Recursive Sherman-Morrison factorization for scattering calculations

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Abstract. A technique based on the Sherman-Morrison formula is presented for developing efficient schemes for scattering calculations in the forward and inverse problems governed by the Helmholtz equation. Previous methods have been based directly on multiple scattering process which experience difficulties with more complex scattering calculations. Our approach is purely algebraic, systematic, and thus robust and easily generalizable to arbitrary scattering systems, among which is the calculation of variations of the Helmholtz equation required for linearization of the inverse scattering problem.

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1. Introduction

Efficient numerical methods for scattering calculations for the Helmholtz equation are either iterative or direct. In two dimensions, a direct fast solver is more attractive and more efficient [1] for problems with multiple incident waves than an iterative approach where each incident wave gives rise to a distinct right hand side for the linear system of equations to which the iterative method is applied. Circumstances for multiple incident waves arise, for example, when we solve the inverse problem, or when we solve an eigenvalue problem to determine the frequencies of propagating modes in a wave guide.

Computationally, a fast, direct solver is useful either for the Helmholtz equation converted to the Lippmann-Schwinger integral equation for volume scattering, or for its related variational calculations used for the inverse problem; see Section 6. Its core processes, which makes it efficient, is the so-called merging and splitting operations [1].

Arithmetically, the merging procedure corresponds to a factorization of the matrix of the linear system of equations, whose solution we seek for the scattering calculation, in a way similar to the LU or QR factorization, except that it is accomplished by divide-and-conquer. Once the matrix is recursively factorized, the back solve is performed also recursively via the splitting procedure.

Traditionally, the merging and splitting formulae are physically motivated and obtained with the help of the law of multiple scattering: The total incident wave to one subscatterer is the superposition of the original incident wave and the scattered waves from other subscatterers; see [1], [2], [3], [4]. We discovered that there exists a purely algebraic process, unrelated to the physically based multiple scattering process, that leads to the merging and splitting formulae. In particular, we now are able to pinpoint to the nature of this recursive matrix factorization: We will call it a recursive Sherman-Morrison factorization, because it turns out that the purely algebraic procedure, the Sherman-Morrison formula, combined with a natural definition of the scattering matrix, is what that matters.

The results presented here are not just about an alternative viewpoint of the merging and splitting formulae – indeed the new approach will give rise to identical merging and splitting formulae for the solution of the Lippmann-Schwinger equation – but also about, and actually critical to, their generalizations to other scattering calculations where the underlying physics becomes obscure, and the law of multiple scattering becomes difficult to apply, due to the complexity of the scattering problems; such is the case, for example, when we compute the variational quantities (37) and (38) associated with the Helmholtz equation for the purpose of its inverse scattering problem.

The paper is organized as follows. In Section 2, we introduce the scattering matrix. Section 3 provides technical tools for the recursive Sherman-Morrison factorization. In Sections 4 and 5, we re-establish the formulae of merging and splitting using the Sherman-Morrison formula. Section 6 applies the techniques and results developed in the preceding sections to a variational calculation directly useful for the efficient numerical solution of the inverse scattering problem for the Helmholtz equation.

2. Mathematical preliminaries

In this section, we introduce the scattering matrix, define several linear operators associated with the Lippmann-Schwinger equation, and provide an explicit expression for calculating the scattering matrix in terms of these linear operators. We also present the Woodbury Formula, more commonly known as the Sherman-Morrison formula, for inverting a linear operator that is a sum of an invertible operator and a low rank outer product.

2.1. Scattering matrix

Let ϕ represent the incident field to the scatterer supported by the domain D, and let ψ represent the scattered field from the scatterer. The scattered field ψ depends linearly on the

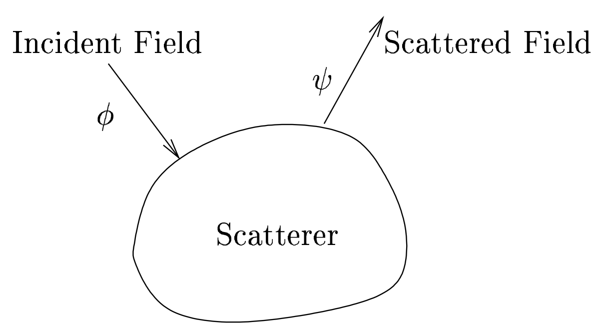

Figure 1. Geometry of wave scattering

given incident field ϕ and the linear map from the pair of the incident field and its normal derivative to the pair of the scattered field and its normal derivative is called *scattering matrix* , defined by the formula

$$\left(\psi, \frac{\partial \psi}{\partial n}\right) = S\left(\phi, \frac{\partial \phi}{\partial n}\right). \tag{1}$$

