DISCRETE AND CONTINUOUS
DYNAMICAL SYSTEMS
Volume **18**, Number **4**, August **2007**

Website: http://aimSciences.org

pp. **627–636**

RAPID PERTURBATIONAL CALCULATIONS FOR THE HELMHOLTZ EQUATION IN TWO DIMENSIONS

Sang-Yeun Shim

Courant Institute of Mathematical Sciences, New York University
251 Mercer Street
New York, NY 10012-1110

Marcos Capistran

Centro de Investigación en Matemáticas, CIMAT A. C.
Jalisco s/n, Mineral de Valenciana, C.P. 36240, Guanajuato
Guanajuato, Mexico

Yu Chen

Courant Institute of Mathematical Sciences, New York University
251 Mercer Street
New York, NY 10012-1110

Abstract. Existing approaches to the solution of the inverse scattering problems in two and three dimensions rely on linearization of the Helmholtz equation, which requires the knowledge of the Fréchet derivative of the far field with respect to the index of refraction. We present an efficient algorithm for this perturbational calculation in two dimensions. Our method is based on the merging and splitting procedures already established for the solution of the Lippmann-Schwinger equation [2], [3], [4]. For an m-by-m wavelength problem, the algorithm obtains perturbations to scattered waves for m distinct incident waves in $O(m^3)$ steps.

1. **Introduction.** Given a well-posed boundary value problem for an elliptic PDE in a bounded domain D, the Fréchet derivative of the solution with respect to the coefficients of the equation is an object of interest in the linearization of inverse problems of the PDE. When the inverse problem is reducible to solving a sequence of linear problems, it is this Fréchet matrix whose construction and inversion will require the bulk of the computation.

Given a positive wave number k and continuous function q in domain D, we consider the scattering problem

$$\Delta v + k^2(1+q)\,v = -k^2 u \tag{1}$$

in a subdomain $\Omega \subset D$, where q is set to zero outside Ω. Arising from a given (total) incident wave u, the solution v of the Helmholtz equation (1) is the scattered wave subject to the Sommerfeld radiation condition. When $\Omega = D$, we will denote by u_0 and v_0 the incident and scattered waves. Let G be the fundamental solution

$$G(x,\xi) = \frac{i}{4} H_0(k\|x-\xi\|) \tag{2}$$

2000 *Mathematics Subject Classification.* Primary: 65R20, 49N45; Secondary: 45Q05.
Key words and phrases. scattering matrix, merging formulae, fast direct algorithms.
The first author was affiliated with Courant Institute, New York University.

of the Helmholtz equation. The incident wave u_0 arises from sources outside D; therefore [1],

$$u_0(x) = \int_{\partial D} G(x,\xi)\alpha_0(\xi)ds(\xi), \quad x \in D \tag{3}$$

where α_0 is the density of equivalent monopoles on the boundary ∂D, to be referred to as the incident source to D. As is well-known, the scattering problem for D can be reformulated as the Lippmann-Schwinger integral equation

$$\beta_0(x) - a(x)\int_D G(x,\xi)\beta_0(\xi)d\xi = a(x)u_0, \tag{4}$$

where $a(x) = -k^2q(x)$ will be also referred to as the scatterer, and the monopole density β_0 in D gives rise to the scattered wave $v_0(x)$

$$v_0(x) = \int_D G(x,\xi)\beta_0(\xi)d\xi, \quad x \in \mathbb{R}^2. \tag{5}$$

The linearization for the inverse scattering problem requires solution of linear equations with the Fréchet derivatives such as $\partial v/\partial a$ as the matrix of the linear system. In two and three dimensions, direct inversion of the matrix is prohibitively expensive; standard iterative methods, such as GMRES or CGN, are the alternatives which require the matrix-vector multiplications.

