\ \Big|\ \big(\big(f, \overline{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}}\big)_0\big)_{n=1}^\infty \in \ell_2\ \Big\}$.

(ii.) $\mathcal{R}\big(B_\kappa^{\frac12}\big)$ *is invariant under the operator* D_κ *iff* $\sum_{n=1}^\infty \big|\big(D_\kappa f, \overline{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}}\big)_0\big|^2 < \infty$ *whenever* $f \in H^0(\Gamma)$ *and* $\sum_{n=1}^\infty \big|\big(f, \overline{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}}\big)_0\big|^2 < \infty$.

(iii.) *If* $\mathcal{R}\big(B_\kappa^{\frac12}\big)$ *is invariant under* D_κ*, then* $\operatorname{Reg} V_n^{\kappa\mathcal{O}}\big|_\Gamma$ *and* $A_\kappa \operatorname{Reg} V_{n,\mathbf{n}}^{\kappa\mathcal{O}}$ *lie in* $\mathcal{R}\big(B_\kappa^{\frac12}\big)$ *for each* n*, so that* $\sum_{m=1}^\infty \big|\big(\operatorname{Reg} V_n^{\kappa\mathcal{O}}\big|_\Gamma, \overline{V_{m,\mathbf{n}}^{\kappa\mathcal{O}}}\big)_0\big|^2 < \infty$ *and* $\sum_{m=1}^\infty \big|\big(\operatorname{Reg} V_{n,\mathbf{n}}^{\kappa\mathcal{O}}, \overline{V_m^{\kappa\mathcal{O}}}\big|_\Gamma\big)_0\big|^2 < \infty$*, for* $n = 1, 2, 3, \ldots$.

Proof: (*i*). Let $f \in \mathcal{R}(B_\kappa^{\frac{1}{2}})$, say, $f = B_\kappa^{\frac{1}{2}}\widetilde{f}$. Then $\big(f, \overline{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}}\big)_0 = \big(\widetilde{f}, B_\kappa^{\frac{1}{2}}\overline{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}}\big)_0$, since $B_\kappa^{\frac{1}{2}}$ is self-adjoint. Upon recalling that $\big(B_\kappa^{\frac{1}{2}}\overline{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}}\big)_{n=1}^\infty$ is an orthonormal basis for $H^0(\Gamma)$, we conclude that $\big((f, \overline{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}})_0\big)_{n=1}^\infty \in \ell_2$. Conversely, suppose that the latter inclusion holds for some $f \in H^0(\Gamma)$. Then we *can* construct an element $\widetilde{f} \in H^0(\Gamma)$ by $\widetilde{f} := \sum_{n=1}^\infty \big(f, \overline{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}}\big)_0 B_\kappa^{\frac{1}{2}}\overline{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}}$, the series converging in $H^0(\Gamma)$. Since $B_\kappa\overline{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}} = U_n^{\kappa\mathcal{O}}$, we compute $B_\kappa^{\frac{1}{2}}\widetilde{f} = \sum_{n=1}^\infty \big(f, \overline{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}}\big)_0 U_n^{\kappa\mathcal{O}}$; but the latter series is just f itself, for, denoting the sum of the series by f_0 and recalling the biorthonormality of $\big(\overline{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}}\big)_{n=1}^\infty$ and $\big(U_n^{\kappa\mathcal{O}}\big)_{n=1}^\infty$, we find that $\big(f_0, \overline{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}}\big)_0 = \big(f, \overline{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}}\big)_0$ for each n, whence the completeness of $\big(\overline{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}}\big)_{n=1}^\infty$ in $H^0(\Gamma)$ implies that $f_0 = f$. Therefore, $B_\kappa^{\frac{1}{2}}\widetilde{f} = f$, so $f \in \mathcal{R}(B_\kappa^{\frac{1}{2}})$.

(*ii*). This clearly follows directly from the characterization of $\mathcal{R}(B_\kappa^{\frac{1}{2}})$ just proven in (*i*).

(*iii*). Suppose that D_κ maps $\mathcal{R}(B_\kappa^{\frac{1}{2}})$ into itself. Then, for any n, since $U_n^{\kappa\mathcal{O}} = B_\kappa\overline{V_{n,\mathbf{n}}^{\kappa\mathcal{O}}}$ belongs to $\mathcal{R}(B_\kappa) \subset \mathcal{R}(B_\kappa^{\frac{1}{2}})$, the relation $(I + D_\kappa)U_n^{\kappa\mathcal{O}} = -\mathrm{i}\kappa\mathrm{Reg}\,V_n^{\kappa\mathcal{O}}\big|_\Gamma$ shows that $\mathrm{Reg}\,V_n^{\kappa\mathcal{O}}\big|_\Gamma \in \mathcal{R}(B_\kappa^{\frac{1}{2}})$. But then the inclusion $A_\kappa\mathrm{Reg}\,V_{n,\mathbf{n}}^{\kappa\mathcal{O}} \in \mathcal{R}(B_\kappa^{\frac{1}{2}})$ follows directly from the definition of $U_n^{\kappa\mathcal{O}}$. □