The pair of the incident field and its derivative will be referred to as *the incident pair* and the pair of the scattered field and its derivative will be referred as *the scattered pair.*

The scattering matrix, S, can be obtained in terms of the scatterer q [1] and of the following three mappings

(i) Linear mapping, G_{vb}, from the incident pair (ϕ, ϕ_n) on the boundary of D to the incident field inside D, defined by

$$G_{vb}(u,v) = \int_{\partial D} \left(v(\xi)G(x,\xi) - u(\xi)\frac{\partial G(x,\xi)}{\partial n(\xi)} \right) ds(\xi) \tag{2}$$

(ii) Linear mapping G_{vv} defined by

$$G_{vv}(\sigma)(x) = \int_D G(x,\xi)\sigma(\xi)d\xi, \tag{3}$$

so that the Lippmann-Schwinger equation

$$\sigma(x) + k^2 q(x) \int_D G(x,\xi)\sigma(\xi)d\xi = -k^2 q(x)\phi(x). \tag{4}$$

can be rewritten as

$$(I - \alpha\, G_{vv})\,\sigma = \alpha\,\phi \tag{5}$$

where

$$\alpha(x) = -k^2 q(x) \tag{6}$$

(iii) Linear mapping G_{bv} from the charge density σ inside D to the scattered pair on the boundary of D, defined by

$$G_{bv}(\sigma)(x) = \int_D \left(G(x,\xi), \frac{\partial G(x,\xi)}{\partial n(x)} \right) \sigma(\xi)d\xi. \tag{7}$$

It follows from the definition of the scattering matrix S that

$$S = G_{bv} \cdot (I - \alpha\, G_{vv})^{-1} \cdot \alpha \cdot G_{vb}. \tag{8}$$

The operators G_{vb}, G_{vv}, G_{bv} will be referred to as *the Green operators.* Obviously, the Green operators are translational invariant.

2.2. Sherman-Morrison formula

Let A, U, V be bounded linear operators. Then

$$(A + UV^T)^{-1} = A^{-1} - A^{-1}U(I + V^T A^{-1}U)^{-1}V^T A^{-1} \tag{9}$$

provided that A and $I + V^T A^{-1} U$ are invertible.

3. Factorizations of G_{vb}, G_{bv}, G_{vv}

As building blocks to the merging and scattering formula, we develop in this section recursive factorizations of G_{vb}, G_{vv}, G_{bv}. Let the domain D be partitioned into m non-overlapping subdomains D_i, $i = 1, \cdots, m$ so that $D = \cup D_i$ (see Figure 2), and let $\tilde{G}_{vb}, \tilde{G}_{vv}, \tilde{G}_{bv}$ be the Green operators for D_i, defined by

$$\tilde{G}_{vb}(u,v) = \int_{\partial D_i} \left(v(\xi)G(x,\xi) - u(\xi)\frac{\partial G(x,\xi)}{\partial n(\xi)} \right) ds(\xi), \tag{10}$$

$$\tilde{G}_{vv}(\sigma)(x) = \int_{D_i} G(x,\xi)\sigma(\xi)d\xi, \tag{11}$$

$$\tilde{G}_{bv}(\sigma)(x) = \int_{D_i} \left(G(x,\xi), \frac{\partial G(x,\xi)}{\partial n(x)} \right) \sigma(\xi)d\xi. \tag{12}$$

In the following subsections, we develop recursive factorizations for the Green operators such that the Green operators for the parent domain are decomposed into product of the Green operators for the subdomains.

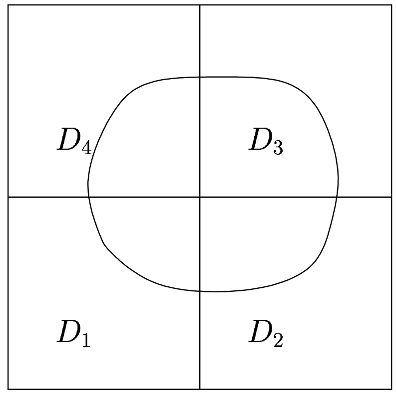

Figure 2. Domain partition: $D = D_1 \cup D_2 \cup D_3 \cup D_4$.

3.1. Factorization of G_{vb}

The operator G_{vb}, mapping the incident pair on the boundary of D to the incident field inside D, is a composition of the following operations.

(i) The incident pair on the boundary of D uniquely determines the incident pair on the boundary of each subdomain D_i, $i = 1, \cdots, m$

(ii) The incident pair on the boundary of each subdomain uniquely determines the incident field inside the subdomain.