In this paper we will present algorithms to efficiently compute the matrix-vector product. We will refer to these matrix-vector multiplications as perturbational calculations. More specifically, let $da = -k^2dq$ be the perturbation to a when q is perturbed by dq. There are two types of perturbational calculations we seek to perform: (i) compute the perturbations to β_0 and consequently to v_0 or its far field, for a given incident wave u_0 to D, and (ii) compute the perturbation to the scattering matrix S (see (9) for its definition) when all the incident waves are considered. We will present an algorithm that computes these perturbations in $O(m^3)$ steps for a m-by-m wavelength problem.

The paper is organized as follows. In §2 we introduce the calculation of perturbations, define the scattering matrix, and construct formulae for their direct, not fast, evaluations. §3 is devoted to a multiple scattering formalism for the perturbations. In §4 we establish the splitting and merging formulae for the perturbations. A fast algorithm is presented in §5 for the rapid computation of the perturbations. Further discussions of the algorithm are given in §6.

2. **The scattering matrix and its perturbation.**

We introduce the scattering matrix and its perturbation, and we examine their computations.

2.1. **The scattering matrix for a subdomain.**

Restricting the scatterer q in the subdomain Ω of D, we represent the incident wave u to Ω as

$$u(x) = \int_{\partial\Omega} G(x,\xi)\alpha(\xi)ds(\xi) := G^{(v,b)}\alpha, \quad x \in \Omega \tag{6}$$

via its equivalent monopole sources on $\partial\Omega$. Note that the superscript (v,b) is to indicate that the linear map $G^{(v,b)}$ is from "boundary" to "volume."

The corresponding scattered wave $v \in C(\mathbb{R}^2)$ can be written

$$v(x) = \int_\Omega G(x,\xi)\beta(\xi)d\xi, \quad x \in \mathbb{R}^2 \tag{7}$$

so that

$$v(x) = \int_\Omega G(x,\xi)\beta(\xi) := G^{(b,v)}\beta, \quad x \in \partial\Omega \tag{8}$$

where the superscript (b, v) is to indicate that the linear map is from "volume" to "boundary." We define the scattering matrix $S : C(\partial\Omega) \mapsto C(\partial\Omega)$ for Ω by the formula

$$v|_{\partial\Omega} = S\alpha. \tag{9}$$

This is a source-to-field definition at the fixed wave number k. Similar to (4), the monopole density β in Ω satisfies the Lippmann-Schwinger equation

$$P\,\beta = aG^{(v,b)}\alpha \tag{10}$$

in Ω, where $P : L_2(\Omega) \mapsto L_2(\Omega)$ are defined by

$$P = I - aG^{(v,v)}, \quad G^{(v,v)}(\beta)(x) = \int_\Omega G(x,\xi)\beta(\xi)d\xi. \tag{11}$$

Hence, the scattering matrix can be obtained by the formula

$$S = G^{(b,v)}P^{-1}aG^{(v,b)} \tag{12}$$

provided that the scattering problem in Ω is well posed, and thus P is invertible, which we will assume throughout the paper.

2.2. **Perturbation of the scattering matrix.** Given a subdomain Ω of D, let u be the total incident wave to Ω due to the original incident wave u_0 and the scattered wave $v|_{D\setminus\Omega}$ from the remainder of D, namely,

$$u = u_0 + v|_{D\setminus\Omega}, \quad \text{on } \Omega. \tag{13}$$

Remark 1. For the total incident wave u to Ω, with multiple scattering between Ω and $D \setminus \Omega$ taken into account, β of (10) is identical to β_0 of (4) restricted to Ω. In other words,

$$\beta = \beta_0|_\Omega. \tag{14}$$

Let the coefficient a be perturbed in D by da, and we define the corresponding perturbations to α, β, and S in Ω, not as the actual amount of change to them but as the differentials

$$d\beta = \frac{\partial\beta}{\partial a}da, \quad d\alpha = \frac{\partial\alpha}{\partial a}da, \quad dS = \frac{\partial S}{\partial a}da. \tag{15}$$

With the perturbation da, the total incident wave u in Ω is subject to change: da gives rise to perturbation to the scattered wave in D, resulting in a perturbation to u by (13). By (10),

$$P\,d\beta = da\big(G^{(v,b)}\alpha + G^{(v,v)}\,\beta\big) + a\,G^{(v,b)}d\alpha, \quad \text{on } \Omega. \tag{16}$$

Remark 2. When $\Omega = D$, the last term of (16) vanishes because $d\alpha_0 = 0$: the original incident source α_0 to D is fixed and thus not subject to change by da.