Remark. Appearing in the original presentation of WATERMAN [18] and repeated often in the literature on these methods is the purported relation

$$\mathcal{Q}^{\kappa\mathcal{O}}\mathcal{T}^{\kappa\mathcal{O}} = -\mathrm{Re}\,\mathcal{Q}^{\kappa\mathcal{O}}, \tag{5.1}$$

claimed to connect the actual transition-matrix defined here in Section 1 and the infinite matrix $\mathcal{Q}^{\kappa\mathcal{O}}$ with elements $\mathcal{Q}_{mn}^{\kappa\mathcal{O}}$ defined in (1.13). That is, the product indicated on the left in (5.1) is intended as (convergent) infinite-matrix multiplication. The "truncated" form of (5.1) is the relation (1.12), already cited as forming the basis for the second Waterman scheme. Alternately, if (5.1) holds and ι is a sequence of coefficients generating a regular incident field as in (1.9), then the corresponding sequence $\sigma := \mathcal{T}^{\kappa\mathcal{O}}\iota$ of scattered-field expansion coefficients will satisfy the infinite linear system expressed by

$$\mathcal{Q}^{\kappa\mathcal{O}}\sigma = -\mathrm{Re}\,\mathcal{Q}^{\kappa\mathcal{O}}\iota. \tag{5.2}$$

It seems to be a common perception that (5.1) and (5.2) are correct in general, and that the "T-matrix method" consists in truncating either of the two systems to get finite systems to solve for, respectively, approximate transition matrices or approximate scattered-field expansion coefficients. By "truncation" here we mean the formal application of the classical *abscnittsmethode* for approximate solution of an infinite system; *cf.*, *e.g.*, [6]. In fact, the "derivation" of (5.1) given in [18] is completely formal, and it is not known just when the relation is correct, just as it is not known exactly when the *abscnittsmethode* can be applied to generate convergent approximations in the indicated manner. In any event, an analysis of the correctness of (5.1) and (5.2) is not necessary for an analysis of the second Waterman scheme. Nevertheless, one can show that (5.1) holds at least whenever the set of traces $\{\mathrm{Reg}\,V_n^{\kappa\mathcal{O}}\big|_\Gamma\}_{n=1}^\infty$ belongs to the range $\mathcal{R}(B_\kappa^{\frac{1}{2}})$; the easy proof of this is given in [5]. Therefore, according to Proposition 5.2.*iii*, (5.1) holds if $\mathcal{R}(B_\kappa^{\frac{1}{2}})$ is invariant under D_κ. By continuing along the lines that we have begun here, one can prove more concerning these questions; since we have not developed any new facts about the convergence of the methods by following this approach through sequence spaces, we shall just roughly indicate some of the results without proof. Thus, by supposing that conditions (C.1) and (C.2) hold, one can show that $\mathcal{Q}^{\kappa\mathcal{O}}$ generates a bounded linear operator in the sequence space ℓ_2 that is also bijective, while the transition matrix and scattered-field expansion coefficients satisfy (5.1) and (5.2), respectively. Moreover, application of the *abscnittsmethode* to, say, (5.2), can be completely justified; the result will be a sequence of "finite-length" elements of ℓ_2 converging to the unique σ satisfying (5.2), whence it also follows easily that the corresponding sequence of far-field patterns will converge to the far-field pattern of the scattered field, just as in the statement of Theorem 5.1.*i*. Finally, in case (C.1) fails to hold, the numerical instability described in Theorem 5.1.*ii* can be established by the same approach.

6. A condition sufficient for (C.2) and its satisfaction for ellipsoidal Γ.

In the preceding section, we established the implications of the condition (C.2), first with condition (C.1) and then under the assumption that (C.1) fails, for the viability, convergence, and numerical stability of the generalized second Waterman scheme. However, we have not yet shown here that there are any domains Ω_- for which (C.2) actually holds. While it appears that (C.2) is a strong restriction on the shape of Ω_-, we can give at present no easily verifiable criterion that is equivalent to this condition. We do, however, have a condition that is sufficient to ensure (C.2) and which can be verified to hold for at least one important class of shapes, *viz.*,

$$\mathcal{R}(B_\kappa) \quad \textit{is invariant under} \quad D_\kappa; \tag{C.2.1}$$

this is the content of Theorems 6.1 and 6.2.

Theorem 6.1. (*i.*) *The condition* (C.2.1) *implies* (C.2).

(*ii.*) *Condition* (C.2.1) *is implied by the operator relation*

$$D_\kappa B_\kappa = B_\kappa \overline{D_\kappa^*}. \tag{C.2.2}$$

(*iii.*) *The operator relation* (C.2.2) *is equivalent to the symmetry condition*

$$\big(V^{\kappa\mathcal{O}}_{m,\mathbf{n}}, \operatorname{Reg} V^{\kappa\mathcal{O}}_{n}\big|_\Gamma\big)_0 = \big(V^{\kappa\mathcal{O}}_{n,\mathbf{n}}, \operatorname{Reg} V^{\kappa\mathcal{O}}_{m}\big|_\Gamma\big)_0 \qquad \textit{for all} \quad m \textit{ and } n = 1,\, 2,\, 3,\, \ldots\,. \tag{C.2.2$'$}$$

Moreover, if (C.2.2)$'$ *holds for some* $\mathcal{O} \in \Omega_-$*, then it is also true with* $\mathcal{O}$ *replaced by any other* $\mathcal{O}' \in \Omega_-$.