Lemma 3.1 *Let R_i be the restriction operator mapping the incident pair on the boundary of D to the incident pair on the boundary of D_i, defined by*

$$R_i(u,v)(x) = \int_{\partial D} \left[v(\xi) \left(G, \frac{\partial G}{\partial n_x} \right) - u(\xi) \left(\frac{\partial G(x,\xi)}{\partial n_\xi} \frac{\partial^2 G(x,\xi)}{\partial n_x \partial n_\xi} \right) \right] ds(\xi). \quad (13)$$

Then

$$G_{vb} = \{\tilde{G}_{vb}\} \begin{bmatrix} R_1 \\ R_2 \\ \vdots \\ R_m \end{bmatrix}, \quad where \{\tilde{G}_{vb}\} =: \begin{bmatrix} \tilde{G}_{vb} & 0 & \cdots & 0 \\ 0 & \tilde{G}_{vb} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & \tilde{G}_{vb} \end{bmatrix}. \quad (14)$$

3.2. Factorization of G_{bv}

The linear map G_{bv}, mapping the charge density inside D to the scattered pair on the boundary of D, is a composition of the following operations.

(i) The charge density inside each subdomain D_i uniquely determines the scattered pair on the boundary of the subdomain

(ii) The scattered pairs on the boundaries of the subdomains D_i, $i = 1, \cdots, m$ uniquely determine the scattered pair on the domain D.

Lemma 3.2 *Let E_i be the extension operator mapping the scattered pair on the boundary of D_i to the scattered pair the boundary of D, defined by*

$$E_i(u,v)(x) = -\int_{\partial D_i} \left[v(\xi) \left(G, \frac{\partial G}{\partial n_x} \right) - u(\xi) \left(\frac{\partial G(x,\xi)}{\partial n_\xi}, \frac{\partial^2 G(x,\xi)}{\partial n_x \partial n_\xi} \right) \right] ds(\xi). \quad (15)$$

Then

$$G_{bv} = \begin{bmatrix} E_1 & E_2 & \cdots & E_m \end{bmatrix} \{\tilde{G}_{bv}\}, \tag{16}$$

where

$$\{\tilde{G}_{bv}\} =: \begin{bmatrix} \tilde{G}_{bv} & 0 & \cdots & 0 \\ 0 & \tilde{G}_{bv} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & \tilde{G}_{bv} \end{bmatrix}. \tag{17}$$

3.3. Factorization of G_{vv}

Let $(G_{vv})_{ij}$ be the linear mapping the charge density inside D_j to the incident field inside D_i, defined by

$$(G_{vv})_{ij}(\sigma)(x) = \int_{D_i} G(x,\xi)\sigma(\xi)d\xi, \quad x \in D_i, \tag{18}$$

and let $\{(G_{vv})_{ij}\}_{i,j=1}^m$ be a block partition of the operator G_{vv} introduced by (18). Then, the linear map $(G_{vv})_{ii}$ is equal to $\tilde{G}_{vv}$ by definition, and the linear map $(G_{vv})_{ij}$, $i \neq j$, mapping the charge density inside D_j to the incident field inside D_i, is a composition of the following operations.

(i) The charge density inside D_j uniquely determines the scattered pair on the boundary of D_j

(ii) The scattered pair on the boundary of D_j uniquely determines the incident pair on the boundary of D_i

(iii) The incident pair on the boundary of D_i uniquely determines the incident field inside D_i

Lemma 3.3 *Let T_{ij} be the translation operator, mapping the scattered pair on the boundary of D_j to the incident pair on D_i, defined by*

$$T_{ij}(u,v)(x) = -\int_{\partial D_j} \left[v(\xi)\left(G, \frac{\partial G}{\partial n_x}\right) - u(\xi)\left(\frac{\partial G(x,\xi)}{\partial n_\xi}, \frac{\partial^2 G(x,\xi)}{\partial n_x \partial n_\xi}\right)\right] ds(\xi). \tag{19}$$

Then

$$(G_{vv})_{ij} = \begin{cases} \tilde{G}_{vb} T_{ij} \tilde{G}_{bv}, & i \neq j, \\ \tilde{G}_{vv}, & i = j. \end{cases} \tag{20}$$

Remark 3.4 *The factorizations of G_{bv}, G_{vb}, G_{vv} are recursive in nature; the operators $\tilde{G}_{bv}, \tilde{G}_{vb}, \tilde{G}_{vv}$ can be factorized in the same manner as the subdomains are further refined.*

4. Merging formula for the scattering matrices

In this section, we develop the merging formula for the scattering matrices based on factorizations of the operators G_{vv}, G_{bv}, and G_{vb} provided in Section 3. The linchpin in our approach is the Sherman-Morrison formula, whereas the target of this development is the scattering matrix: To calculate the scattering matrix of a scatterer by merging the scattering matrices of its subscatterers.