By (9), the perturbation to S satisfies

$$dv = dS\ \alpha + Sd\alpha, \tag{17}$$

where $dv = G^{(b,v)}d\beta$ due to (8). By (16),

$$dS = G^{(b,v)}P^{-1}da(1 + G^{(v,v)}P^{-1}a)G^{(v,b)}. \tag{18}$$

Remark 3. By (12) and (18), S and dS depend on the scatterer a and its perturbation da only inside Ω.

Given the coefficient $a = -k^2 q$ and the incident source α, β can be obtained by solving the well-posed second kind integral equation (10). For an m-by-m wavelength problem in a square domain D in two dimensions discretized by an $n \times n$ mesh with $n = O(m)$, the solution of (10) requires inverting P of size $n^2 \times n^2$. Standard methods such as LU-factorization of P requires $O(n^6)$ steps. Fast, recursive factorization of P exists [2], which is based on a merging and splitting mechanism in $O(n^3)$ steps; its back solving requires $O(n^2 \log n)$ steps to obtain a β for an incident wave. This fast factorization also constructs the scattering matrix S for D in $O(n^3)$ steps.

In the remainder of the paper we develop a merging and splitting apparatus for, among other things, a rapid matrix-vector multiplication

$$\frac{\partial S}{\partial a} da := G^{(b,v)} P^{-1} da (1 + G^{(v,v)} P^{-1} a) G^{(v,b)} \tag{19}$$

for the Fréchet matrix $\partial S/\partial a$ and an arbitrary vector da in $O(n^3)$ steps.

Remark 4. When a square domain D is discretized by an $n \times n$ mesh, there will be about $4n$ boundary points on the mesh; da on the left of (19) is a vector of size $n^2 \times 1$, whereas a and da on the right are diagonal matrices of size $n^2 \times n^2$. The matrix $\partial S/\partial a$ is $(4n)^2 \times n^2$; $G^{(b,v)}$ is $4n \times n^2$; P and $G^{(b,v)}$ are $n^2 \times n^2$; and $G^{(v,b)}$ is $n^2 \times 4n$. The matrix-vector multiplication by (19), even if P^{-1} is available as a $n^2 \times n^2$ matrix, will cost $O(n^6)$ steps.

3. Multiple scattering.

We establish a merging and splitting formalism, similar to that of [2], for the perturbational calculation (18). In other words, the merging and splitting formulae of [2] are useful for rapid solution of (10), whereas here our formulae to be developed will be used for rapid solution of (16). Throughout this section, perturbations of variables are all due to a perturbation da of a over D.

3.1. Analytical machinery.

Let Ω be a subdomain of D, consisting of m nonoverlapping scatterers in Ω_i with $\Omega = \cup_i \Omega_i$. A wave in the free space outside a domain A, arising from sources inside A, is referred to as an outgoing wave from A. We require the three operators

1. Restriction $R_i : C(\partial\Omega) \mapsto C(\partial\Omega_i)$, to map an incident source α on $\partial\Omega$ (see (6)) to that on $\partial\Omega_i$.
2. Extension $E_i : C(\partial\Omega_i) \mapsto C(\partial\Omega)$, to map the boundary value on $\partial\Omega_i$ of an outgoing wave v from Ω_i to that on $\partial\Omega$ of the same outgoing wave.
3. Translation $T_{ji} : C(\partial\Omega_i) \mapsto C(\partial\Omega_j)$, $i \neq j$, to map the boundary value on $\partial\Omega_i$ of an outgoing wave v from Ω_i to the incident monopole source α_j on $\partial\Omega_j$ for the same wave v in Ω_j, now regarded as an incident wave to Ω_j.