Proof: (*i*). To show that (C.2.1) implies (C.2) it is convenient to appeal to (a simple extension of) a result of Lax [10]:

Lemma 6.1. *Let* $\big(B, \|\cdot\|_B\big)$ *be a Banach space and* $\big(H, (\,\cdot\,,\,\cdot\,)_H\big)$ *a Hilbert space with* $B \subset H$, B *dense in* H*, and the natural injection map of* B *into* H *bounded. Let the operators* L_1 *and* $L_2 \in \mathcal{B}(B)$ *be formally adjoint when regarded as densely defined and acting in* H*. That is, with* $\widehat{L}_k : \{B \subset H\} \to H$ *given by* $\widehat{L}_k f := L_k f$ *for each* $f \in B$*,* $k = 1$ *and* 2*, it is supposed that*

$$\big(\widehat{L}_1 f, h\big)_H = \big(f, \widehat{L}_2 h\big)_H \qquad \text{for} \quad f,\, h \in B. \tag{6.1}$$

Then

(*i.*) $\widehat{L}_1$ *and* $\widehat{L}_2$ *are bounded, and so possess unique extensions to elements of* $\mathcal{B}(H)$*, which we denote again by* $\widehat{L}_1$ *and* $\widehat{L}_2$*, respectively; these extensions have norms not exceeding* $\big\{\|L_1\|_B \|L_2\|_B\big\}^{\frac{1}{2}}$ *and are related by* $\widehat{L}_2 = \widehat{L}_1{}^*$;

(*ii.*) *if either* L_1 *or* L_2 *is compact (in* B*), then both* $\widehat{L}_1$ *and* $\widehat{L}_2$ *are compact (in* H*).*

Proof: The proof of Lemma 6.1 appears at the end of this section.

Returning to the proof of Theorem 6.1.*i*, let (C.2.1) hold. As we have observed, $\mathcal{R}(B_\kappa)$ is closed under complex conjugation because B_κ is self-conjugate, and so $\mathcal{R}(B_\kappa)$ is also invariant under $\overline{D}_\kappa$. This means that the domain of the operator $B_\kappa^{-1}\overline{D}_\kappa B_\kappa$ is all of $L_2(\Gamma)$; since the operator is also closed, it follows that it is in $\mathcal{B}\big(H^0(\Gamma)\big)$. In the statement of Lemma 6.1, take $B = H^0(\Gamma)$, $H = H^-_{\mathcal{N}}(\Gamma)$, $L_1 = \overline{D_\kappa^*}$, and $L_2 = B_\kappa^{-1}\overline{D}_\kappa B_\kappa$. To see that the hypotheses of Lemma 6.1 are fulfilled with these choices, we need only check that the two operators are formal adjoints with respect to the inner product of $H^-_{\mathcal{N}}(\Gamma)$. Accordingly, for f and $h \in L_2(\Gamma)$ we compute

$$\big(\overline{D^*_\kappa} f, h\big)^{\mathcal{N}}_- = \big(f, \overline{D}_\kappa B_\kappa h\big)_0 = \big(f, B_\kappa B_\kappa^{-1} \overline{D}_\kappa B_\kappa h\big)_0 = \big(f, B_\kappa^{-1} \overline{D}_\kappa B_\kappa h\big)^{\mathcal{N}}_-,$$

as required. Now, with the compactness of $\overline{D^*_\kappa}$ in $H^0(\Gamma)$, Lemma 6.1 shows that (C.2) must be true.

(ii). This statement is obvious.

(iii). It is easy to show that (C.2.2) and (C.2.2)′ are equivalent. In fact, we can draw the conclusion from the pairwise equivalence of the following chain of assertions, which follows by recalling the completeness of $\big(V^{\kappa\mathcal{O}}_{n,\mathbf{n}}\big)_{n=1}^{\infty}$ in $H^0(\Gamma)$, relation (1.6), and the fact that the regular solutions $\operatorname{Reg} V^{\kappa\mathcal{O}}_n$ are real-valued:

$$B_\kappa \overline{D^*_\kappa} = D_\kappa B_\kappa;$$

$$\frac{\mathrm{i}}{\kappa} B_\kappa \big(I + \overline{D^*_\kappa}\big) = \frac{\mathrm{i}}{\kappa}\big(I + D_\kappa\big) B_\kappa;$$

$$\frac{\mathrm{i}}{\kappa} B_\kappa \big(I + \overline{D^*_\kappa}\big) \overline{V^{\kappa\mathcal{O}}_{m,\mathbf{n}}} = \frac{\mathrm{i}}{\kappa}\big(I + D_\kappa\big) B_\kappa \overline{V^{\kappa\mathcal{O}}_{m,\mathbf{n}}} = \operatorname{Reg} V^{\kappa\mathcal{O}}_m|_\Gamma \qquad \text{for} \quad m = 1, 2, 3, \dots ;$$

$$\Big(V^{\kappa\mathcal{O}}_{n,\mathbf{n}}, \frac{\mathrm{i}}{\kappa} B_\kappa \big(I + \overline{D^*_\kappa}\big) \overline{V^{\kappa\mathcal{O}}_{m,\mathbf{n}}}\Big)_0 = \big(V^{\kappa\mathcal{O}}_{n,\mathbf{n}}, \operatorname{Reg} V^{\kappa\mathcal{O}}_m|_\Gamma\big)_0 \qquad \text{for} \quad m,\, n = 1, 2, 3, \dots ;$$

and, finally,

$$\begin{aligned} \big(V^{\kappa\mathcal{O}}_{m,\mathbf{n}}, \operatorname{Reg} V^{\kappa\mathcal{O}}_n|_\Gamma\big)_0 &= \big(\operatorname{Reg} V^{\kappa\mathcal{O}}_n|_\Gamma, \overline{V^{\kappa\mathcal{O}}_{m,\mathbf{n}}}\big)_0 \\ &= \Big(-\frac{\mathrm{i}}{\kappa}\big(I + \overline{D}_\kappa\big) B_\kappa V^{\kappa\mathcal{O}}_{n,\mathbf{n}}, \overline{V^{\kappa\mathcal{O}}_{m,\mathbf{n}}}\Big)_0 = \Big(V^{\kappa\mathcal{O}}_{n,\mathbf{n}}, \frac{\mathrm{i}}{\kappa} B_\kappa \big(I + \overline{D^*_\kappa}\big) \overline{V^{\kappa\mathcal{O}}_{m,\mathbf{n}}}\Big)_0 \\ &= \big(V^{\kappa\mathcal{O}}_{n,\mathbf{n}}, \operatorname{Reg} V^{\kappa\mathcal{O}}_m|_\Gamma\big)_0 \qquad \text{for} \quad m,\, n = 1, 2, 3, \dots . \end{aligned}$$