Theorem 4.1 (Merging Formula) *Let S be the scattering matrix for D given in (8), let α_i be the restriction of α on the subdomain D_i, and let S_i be the scattering matrix for subdomain D_i. Furthermore, let*

$$[T_{ij}] = \begin{bmatrix} 0 & T_{12} & \cdots & T_{1m} \\ T_{21} & 0 & \cdots & T_{2m} \\ \cdots & \cdots & \cdots & \cdots \\ T_{m1} & T_{m2} & \cdots & 0 \end{bmatrix}, \quad \{S_i\} = \begin{bmatrix} S_1 & 0 & \cdots & 0 \\ 0 & S_2 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & S_m \end{bmatrix}. \tag{21}$$

Then

$$S = \begin{bmatrix} E_1 & E_2 & \cdots & E_m \end{bmatrix} \{S_i\} \Big(I - [T_{ij}]\{S_i\} \Big)^{-1} \begin{bmatrix} R_1 \\ R_2 \\ \vdots \\ R_m \end{bmatrix}. \tag{22}$$

The proof of the merging formula (22) is technical, and is organized in the following two lemmas, where the critical step is to establish a factorization of $(I - \alpha\, G_{vv})^{-1}$ using Sherman-Morrison formula.

Lemma 4.2

$$I - \alpha\, G_{vv} = \{I_i - \alpha_i \tilde{G}_{vv}\} - \{\alpha_i\}\{\tilde{G}_{vb}\}[T_{ij}]\{\tilde{G}_{bv}\} \tag{23}$$

Proof. Separating G_{vv} in diagonal and off-diagonal blocks

$$\begin{aligned} G_{vv} &= \{(G_{vv})_{ii}\} + [(G_{vv})_{ij}] \\ &= \{\tilde{G}_{vv}\} + [\tilde{G}_{vb} T_{ij} \tilde{G}_{bv}] \quad \text{(By Lemma 3.3)} \\ &= \{\tilde{G}_{vv}\} + \{\tilde{G}_{vb}\}[T_{ij}]\{\tilde{G}_{bv}\} \end{aligned} \tag{24}$$

we obtain

$$\begin{aligned} I - \alpha\, G_{vv} &= \{I_i\} - \{\alpha_i\}\Big(\{\tilde{G}_{vv}\} + \{\tilde{G}_{vb}\}[T_{ij}]\{\tilde{G}_{bv}\}\Big) \\ &= \{I_i\} - \{\alpha_i\}\{\tilde{G}_{vv}\} - \{\alpha_i\}\{\tilde{G}_{vb}\}[T_{ij}]\{\tilde{G}_{bv}\} \\ &= \{I_i - \alpha_i \tilde{G}_{vv}\} - \{\alpha_i\}\{\tilde{G}_{vb}\}[T_{ij}]\{\tilde{G}_{bv}\}. \end{aligned} \tag{25}$$

Lemma 4.3

$$\begin{aligned} (I_i - \alpha_i \tilde{G}_{vv})^{-1} = \{I_i - \alpha_i \tilde{G}_{vv}\}^{-1} + \{I_i - \alpha_i \tilde{G}_{vv}\}^{-1}\{\alpha_i\}\{\tilde{G}_{vb}\} \times \\ \Big(I - [T_{ij}]\{\tilde{G}_{bv}\}\{I_i - \alpha_i \tilde{G}_{vv}\}^{-1}\{\alpha_i\}\{\tilde{G}_{vb}\} \Big)^{-1} \times \\ [T_{ij}]\{\tilde{G}_{bv}\}\{I_i - \alpha_i \tilde{G}_{vv}\}^{-1}. \end{aligned} \tag{26}$$

Proof. Apply Sherman-Morrison formula (9) to the right hand side of (23) with

$$A = \{I_i - \alpha_i \tilde{G}_{vv}\}, \quad U = -\{\alpha_i\}\{\tilde{G}_{vb}\}, \quad V^T = [T_{ij}]\{\tilde{G}_{bv}\}. \tag{27}$$