Remark 5. These three operators can be constructed, e.g., by solving standard boundary integral equations [1]. They are independent of the scatterer q, dependent only on the relative positions of Ω_i, Ω_j, and their parent Ω.

Denote by S, $dS : C(\partial\Omega) \mapsto C(\partial\Omega)$ the scattering matrices and its perturbation on Ω, and by S_i, $dS_i : C(\partial\Omega_i) \mapsto C(\partial\Omega_i)$ the scattering matrices and their perturbations on Ω_i. By (12) and (18),

$$S_i = G_i^{(b,v)} \cdot P_i^{-1} \cdot a_i \cdot G_i^{(v,b)} \tag{20}$$

$$dS_i = G_i^{(b,v)} \cdot P_i^{-1} \cdot da_i \cdot (1 + G_i^{(v,v)} P_{ii}^{-1} a_i) \cdot G_i^{(v,b)}, \tag{21}$$

where $G_i^{(v,b)} : C(\partial\Omega_i) \mapsto C(\Omega_i)$ is defined by

$$\big[G_i^{(v,b)}\alpha_i\big](x) = \int_{\partial\Omega_i} G(x,\xi)\alpha_i(\xi)ds(\xi) \tag{22}$$

and $G_i^{(b,v)} : L_2(\Omega_i) \mapsto L_2(\partial\Omega_i)$ is defined by

$$\big[G_i^{(b,v)}\,\beta\big](x) = \int_{\Omega_i} G(x,\xi)\beta(\xi)d\xi. \tag{23}$$

Let u be the total incident wave (due to u_0) to Ω, and let α be its equivalent incident source on $\partial\Omega$. Let β_i, $d\beta_i$, a_i, da_i be restrictions to Ω_i

$$\beta_i = \beta|_{\Omega_i}, \quad d\beta_i = d\beta|_{\Omega_i} \tag{24}$$

$$a_i = a|_{\Omega_i}, \quad da_i = da|_{\Omega_i}. \tag{25}$$

By Remark 1,

$$\beta_i = \beta|_{\Omega_i} = \beta_0|_{\Omega_i}. \tag{26}$$

Let α_{i0}, $d\alpha_{i0} \in C(\partial\Omega_i)$ be defined by

$$\alpha_{i0} = R_i\alpha, \quad d\alpha_{i0} = R_i d\alpha. \tag{27}$$

In the case of Ω containing two subscatterers Ω_1 and Ω_2, (10) and (16) are rewritten

$$\begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} a_1 G_1^{(v,b)}\alpha_{10} \\ a_2 G_2^{(v,b)}\alpha_{20} \end{bmatrix} \tag{28}$$

and

$$\begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix} \begin{bmatrix} d\beta_1 \\ d\beta_2 \end{bmatrix} = \begin{bmatrix} a_1 G_1^{(v,b)} d\alpha_{10} + da_1 G_1^{(v,b)}\alpha_{10} \\ a_2 G_2^{(v,b)} d\alpha_{20} + da_2 G_2^{(v,b)}\alpha_{20} \end{bmatrix} + \begin{bmatrix} da_1\big(G_{11}^{(v,v)}\beta_1 + G_{12}^{(v,v)}\beta_2\big) \\ da_2\big(G_{22}^{(v,v)}\beta_2 + G_{21}^{(v,v)}\beta_1\big) \end{bmatrix}, \tag{29}$$

where $P_{ji} : L_2(\Omega_i) \mapsto L_2(\Omega_j)$ is defined by

$$[P_{ji}\,\beta](x) := \big(\delta_{ji}I - a_j G_{ji}^{(v,v)}\big)\beta := \delta_{ji}\beta(x) - a_j(x)\int_{\Omega_i} G(x,\xi)\beta(\xi)d\xi. \tag{30}$$