The final assertion of (iii) now follows from the equivalence of (C.2.2) and (C.2.2)′, since condition (C.2.2) is independent of the choice of $\mathcal{O} \in \Omega_-$. This completes the proof. ∎

We finish the development of our concrete sufficient condition for (C.2) and the conclusions of Theorem 5.1 on the viability, convergence, and numerical stability of (gW.II) by recalling that the symmetry condition (C.2.2)′ obtains whenever Γ is an ellipsoid, as pointed out by WATERMAN [18].

Theorem 6.2. *The equivalent conditions* (C.2.2) *and* (C.2.2)′ *hold whenever the boundary* Γ *is ellipsoidal. Therefore, when* Γ *is an ellipsoid condition* (C.2) *obtains, so that statements* (i) *and* (ii) *of Theorem 5.1 hold in that case.*

Proof: Because the complete reasoning is somewhat lengthy, we have relegated to the Appendix an amplification of Waterman's argument showing that the symmetry condition (C.2.2)′ holds when Γ is ellipsoidal. The remaining statements of the Theorem follow immediately from this, by Theorem 6.1. ∎

Finally, we supply a proof of Lemma 6.1. For this, we will rely on

Lemma 6.2. *Let* $\big(B, \|\cdot\|_B\big)$ *and* $\big(H, (\,\cdot\,,\,\cdot\,)_H\big)$ *be, respectively, a Banach space and a Hilbert space related as in Lemma 6.1. Let* $L \in \mathcal{B}\big(B\big)$ *be symmetric when regarded as densely defined and acting in* H*. That is, with* $\widehat{L} : \big\{B \subset H\big\} \to H$ *defined by* $\widehat{L}f := Lf$ *for each* $f \in B$*, it is supposed that*

$$\big(\widehat{L}f, h\big)_H = \big(f, \widehat{L}h\big)_H \qquad \text{for} \quad f,\, h \in B. \tag{6.2}$$

Then

(*i.*) *$\widehat{L}$ is bounded, with norm not exceeding $\|L\|_{\mathcal{B}(B)}$, and so possesses a unique extension to an element of $\mathcal{B}(H)$, which we denote again by $\widehat{L}$, with $\|\widehat{L}\|_{\mathcal{B}(H)} \le \|L\|_{\mathcal{B}(B)}$;*

(*ii.*) *if L is compact (in B), then $\widehat{L}$ is compact (in H).*

Proof: Statements (i) and (ii) are, respectively, Theorem I and Corollary II of LAX [10]. □

Proof of Lemma 6.1: The first part of the statement of (i) is noted in [10], along with a proof; we choose to employ instead the approach taken in [7, Theorem 2.13] for establishing the result, since this leads to an easy proof of (ii). Let $L := L_2L_1 \in \mathcal{B}(B)$, and define $\widehat{L} := \widehat{L}_2\widehat{L}_1 : \{B \subset H\} \to H$, so $\widehat{L}f = Lf$ for each $f \in B$, and $\widehat{L}$ is just L regarded as acting in H. With (6.1) it is easy to check that (6.2) holds, so $\widehat{L}$ is symmetric, and we may apply Lemma 6.2 to conclude that $\widehat{L}$ is bounded. Denoting its continuous extension in $\mathcal{B}(H)$ again by $\widehat{L}$, we see that $\|\widehat{L}\|_{\mathcal{B}(H)} \le \|L\|_{\mathcal{B}(B)} \le \|L_1\|_{\mathcal{B}(B)}\|L_2\|_{\mathcal{B}(B)}$. Now the boundedness of $\widehat{L}_1$ follows from

$$\|\widehat{L}_1 f\|_H^2 = (\widehat{L}_1 f, \widehat{L}_1 f)_H = (f, \widehat{L} f)_H \le \|\widehat{L}\|_{\mathcal{B}(H)}\|f\|_H^2 \le \|L_1\|_{\mathcal{B}(B)}\|L_2\|_{\mathcal{B}(B)}\|f\|_H^2 \qquad \text{for} \quad f \in B,$$

along with the claimed estimate for the norm of $\widehat{L}_1$. The boundedness of $\widehat{L}_2$ is proven in the same manner. Denote the bounded extensions again by $\widehat{L}_1, \widehat{L}_2 \in \mathcal{B}(H)$. Since B is dense in H, the equality (6.1) extends to hold for all $f, h \in H$, whence we conclude that $\widehat{L}_2 = \widehat{L}_1^*$. To prove the compactness assertion, we note first that the definition $\widehat{L} := \widehat{L}_2\widehat{L}_1$ extends to hold on all of H as $\widehat{L} = \widehat{L}_1^*\widehat{L}_1$. Consequently, if either L_1 or L_2 is compact, then $L := L_2L_1$ is compact, so Lemma 6.2 says that $\widehat{L}$, *i.e.*, $\widehat{L}_1^*\widehat{L}_1$, is compact; the compactness of $\widehat{L}_1$ follows from this (*cf.*, *e.g.*, [19, Theorem 6.4(c)]), along with that of $\widehat{L}_2 = \widehat{L}_1^*$. □

Appendix. Satisfaction of the symmetry condition (C.2.2)$'$ when Γ is an ellipsoid.