Now, we complete the proof of the merging formula (22) by applying Lemmas lem-decomp and 4.3 to (8). Indeed, substituting (14), (16), (26) into (8) we obtain

$$\begin{aligned} S &= [E_1 \cdots E_m]\, \{\tilde{G}_{bv}\}(I - \alpha\, G_{vv})^{-1} \alpha\, \{\tilde{G}_{vb}\}\, [R_1^T \cdots R_m^T]^T \\ &= [E_1 \cdots E_m]\, \{\tilde{G}_{bv}\}\{I_i - \alpha_i \tilde{G}_{vv}\}^{-1} \alpha\, \{\tilde{G}_{vb}\}\, [R_1^T \cdots R_m^T]^T \\ &\quad + [E_1 \cdots E_m]\, \{\tilde{G}_{bv}\}\{I_i - \alpha_i \tilde{G}_{vv}\}^{-1}\, \{\alpha_i\}\{\tilde{G}_{vb}\} \times \end{aligned}$$

$$\left(I - [T_{ij}]\{\tilde{G}_{bv}\}\{I_i - \alpha_i \tilde{G}_{vv}\}^{-1}\{\alpha_i\}\{\tilde{G}_{vb}\}\right)^{-1} \times$$
$$[T_{ij}]\{\tilde{G}_{bv}\}\{I_i - \alpha_i \tilde{G}_{vv}\}^{-1}\alpha\,\{\tilde{G}_{vb}\}\,[R_1^T \cdots R_m^T]^T$$
$$= [E_1 \cdots E_m]\,\{\tilde{G}_{bv}\}(I - \alpha\, G_{vv})^{-1}\alpha\,\{\tilde{G}_{vb}\} \times$$
$$\left(I - [T_{ij}]\{\tilde{G}_{bv}\}\{I_i - \alpha_i \tilde{G}_{vv}\}^{-1}\{\alpha_i\}\{\tilde{G}_{vb}\}\right)^{-1} \times [R_1^T \cdots R_m^T]^T \tag{28}$$

Thus the merging formula (22) follows immediately from the definition of the scattering matrix

$$\{S_i\} = \{\tilde{G}_{bv}\}\{I_i - \alpha_i \tilde{G}_{vv}\}^{-1}\{\alpha_i\}\{\tilde{G}_{vb}\} \tag{29}$$

5. Splitting formula

In order to establish the splitting formula, we consider the solution σ of the Lippmann-Schwinger equation

$$(I - \alpha\, G_{vv})\sigma(x) = \alpha\, \phi(x), \quad x \in D, \tag{30}$$

given by the formula

$$\sigma = (I - \alpha\, G_{vv})^{-1}\alpha\, \phi.$$
$$= (I - \alpha\, G_{vv})^{-1}\, \alpha\, G_{bv}(\phi, \phi_n). \tag{31}$$

Theorem 5.1 (Splitting Formula) *Let Σ be the linear mapping the incident pair on ∂D to the solution of the Lippmann-Schwinger equation inside D, and let Σ_i be the linear mapping the incident pair on ∂D_i to the solution of the Lippmann-Schwinger equation inside D_i, defined by*

$$\Sigma \quad = (I - \alpha\, G_{vv})^{-1}\alpha\, G_{bv}, \tag{32}$$
$$\{\Sigma_i\} = \{I_i - \alpha_i \tilde{G}_{vv}\}^{-1}\{\alpha_i\}\{\tilde{G}_{bv}\}. \tag{33}$$

Then

$$\Sigma = \{\Sigma_i\}\left(I - [T_{ij}]\{S_i\}\right)^{-1} \left[\begin{array}{ccc} R_1^T & \ldots & R_m^T \end{array}\right]^T. \tag{34}$$

Proof. Substituting (2), (26) into (32) yields

$$\Sigma = (I - \alpha\, G_{vv})^{-1}\alpha\,\{\tilde{G}_{vb}\}\,[R_1^T \cdots R_m^T]^T$$
$$= \{I_i - \alpha_i \tilde{G}_{vv}\}^{-1}\alpha\,\{\tilde{G}_{vb}\}\,[R_1^T \cdots R_m^T]^T + \{I_i - \alpha_i \tilde{G}_{vv}\}^{-1}\,\{\alpha_i\}\{\tilde{G}_{vb}\} \times$$
$$\left(I - [T_{ij}]\{\tilde{G}_{bv}\}\{I_i - \alpha_i \tilde{G}_{vv}\}^{-1}\{\alpha_i\}\{\tilde{G}_{vb}\}\right)^{-1} \times$$
$$[T_{ij}]\{\tilde{G}_{bv}\}\{I_i - \alpha_i \tilde{G}_{vv}\}^{-1}\alpha\,\{\tilde{G}_{vb}\}\,[R_1^T \cdots R_m^T]^T$$
$$= \{I_i - \alpha_i \tilde{G}_{vv}\}^{-1}\alpha\,\{\tilde{G}_{vb}\} \times$$
$$\left(I - [T_{ij}]\{\tilde{G}_{bv}\}\{I_i - \alpha_i \tilde{G}_{vv}\}^{-1}\{\alpha_i\}\{\tilde{G}_{vb}\}\right)^{-1} \times [R_1^T \cdots R_m^T]^T$$
$$= \{\Sigma_i\}\left(I - [T_{ij}]\{S_i\}\right)^{-1}\,[R_1^T \cdots R_m^T]^T. \tag{35}$$

6. Recursive Sherman-Morrison for perturbations

The variational calculations related to the Helmholtz equation is necessary for the linearization of the inverse problem, whereas their efficient computation is critical to numerical inversion. A standard variational calculation computes the perturbation of the scattering data – the scattering matrix – due to a perturbation of the scatterer q, or its scaled version α. In other words, we wish to efficiently compute the Frechet derivative for linearization, and invert it for inversion.