3.2. **Multiple scattering between subscatterers.** Let $u_i \in C(\Omega_i)$ be the total incident wave (due to u_0) to Ω_i, and let $\alpha_i \in C(\partial\Omega_i)$ be the incident source. It follows immediately from (10) and (16), with Ω replaced by Ω_i, that

$$P_{ii}\ \beta_i = a_i G_i^{(v,b)}\alpha_i \tag{31}$$

$$P_{ii}\ d\beta_i = a_i G_i^{(v,b)} d\alpha_i + da_i\big(G_i^{(v,b)}\alpha_i + G_{ii}^{(v,v)}\,\beta_i\big). \tag{32}$$

Remark 6. There are two types, or descriptions, of the total incident wave u_i to Ω_i. The first is due to the total incident wave u to Ω, where u itself is due to u_0, with the multiple scattering in D accounted for; we will refer to the first type as due to u_0. The second is due to an arbitrary incident wave u to Ω standing alone; there is no multiple scattering coming from exterior of Ω, but there is multiple scattering among Ω_j, $j = 1 : m$, in Ω. For the first type, (26) holds, whereas for the second, only the first equality holds: $\beta_i = \beta|_{\Omega_i}$.

The knowledge of the total incident wave (due to u_0) to a subdomain allows us, by (31) and (32), to solve the scattering problem in the subdomain independently of the rest of D. The following definition is motivated by the idea of splitting: Determine α_i of Ω_i from α of the parent Ω.

Definition 3.1. Let $W_m = [C(\partial\Omega_1), C(\partial\Omega_2),\ \ldots,\ C(\partial\Omega_m)]$, and let the operators

$$T,\, T_s,\, dT_s : W_m \mapsto W_m, \quad R,\ S_p,\ dS_p : C(\partial D) \mapsto W_m \tag{33}$$

be defined by the formulae

$$T = \begin{bmatrix} 0 & -T_{12} & \cdots & -T_{1m} \\ -T_{21} & 0 & \cdots & -T_{2m} \\ \vdots & \vdots & \cdots & \vdots \\ -T_{m1} & -T_{m2} & \cdots & 0 \end{bmatrix}, \qquad R = \begin{bmatrix} R_1 \\ R_2 \\ \vdots \\ R_m \end{bmatrix} \tag{34}$$

$$T_s = \begin{bmatrix} 0 & -T_{12}S_2 & \cdots & -T_{1m}S_m \\ -T_{21}S_1 & 0 & \cdots & -T_{2m}S_m \\ \vdots & \vdots & \cdots & \vdots \\ -T_{m1}S_1 & -T_{m2}S_2 & \cdots & 0 \end{bmatrix} = T\,\mathbf{diag}\{S_j\}\,, \tag{35}$$

$$dT_s = \begin{bmatrix} 0 & -T_{12}\,dS_2 & \cdots & -T_{1m}\,dS_m \\ -T_{21}\,dS_1 & 0 & \cdots & -T_{2m}\,dS_m \\ \vdots & \vdots & \cdots & \vdots \\ -T_{m1}\,dS_1 & -T_{m2}\,dS_2 & \cdots & 0 \end{bmatrix} = T\,\mathbf{diag}\{dS_j\} \tag{36}$$

$$S_p = (I - T_s)^{-1}R, \qquad dS_p = (I - T_s)^{-1}\,dT_s\,S_p, \tag{37}$$

where $S_p,\ dS_p$ will be referred to as the splitting operators, provided that $I - T_s$ is invertible.