In this Appendix, we fill in some of the details in the reasoning given by WATERMAN [18] to show that the symmmetry condition (C.2.2)$'$ holds whenever the boundary $\Gamma := \partial\Omega_-$ is an ellipsoid.

It is more convenient now to work in the double-index notation. Thus, setting

$$\mathcal{Q}_{kn}^{lm} := \big(V_{kn},_{\mathbf{n}}^{\kappa\mathcal{O}}, \operatorname{Reg} V_{lm}^{\kappa\mathcal{O}}\big|_{\Gamma}\big)_0 = \int_{\Gamma} V_{kn},_{\mathbf{n}}^{\kappa\mathcal{O}} \operatorname{Reg} V_{lm}^{\kappa\mathcal{O}}\, d\lambda_{\Gamma},$$

we want to prove that the difference $\widetilde{\mathcal{D}}_{kn}^{lm} := \mathcal{Q}_{kn}^{lm} - \mathcal{Q}_{lm}^{kn}$ vanishes for any ellipsoid Γ whenever k and l are nonnegative integers and the integers m and n satisfy $-k \le n \le k$ and $-l \le m \le l$. Since it is easy to see that

$$\begin{aligned}\int_{\Gamma} V_{kn},_{\mathbf{n}}^{\kappa\mathcal{O}} \operatorname{Reg} V_{lm}^{\kappa\mathcal{O}}\, d\lambda_{\Gamma} &= \frac{1}{2}\left\{\int_{\Gamma}\left(V_{kn}^{\kappa\mathcal{O}} \operatorname{Reg} V_{lm}^{\kappa\mathcal{O}}\right),_{\mathbf{n}} d\lambda_{\Gamma} - \int_{\Gamma}\left(V_{kn}^{\kappa\mathcal{O}} \operatorname{Reg} V_{lm},_{\mathbf{n}}^{\kappa\mathcal{O}} - V_{kn},_{\mathbf{n}}^{\kappa\mathcal{O}} \operatorname{Reg} V_{lm}^{\kappa\mathcal{O}}\right) d\lambda_{\Gamma}\right\}\\ &= \frac{1}{2}\int_{\Gamma}\left(V_{kn}^{\kappa\mathcal{O}} \operatorname{Reg} V_{lm}^{\kappa\mathcal{O}}\right),_{\mathbf{n}} d\lambda_{\Gamma} + \frac{\mathrm{i}}{\kappa}\delta_{kn}^{lm},\end{aligned}$$

we get

$$\widetilde{\mathcal{D}}_{kn}^{lm} := \mathcal{Q}_{kn}^{lm} - \mathcal{Q}_{lm}^{kn} = \frac{1}{2}\int_{\Gamma}\left(V_{kn}^{\kappa\mathcal{O}} \operatorname{Reg} V_{lm}^{\kappa\mathcal{O}} - V_{lm}^{\kappa\mathcal{O}} \operatorname{Reg} V_{kn}^{\kappa\mathcal{O}}\right),_{\mathbf{n}} d\lambda_{\Gamma}.$$

From the latter expression it is already obvious that $\widetilde{\mathcal{D}}_{ln}^{lm} = 0$.

For the time being, we suppose merely that Γ is starlike with respect to the point $\mathcal{O} \in \Omega_-$ and symmetric with respect to each of three mutually orthogonal planes passing through $\mathcal{O}$. Relative to an origin located at $\mathcal{O}$, let Γ be described as the graph of the mapping given on the unit sphere Σ_1 by $\hat{\mathbf{e}} \mapsto \mathrm{r}_{\Gamma}(\hat{\mathbf{e}})\hat{\mathbf{e}}$, in which r_{Γ} is a positive real function of class C^2 on Σ_1. Then, by setting up the integral in spherical coördinates and merely invoking the properties of r_{Γ} that are implied by the geometric assumptions listed, one discovers that $\widetilde{\mathcal{D}}_{kn}^{lm} = 0$ if (1) k and l are of opposite parity or if (2) m and n are of opposite parity or if (3) one of m and n is nonnegative while the other is negative. Consequently, writing

$$\mathcal{D}_{lsmn} := \widetilde{\mathcal{D}}_{l+2s\,n}^{lm} = \int_{\Gamma} F_{lsmn},_{\mathbf{n}}\, d\lambda_{\Gamma},$$

in which F_{lsmn} is given in $\mathbb{R}^3 \setminus \{\mathcal{O}\}$ by

$$F_{lsmn}(\varrho\,\hat{\mathbf{e}}) := \mathrm{i}\left\{j_l(\kappa\varrho)\, y_{l+2s}(\kappa\varrho) - j_{l+2s}(\kappa\varrho)\, y_l(\kappa\varrho)\right\} \widehat{Y}_{lm}(\hat{\mathbf{e}})\, \widehat{Y}_{l+2s\,n}(\hat{\mathbf{e}}) \qquad \text{for} \quad \varrho > 0, \quad \hat{\mathbf{e}} \in \Sigma_1,$$

where ϱ denotes distance measured from $\mathcal{O}$, the proof is reduced to showing that

$$\mathcal{D}_{lsmn} = 0 \qquad \textit{for} \qquad \begin{cases} |m| \le l, \quad |n| \le l + 2s, \quad l \ge 0, \quad \textit{and} \quad s \ge 1, \\ \textit{with } m \textit{ and } n \textit{ of the same parity} \quad \textit{and} \quad \textit{both either} \ge 0 \textit{ or} < 0, \\ \textit{when } \Gamma \textit{ is an ellipsoid.} \end{cases} \tag{A.1}$$

From this point we suppose that the integers l, s, m, and n are fixed as in (A.1).