In this section, we address the issue of efficient calculation of variations (37) and (38) by applying the technique of recursive Sherman-Morrison factorization which we have developed in the preceding sections. The formulae we provide here for efficient calculation of variations, which appears to have not been established elsewhere, play a similar role to the merging and splitting formulae for efficient solution of the Lippmann-Schwinger equation. Their derivations are purely algebraic, and thus avoid appealing directly to the underlying multiple scattering process [1] which becomes difficult here due to the algebraic complexity of the variational calculation (37) and (38).

Let $\mathcal{L}_\alpha$ be the variational, or Frechet, derivative of the scattering matrix $S(\alpha)$ with respect to the rescaled scatterer α so that

$$\delta S = \mathcal{L}_\alpha(\delta\alpha) + O((\delta\alpha)^2). \tag{36}$$

The explicit expressions of the derivative $\mathcal{L}_\alpha$ and its conjugate $\mathcal{L}_\alpha^*$ can be obtained by applying standard variational calculus to (8)

$$\begin{aligned}\mathcal{L}_\alpha(\delta\alpha) &= G_{bv}(I - \alpha\, G_{vv})^{-1}(\delta\alpha)(I + G_{vv}(I - \alpha\, G_{vv})^{-1}\alpha)G_{vb}\\ &= G_{bv}(I - \alpha\, G_{vv})^{-1}(\delta\alpha)(I - G_{vv}\alpha)^{-1}G_{vb},\end{aligned} \tag{37}$$

$$\mathcal{L}_\alpha^*(\delta S) = diag\left(\left(G_{bv}(I - \alpha\, G_{vv})^{-1}\right)^* \delta S \left((I - G_{vv}\alpha)^{-1}G_{vb}\right)^*\right). \tag{38}$$

Remark 6.1 *The operator (37) is required in the standard linearization step for the solution of the inverse problem, whereas its conjugation (38) is required when we solve the linear system*

$$\delta S = \mathcal{L}_\alpha(\delta\alpha) \tag{39}$$

for $\delta\alpha$ iteratively via the conjugate gradient method applied to the normal equation.

Numerical computation for $\mathcal{L}_\alpha(\delta\alpha)$ and (38) is prohibitive – it requires inverting operators such as $(I - \alpha\, G_{vv})$. Theorems 6.2 and 6.3 provide procedures necessary for efficient calculations of (37) and (38). These procedures algebraically resemble those of merging and splitting of Sections 4, 5, and will be so referred to.

Theorem 6.2 (Merging formula for perturbation of scattering matrix) *Let $\delta\alpha_i$ be the restriction of $\delta\alpha$ on the i-th subdomain, and let $\tilde{\mathcal{L}}_{\alpha_i}$ be the variational derivative of S_i, defined by*

$$\tilde{\mathcal{L}}_{\alpha_i}(\delta\alpha_i) = \tilde{G}_{bv}(I_i - \alpha_i\tilde{G}_{vv})^{-1}(\delta\alpha_i)(I_i - \tilde{G}_{vv}\alpha_i)^{-1}\tilde{G}_{vb}. \tag{40}$$

Then

$$\begin{aligned}\mathcal{L}_\alpha(\delta\alpha) = \begin{bmatrix} E_1 & \cdots & E_m \end{bmatrix} \Big(I - \{S_i\}[T_{ij}]\Big)^{-1}\{\tilde{\mathcal{L}}_{\alpha_i}(\alpha_i)\} \times \\ \Big(I - [T_{ij}]\{S_i\}\Big)^{-1} \begin{bmatrix} R_1^T & \cdots & R_m^T \end{bmatrix}^T\end{aligned} \tag{41}$$