Lemma 3.2. *Let $I - T_s$ be invertible. Then $[\alpha_1, \alpha_2, \ldots, \alpha_m]$ is a unique solution of*

$$\alpha_i = \alpha_{i0} + \sum_{j\neq i} T_{ij}S_j\alpha_j, \tag{38}$$

and its perturbation $[d\alpha_1, d\alpha_2, \ldots, d\alpha_m]$ is a unique solution of

$$d\alpha_i = d\alpha_{i0} + \sum_{j\neq i} T_{ij}\big(dS_j\alpha_j + S_j d\alpha_j\big). \tag{39}$$

Proof. We only need to prove (38), with its perturbation being (39). By (28),

$$\begin{aligned} P_{ii}\beta_i &= a_i G_i^{(v,b)}\alpha_{i0} - \sum_{j\neq i} P_{ij}\beta_j \\ &= a_i G_i^{(v,b)}\alpha_{i0} + \sum_{j\neq i} a_i G_{ij}^{(v,v)}\beta_j \\ &= a_i G_i^{(v,b)}\alpha_{i0} + \sum_{j\neq i} a_i G_i^{(v,b)} T_{ij} G_j^{(b,v)}\beta_j \\ &= a_i G_i^{(v,b)}\alpha_{i0} + \sum_{j\neq i} a_i G_i^{(v,b)} T_{ij} S_j \alpha_j \\ &= a_i G_i^{(v,b)} \left[\alpha_{i0} + \sum_{j\neq i} T_{ij} S_j \alpha_j \right]. \end{aligned} \tag{40}$$

Now, (38) follows immediately from (31). □

4. **Merging and splitting formulae.** By Remark 3, S_i and dS_i, for the subdomain Ω_i of Ω, depend on the scatterer a and its perturbation da only inside Ω_i. Merging is a procedure to obtain S and dS for Ω from S_i and dS_i, $i = 1 : m$. This procedure is also required in splitting the incident waves, which we will examine next.

4.1. **Splitting incident waves.** Given the pair $[\alpha, d\alpha]$ for the total incident wave u to Ω, splitting is a procedure to obtain the pairs $[\alpha_i, d\alpha_i]$ for the total incident wave u_i (due to u_0) to the children Ω_i, $i = 1 : m$. This procedure requires the knowledge of S_i and dS_i, $i = 1 : m$.

Theorem 4.1. Splitting the incident wave *Let $I - T_s$ be invertible. Then*

$$\{\alpha_j\} := \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_m \end{bmatrix} = S_p\,\alpha, \quad \{d\alpha_j\} := \begin{bmatrix} d\alpha_1 \\ d\alpha_2 \\ \vdots \\ d\alpha_m \end{bmatrix} = [S_p \;\; dS_p] \begin{bmatrix} d\alpha \\ \alpha \end{bmatrix}. \tag{41}$$

Proof. By (38) and (27),

$$\alpha_i - \sum_{j\neq i} T_{ij} S_j\,\alpha_j = R_i \alpha. \tag{42}$$

The first part of (41) follows immediately from (37). Similarly, by (39) and (27)

$$d\alpha_i - \sum_{j\neq i} T_{ij} S_j\,d\alpha_j = R_i\,d\alpha + \sum_{j\neq i} T_{ij} dS_j \alpha_j, \tag{43}$$

which by (37) and (36) can be rewritten

$$(I - T_s)\;\{d\alpha_j\} = R\,d\alpha + dT_s\;\{\alpha_j\} = R\,d\alpha + dT_s\,S_p\,\alpha. \tag{44}$$

Now the second part of (41) follows directly from (37). □

Remark 7. The first part of (41) can also be used to split an arbitrary incident source α to Ω, resulting in the total incident source α_i to Ω_i, where α_i is due to α and not to α_0 (see Remark 6).