Now, according to WATSON [20, pp. 296, 297], for $k \ge 0$ we can write

$$J_{\nu}(z)Y_{\nu+1+k}(z) - J_{\nu+1+k}(z)Y_{\nu}(z) = -\frac{2}{\pi z}R_{k,\nu+1}(z),$$

wherein (the "Lommel polynomial") $R_{k,\mu}$ is of the form

$$R_{k,\mu}(z) := \sum_{q=0}^{[\frac{k}{2}]} \tilde{c}_k^{\mu}(q) z^{-k+2q},$$

with $[\,\cdot\,]$ denoting the greatest-integer function; explicit expressions for the coefficients $\tilde{c}_k^{\mu}(q)$ can be found in [20], but are not needed here. Therefore, since $j_l(z) := \{\pi/2z\}^{\frac{1}{2}} J_{l+\frac{1}{2}}(z)$, and correspondingly for $y_l(z)$, for the spherical functions we have

$$j_l(z)\, y_{l+p}(z) - j_{l+p}(z)\, y_l(z) = -\frac{1}{z^2} R_{p-1,l+\frac{3}{2}}(z) = -\sum_{q=0}^{[\frac{p-1}{2}]} \tilde{c}_{p-1}^{\,l+\frac{3}{2}}(q) z^{-p+2q-1}.$$

In particular, for the combination of present interest we find an expansion of the form

$$j_l(z)\, y_{l+2s}(z) - j_{l+2s}(z)\, y_l(z) = \sum_{q=0}^{s-1} c_s^l(q) \left(\frac{1}{z}\right)^{2(s-q)+1}. \tag{A.2}$$

Next, we require the (generalized-Fourier) expansions of products of the basic spherical-surface harmonics in terms of the same spherical-surface harmonics, for which we appeal to the results cited by MESSIAH [12]. In the latter book, the complex orthonormal spherical-surface harmonics $\{\, \widetilde{Y}_l^m \mid |m| \le l,\ l = 0, 1, 2, \ldots \,\}$ are defined by

$$\widetilde{Y}_l^m(\hat{\mathbf{e}}) := \left\{ \begin{matrix} (-1)^m \\ 1 \end{matrix} \right\} \left(\frac{2l+1}{4\pi} \frac{(l-|m|)!}{(l+|m|)!} \right)^{\frac{1}{2}} P_l^{|m|}(\cos\theta_{\hat{\mathbf{e}}}) \exp(im\phi_{\hat{\mathbf{e}}}) \qquad \text{for} \quad \left\{ \begin{matrix} m \ge 0 \\ m < 0 \end{matrix} \right\}, \quad \hat{\mathbf{e}} \in \Sigma_1.$$

For the products of these spherical harmonics, Messiah gives the expansion

$$\widetilde{Y}_{l_1}^{m_1} \widetilde{Y}_{l_2}^{m_2} = \sum_{p=|l_1-l_2|}^{l_1+l_2} \sum_{q=-p}^{p} \left\{ \frac{(2l_1+1)(2l_2+1)}{4\pi(2p+1)} \right\}^{\frac{1}{2}} \langle\, l_1\, l_2\, 0\, 0 \,|\, p\, 0 \,\rangle \langle\, l_1\, l_2\, m_1\, m_2 \,|\, p\, q \,\rangle \widetilde{Y}_p^q$$

$$\text{for} \quad |m_1| \le l_1, \quad |m_2| \le l_2, \quad l_1, l_2 = 0, 1, 2, \ldots\,, \tag{A.3}$$

in which the Clebsch-Gordon coefficients $\langle\, l_1\, l_2\, m_1\, m_2 \,|\, p\, q \,\rangle$ are defined for $|m_1| \le l_1$, $|m_2| \le l_2$, $|q| \le p$, and l_1, l_2, $p = 0, 1, 2, \ldots$, and satisfy

$$\langle\, l_1\, l_2\, m_1\, m_2 \,|\, p\, q \,\rangle = 0 \qquad \text{if} \quad q \ne m_1 + m_2 \quad \text{or} \quad p < |l_1 - l_2| \quad \text{or} \quad p > l_1 + l_2 \tag{A.4}$$

and

$$\langle\, l_1\, l_2\, m_1\, m_2 \,|\, p\, q \,\rangle = (-1)^{l_1+l_2+p} \langle\, l_1\, l_2\ {-m_1}\ {-m_2} \,|\, p\ {-q} \,\rangle; \tag{A.5}$$

the latter equality shows that $\langle\, l_1\, l_2\, 0\, 0 \,|\, p\, 0 \,\rangle = 0$ if $l_1 + l_2$ and p are of opposite parity. Then, with $\pi(q)$ denoting the parity of the integer q, by also accounting for (A.4) the expansion in (A.3) can be written in the form

$$\widetilde{Y}_{l_1}^{m_1} \widetilde{Y}_{l_2}^{m_2} = \sum_{\substack{p=\max\{|m_1+m_2|,|l_1-l_2|\} \\ \pi(p)=\pi(l_1+l_2)}}^{l_1+l_2} \left\{ \frac{(2l_1+1)(2l_2+1)}{4\pi(2p+1)} \right\}^{\frac{1}{2}} \langle\, l_1\, l_2\, 0\, 0 \,|\, p\, 0 \,\rangle \langle\, l_1\, l_2\, m_1\, m_2 \,|\, p\ \ m_1 + m_2 \,\rangle \widetilde{Y}_p^{m_1+m_2}$$

$$\text{for} \quad |m_1| \le l_1, \quad |m_2| \le l_2, \quad l_1, l_2 = 0, 1, 2, \ldots\,. \tag{A.6}$$