Theorem 6.3 (**Splitting formula for the conjugate operation**) *Let $\mathcal{L}^*_{\alpha_i}$ be defined by*

$$\mathcal{L}^*_{\alpha_i}(\delta S_i) = diag\left(\left(\tilde{G}_{bv}(I_i - \alpha_i\tilde{G}_{vv})^{-1}\right)^* \delta S_i \left((I_i - \tilde{G}_{vv}\alpha_i)^{-1}\tilde{G}_{vb}\right)^*\right), \qquad (42)$$

and let $\mathcal{L}^*_\alpha(\delta S)|_{D_i}$ be the restriction of $\mathcal{L}^*_\alpha(\delta S)$ on the i-th subdomain. Then

$$\mathcal{L}^*_\alpha(\delta S)|_{D_i} = \tilde{\mathcal{L}}^*_{\alpha_i}([S_p(\delta S)]_{ii}), \qquad (43)$$

where

$$S_p(\delta S) = \left(\begin{bmatrix} E_1 & \cdots & E_m \end{bmatrix} \left(I - \{S_i\}[T_{ij}]\right)^{-1}\right)(\delta S) \times \left(\left(I - [T_{ij}]\{S_i\}\right)^{-1} \begin{bmatrix} R_1^T & \cdots & R_m^T \end{bmatrix}^T\right), \qquad (44)$$

and $[S_p(\delta S)]_{ii}$ is the i-th diagonal block of $S_p(\delta S)$.

The proofs of Theorems 6.2 and 6.3 are organized in the following two lemmas, where the critical step is to establish recursive factorizations for $G_{bv}(I - \alpha\, G_{vv})^{-1}$ and $(I - G_{vv}\alpha)^{-1}G_{vb}$.

Lemma 6.4

$$G_{bv}(I - \alpha\, G_{vv})^{-1} = \begin{bmatrix} E_1 & \cdots & E_m \end{bmatrix} \left(I - \{S_i\}[T_{ij}]\right)^{-1} \{\tilde{G}_{bv}\}\{I - \alpha_i\tilde{G}_{vv}\}^{-1} \qquad (45)$$

Proof. It follows from (26) and Lemma 3.2 that

$$\begin{aligned} G_{bv}\,(I - \alpha\, G_{vv})^{-1} &= [E_1 \cdots E_m]\,\{\tilde{G}_{bv}\}(I - \alpha\, G_{vv})^{-1} \\ &= [E_1 \cdots E_m]\,\{\tilde{G}_{bv}\}\{I_i - \alpha_i\tilde{G}_{vv}\}^{-1} + [E_1 \cdots E_m]\{\tilde{G}_{bv}\} \times \\ &\quad \{I_i - \alpha_i\tilde{G}_{vv}\}^{-1}\,\{\alpha_i\}\{\tilde{G}_{vb}\} \times \\ &\quad \left(I - [T_{ij}]\{\tilde{G}_{bv}\}\{I_i - \alpha_i\tilde{G}_{vv}\}^{-1}\{\alpha_i\}\{\tilde{G}_{vb}\}\right)^{-1} \times \\ &\quad [T_{ij}]\{\tilde{G}_{bv}\}\{I_i - \alpha_i\tilde{G}_{vv}\}^{-1} \\ &= [E_1 \cdots E_m]\,\{\tilde{G}_{bv}\}\{I_i - \alpha_i\tilde{G}_{vv}\}^{-1} + [E_1 \cdots E_m] \times \\ &\quad \{S_i\}\left(I - [T_{ij}]\{S_i\}\right)^{-1}[T_{ij}]\{\tilde{G}_{bv}\}\{I_i - \alpha_i\tilde{G}_{vv}\}^{-1} \\ &= [E_1 \cdots E_m]\left(I + \{S_i\}\left(I - [T_{ij}]\{S_i\}\right)^{-1}[T_{ij}]\right) \times \\ &\quad \{\tilde{G}_{bv}\}\{I_i - \alpha_i\tilde{G}_{vv}\}^{-1} \\ &= [E_1 \cdots E_m]\left(I - \{S_i\}[T_{ij}]\right)^{-1}\{\tilde{G}_{bv}\}\{I_i - \alpha_i\tilde{G}_{vv}\}^{-1}. \end{aligned} \qquad (46)$$

Lemma 6.5

$$(I + G_{vv}(I - \alpha\, G_{vv})^{-1}\alpha)G_{vb} = (I + \{\tilde{G}_{vv}\}\{I - \alpha_i\tilde{G}_{vv}\}^{-1}\{\alpha_i\})\{\tilde{G}_{vb}\} \times \left[I - [T_{ij}]\{S_i\}\right]^{-1} \begin{bmatrix} R_1^T & \cdots & R_m^T \end{bmatrix}^T. \qquad (47)$$

Proof. The splitting formula (34) implies that

$$\begin{aligned} &(I - \alpha\, G_{vv})^{-1}\alpha\, G_{vb} \\ &= \{I_i - \alpha_i\tilde{G}_{vv}\}^{-1}\{\alpha_i\}\{\tilde{G}_{vb}\}\left(I - [T_{ij}]\{S_i\}\right)^{-1}[R_1^T \cdots R_m^T]^T. \end{aligned} \qquad (48)$$