One can easily verify that the real $H^0(\Sigma_1)$-orthonormal spherical-surface harmonics $\{\widehat{Y}_{lm}\}$ defined in Section 1 are given in terms of the complex orthonormal spherical-surface harmonics defined above by

$$\widehat{Y}_{lm} = \begin{cases} \widetilde{Y}_l^0 & \text{for } m = 0, \\ \dfrac{1}{\sqrt{2}}\{(-1)^m \widetilde{Y}_l^m + \widetilde{Y}_l^{-m}\} & \text{for } m = 1, \ldots, l, \\ \dfrac{\mathrm{i}}{\sqrt{2}}\{(-1)^m \widetilde{Y}_l^{-m} - \widetilde{Y}_l^m\} & \text{for } m = -l, \ldots, -1, \end{cases} \qquad \text{for} \quad l = 0,\, 1,\, 2,\, \ldots\,.$$

By using the latter relations with (A.6) and keeping in mind (A.5), when m_1 and m_2 are either both nonnegative or both negative one arrives at an expansion of the form

$$\widehat{Y}_{l_1 m_1} \widehat{Y}_{l_2 m_2} = \sum_{\substack{p=\max\{|m_1+m_2|,|l_1-l_2|\} \\ \pi(p)=\pi(l_1+l_2)}}^{l_1+l_2} a_{l_1 l_2}^{m_1 m_2}(p) \widehat{Y}_{p\,|m_1+m_2|} + \sum_{\substack{p=\max\{|m_1-m_2|,|l_1-l_2|\} \\ \pi(p)=\pi(l_1+l_2)}}^{l_1+l_2} b_{l_1 l_2}^{m_1 m_2}(p) \widehat{Y}_{p\,|m_1-m_2|}$$

$$(\text{with} \quad m_1 \text{ and } m_2 \quad \text{either} \quad \text{both} \geq 0 \quad \text{or} \quad \text{both} < 0), \qquad \text{(A.7)}$$

the second sum being absent if $m_1 m_2 = 0$; specific expressions for the coefficients are easily worked out, but are not required for present purposes. Of course, the sums here are over even values of the index p if $\pi(l_1) = \pi(l_2)$, which holds in the cases of interest to us. Since we have restricted l, s, m, and n as in (A.1), with (A.2) and (A.7) the difference $\mathcal{D}_{lsmn}$ can be expressed as a finite linear combination of integrals of the form $\int_\Gamma F_{pq}^\alpha{}_{,\mathbf{n}}\, d\lambda_\Gamma$, in which F_{pq}^α is given by $F_{pq}^\alpha(\varrho\,\hat{\mathbf{e}}) := \widehat{Y}_{pq}(\hat{\mathbf{e}})/\varrho^\alpha$ for $\varrho > 0$ and $\hat{\mathbf{e}} \in \Sigma_1$ (ϱ again denoting distance from $\mathcal{O} \in \Omega_-$), and in no term of the sum do we find $\alpha < 3$. For such an integral, using the function r_Γ describing the boundary Γ that is here star-shaped with respect to $\mathcal{O}$, one computes

$$\int_\Gamma F_{pq}^\alpha{}_{,\mathbf{n}}\, d\lambda_\Gamma = \left\{ \frac{p(p+1)}{\alpha - 1} - \alpha \right\} \int_{\Sigma_1} \frac{\widehat{Y}_{pq}}{\mathrm{r}_\Gamma^{\alpha-1}}\, d\lambda_{\Sigma_1} \qquad (\alpha \neq 1);$$

note that the integral on the left therefore vanishes when $\alpha = p + 1$ for $p \neq 0$ (which can also be shown by using the fact that F_{pq}^{p+1} is harmonic in $\mathbb{R}^3 \setminus \{\mathcal{O}\}$, as observed in [18]). Thus, with the indices satisfying the conditions of (A.1), we get

$$\mathcal{D}_{lsmn} = \mathrm{i} \sum_{q=0}^{s-1} \sum_{\substack{p=\max\{|m+n|,2s\} \\ p \text{ even}}}^{2(l+s)} \frac{c_s^l(q)\, a_{l\,l+2s}^{mn}(p)}{\kappa^{2(s-q)+1}} \left\{ \frac{p(p+1)}{2(s-q)} - 2(s-q) - 1 \right\} \int_{\Sigma_1} \frac{\widehat{Y}_{p\,|m+n|}}{\mathrm{r}_\Gamma^{2(s-q)}}\, d\lambda_{\Sigma_1}$$

$$+\mathrm{i} \sum_{q=0}^{s-1} \sum_{\substack{p=\max\{|m-n|,2s\} \\ p \text{ even}}}^{2(l+s)} \frac{c_s^l(q)\, b_{l\,l+2s}^{mn}(p)}{\kappa^{2(s-q)+1}} \left\{ \frac{p(p+1)}{2(s-q)} - 2(s-q) - 1 \right\} \int_{\Sigma_1} \frac{\widehat{Y}_{p\,|m-n|}}{\mathrm{r}_\Gamma^{2(s-q)}}\, d\lambda_{\Sigma_1}; \qquad \text{(A.8)}$$

note that $|m + n|$ and $|m - n|$ are even, while the second sum is absent if $mn = 0$.

Finally, let us suppose that Γ is an ellipsoid. Then we have already effectively required that $\mathcal{O}$ lie at the center of the ellipsoid, and it is easy to check that the coördinate system can be oriented so that the function r_Γ describing Γ satisfies

$$\frac{1}{\mathrm{r}_\Gamma^2} = \beta_1 \widehat{Y}_{00} + \beta_2 \widehat{Y}_{20} + \beta_3 \widehat{Y}_{22},$$

in which the coefficients are given in terms of the lengths a_1, a_2, and a_3 of the semi-axes of the ellipsoid, aligned along the respective axes of the associated cartesian system, as

$$\beta_1 := \frac{2}{3}\sqrt{\pi}\left(\frac{1}{a_1^2}+\frac{1}{a_2^2}+\frac{1}{a_3^2}\right), \quad \beta_2 := \frac{2}{3}\sqrt{\frac{\pi}{5}}\left(\frac{2}{a_3^2}-\frac{1}{a_1^2}-\frac{1}{a_2^2}\right), \quad \text{and} \quad \beta_3 := \frac{2}{3}\sqrt{\frac{3\pi}{5}}\left(\frac{1}{a_1^2}-\frac{1}{a_2^2}\right).$$

Thus, on the basis of (A.7) one can prove by induction that $1/\mathrm{r}_\Gamma^{2N}$ can be written as a linear combination of the spherical-surface harmonics $\{\widehat{Y}_{2k\,2j}\}_{0\leq j,k\leq N}$ alone, for each positive integer N. In particular, for $0 \leq q \leq (s-1)$ the function $1/\mathrm{r}_\Gamma^{2(s-q)}$ has an expansion involving only the spherical-surface harmonics $\{\widehat{Y}_{2k\,2j}\}_{0\leq j,k\leq (s-q)}$. On the other hand, the inequality $p \geq 2s$ holds in each term of the sums in (A.8), whence it is clear that the only terms in those sums that will not vanish by virtue of the orthogonality of the spherical-surface harmonics are those with $p = 2s$ and $q = 0$ (and the first sum has no such term if $|m+n| > 2s$, while the second fails to have such a term if $|m-n| > 2s$). But the factor $\{p(p+1)/2(s-q)\} - 2(s-q) - 1$ in the coefficient of those remaining terms vanishes when $p = 2s$ and $q = 0$, so that (A.1) does indeed hold.

This establishes the symmetry condition (C.2.2)$'$ for ellipsoids and completes the proof of Theorem 6.2.

References

1. Abramowitz, M., and I. A. Stegun, editors, *Handbook of Mathematical Functions*, National Bureau of Standards, Washington, DC, 1972.
2. Colton, D., and R. Kress, *Integral Equation Methods in Scattering Theory*, Wiley-Interscience, New York, 1983.
3. Colton, D., and P. Monk, The numerical solution of the three-dimensional inverse scattering problem for time harmonic acoustic waves, *SIAM J. Sci. Stat. Comput.* **8** (1987), 278–291.
4. Dallas, A. G., The Waterman algorithm for approximation of the transition matrix in scattering by obstacles, XXIInd General Assembly of the International Union of Radio Science, Tel Aviv, 1987.
5. Dallas, A. G., Basis properties of traces and normal derivatives of spherical-separable solutions of the Helmholtz equation, Technical Report No. 2000-6, Department of Mathematical Sciences, University of Delaware, Newark, DE, January, 2000.
6. Hellinger, E., and O. Toeplitz, *Integralgleichungen und Gleichungen mit unendlichvielen Unbekannten*, Encyklopädie der Mathematischen Wissenschaften II C13, 1335–1616, 1928. Reprinted by Chelsea Pub. Co., New York.
7. Kirsch, A., *Generalized Boundary Value and Control Problems for the Helmholtz Equation*, Habilitationsschrift, Institut für Numerische und Angewandte Mathematik der Georg-August-Universität Göttingen, Göttingen, 1984.
8. Krasnosel'skiĭ, M. A., G. M. Vainikko, P. P. Zabreiko, Ya. B. Rutitskiĭ, and V. Ya. Stetsenko, *Approximate Solutions of Operator Equations*, Wolters-Noordhoff, Groningen, 1972.
9. Kristensson, G., A. G. Ramm, and S. Ström, Convergence of the T-matrix approach in scattering theory, II, *J. Math. Phys.* **24** (1983), 2619–2631.
10. Lax, P. D., Symmetrizable linear transformations, *Comm. Pure Appl. Math.* **7** (1954), 633–647.
11. Marti, Jürg T., *Introduction to the Theory of Bases*, Springer-Verlag New York, Inc., New York, 1969.
12. Messiah, A., *Quantum Mechanics*, North-Holland, Amsterdam, 1962.
13. Müller, C., and H. Kersten, Zwei Klassen vollständiger Funktionensysteme zur Behandlung der Randwertaufgaben der Schwingungsgleichen $\Delta u + k^2 u = 0$, *Math. Methods Appl. Sci.* **2** (1980), 47–67.
14. Ramm, A. G., *Scattering by Obstacles*, D. Reidel Pub. Co., Dordrecht, 1986.
15. Sarkissian, A., A. G. Dallas, and R. E. Kleinman, Numerical search for a breakdown of the Waterman algorithm for approximating the T-matrix of a rigid obstacle, 112th Meeting of the Acoustical Society of America, Anaheim, CA, 1986.
16. Vekua, I. N., *New Methods for Solving Elliptic Equations*, North-Holland Publishing Company, Amsterdam, 1967.
17. Waterman, P. C., Matrix formulation of electromagnetic scattering, *Proc. IEEE* **53** (1965), 805–812.
18. Waterman, P. C., New formulation of acoustic scattering, *J. Acoust. Soc. Am.* **45** (1969), 1417–1429.
19. Weidmann, J., *Linear Operators in Hilbert Spaces*, Springer-Verlag, New York–Heidelberg–Berlin, 1980.
20. Watson, G. N., *A Treatise on the Theory of Bessel Functions*, 2nd ed., Cambridge University Press, Cambridge, 1944.