Substitute (48) into (47) and separate G_{vv} into diagonal and off-diagonal parts by writing $G_{vv} = \{\tilde{G}_{vv}\} + [G_{vv}]$, and we obtain

$$\begin{aligned}(I + G_{vv}(I - \alpha\, G_{vv})^{-1}\alpha)G_{vb} &= \{\tilde{G}_{vb}\}\,[R_1^T \cdots R_m^T]^T \\ &+ \{\tilde{G}_{vv}\}\{I_i - \alpha_i\tilde{G}_{vv}\}^{-1}\{\alpha_i\}\{\tilde{G}_{vb}\}\Big(I - [T_{ij}]\{S_i\}\Big)^{-1}[R_1^T \cdots R_m^T]^T \\ &+ [G_{vv}]\{I_i - \alpha_i\tilde{G}_{vv}\}^{-1}\{\alpha_i\}\{\tilde{G}_{vb}\}\Big(I - [T_{ij}]\{S_i\}\Big)^{-1}[R_1^T \cdots R_m^T]^T \end{aligned} \tag{49}$$

With $[G_{vv}] = \{\tilde{G}_{vb}\}[T_{ij}]\{\tilde{G}_{bv}\}$, the last term on the right hand side of (49) can be written as

$$\begin{aligned}&[G_{vv}]\{I_i - \alpha_i\tilde{G}_{vv}\}^{-1}\{\alpha_i\}\{\tilde{G}_{vb}\}\Big(I - [T_{ij}]\{S_i\}\Big)^{-1}[R_1^T \cdots R_m^T]^T \\ &= \{\tilde{G}_{vb}\}[T_{ij}]\{\tilde{G}_{bv}\}\{I_i - \alpha_i\tilde{G}_{vv}\}^{-1}\{\alpha_i\}\{\tilde{G}_{vb}\}\Big(I - [T_{ij}]\{S_i\}\Big)^{-1}[R_1^T \cdots R_m^T]^T \\ &= \{\tilde{G}_{vb}\}[T_{ij}]\{S_i\}\Big(I - [T_{ij}]\{S_i\}\Big)^{-1}[R_1^T \cdots R_m^T]^T \end{aligned} \tag{50}$$

The first two terms of the right hand side of (49) can be further simplified

$$\begin{aligned}&\{\tilde{G}_{vb}\}\,[R_1^T \cdots R_m^T]^T + \{\tilde{G}_{vb}\}[T_{ij}]\{S_i\}\Big(I - [T_{ij}]\{S_i\}\Big)^{-1}[R_1^T \cdots R_m^T]^T \\ &= \{\tilde{G}_{vb}\}\left(I + [T_{ij}]\{S_i\}\Big(I - [T_{ij}]\{S_i\}\Big)^{-1}\right)[R_1^T \cdots R_m^T]^T \\ &= \{\tilde{G}_{vb}\}\Big(I - [T_{ij}]\{S_i\}\Big)^{-1}[R_1^T \cdots R_m^T]^T \end{aligned} \tag{51}$$

Thus, substituting (50) and (51) into (49) we obtain

$$\begin{aligned}(I + G_{vv}(I - \alpha\, G_{vv})^{-1}\alpha)G_{vb} &= \{\tilde{G}_{vb}\}\Big(I - [T_{ij}]\{S_i\}\Big)^{-1}[R_1^T \cdots R_m^T]^T \\ &+ \{\tilde{G}_{vv}\}\{I_i - \alpha_i\tilde{G}_{vv}\}^{-1}\{\alpha_i\}\{\tilde{G}_{vb}\}\Big(I - [T_{ij}]\{S_i\}\Big)^{-1}[R_1^T \cdots R_m^T]^T \\ &= (I + \{\tilde{G}_{vv}\}\{I_i - \alpha_i\tilde{G}_{vv}\}^{-1}\{\alpha_i\})\{\tilde{G}_{vb}\}\Big(I - [T_{ij}]\{S_i\}\Big)^{-1}[R_1^T \cdots R_m^T]^T \end{aligned} \tag{52}$$

Theorems 6.2 and 6.3 follow immediately from (45), (37), and (47), (38).

Remark 6.6 *Theorems 6.2 and 6.3 enable efficient calculations of the variational quantities (37) and (38) by recursively traversing up and down a hierarchy of subdomains of the scatterer; see [1] for more details. For an m-by-m wavelength, two dimensional calculation, it requires $O(m^3)$ flops to evaluate (37) and (38); in other words, the evaluation of the Frechet derivative and its conjugation costs $O(m^3)$ flops. This procedure has been implemented numerically, and found useful for the numerical solution of the inverse problem. We will present it in a separate paper.*

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