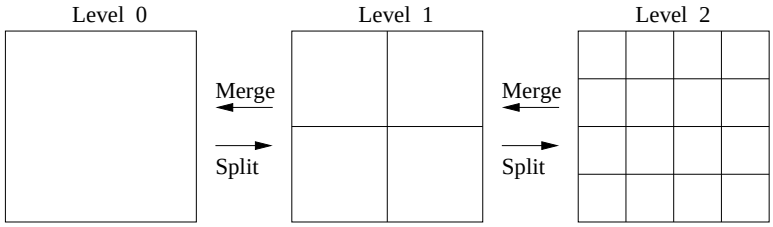

FIGURE 1. A hierarchy of partitions of D, $L = 2$

4.2. **Merging the scattering matrices.** We now present formulae for merging disjoint scatterers Ω_i; namely, to calculate the scattering matrices S, dS of Ω from the scattering matrices S_i, dS_i of Ω_i.

Theorem 4.2. Merge scattering matrices *Given the scattering matrices S_i, dS_i of the subscatterers Ω_i, $i = 1 : m$, the scattering matrices S, dS of $\Omega = \cup_i \Omega_i$ can be obtained by the formulae*

$$S = [E_1,\ E_2,\ \cdots,\ E_m]\,\mathbf{diag}\{S_j\}\,S_p \tag{45}$$

$$dS = [E_1,\ E_2,\ \cdots,\ E_m]\big[I - \mathbf{diag}\{S_j\}\,T\big]^{-1}\,\mathbf{diag}\{dS_j\}\,S_p. \tag{46}$$

Proof. Let u be an (arbitrary) incident wave to Ω, and let α be its incident source on $\partial\Omega$. Let β be a solution to (10), and let v be the scattered wave arising from the monopole density β in Ω, so that (9) holds. Let α_i, $d\alpha_i$ be the total incident source and its perturbation on $\partial\Omega_i$ (due to the arbitrary α) so that $\{\alpha_j\} = S_p\,\alpha$ by Remark 7. Let β_i, $d\beta_i$ be the corresponding monopole density in Ω_i, which gives rise to the scattered wave v_i so that

$$v_i|_{\partial\Omega_i} = S_i\alpha_i. \tag{47}$$

By Remark 6, $\beta_i = \beta|_{\Omega_i}$. Hence,

$$\begin{aligned} v|_{\partial\Omega} &= G^{(b,v)}\beta = \sum_{i=1}^{m} E_i G_i^{(b,v)}\beta_i = \sum_{i=1}^{m} E_i S_i\,\alpha_i \\ &= [E_1,\ E_2,\ \cdots,\ E_m]\mathbf{diag}\{S_j\}\ \{\alpha_i\} \\ &= [E_1,\ E_2,\ \cdots,\ E_m]\mathbf{diag}\{S_j\}\ S_p\alpha. \end{aligned}$$

Now (45) follows from (9); (46) can be proved in a similar way. □

5. **A fast algorithm for perturbational calculations.** Fast algorithms for the solution of the Helmholtz equation in two dimensions exist [2], [3], [4]. Our merging and splitting formulae will be used for the perturbational calculations in a way similar to how the merging and splitting formulae of [2] are used for the solution of the Helmholtz equation. In this section, we will construct a fast algorithm for perturbational calculations, namely, to evaluate the matrix-vector products (15) where $d\beta$ and dS are defined by (16) and (19), for arbitrary da. We will also outline the computational cost, when the various linear operators involved in the algorithm are properly discretized. We will, however, not elaborate on the underlying quadrature issues for singular integrals required for discretizing the Lippmann-Schwinger equation, and for partitioning D into non-overlapping subdomains. The complexity of the algorithm is similar to that of [2], where its more detailed analysis is available.

To illustrate, let's assume that D is a square domain that is partitioned hierarchically as shown in Figure 1, so that there will be 4^ℓ subscatterers on level $\ell = 0, 1, \ldots, L$ for some integer $L > 0$, which is the depth of the hierarchy. Level 0 is referred to as the top level and Level L as the bottom level.

If D is sampled by a mesh of size $n \times n$, L can be chosen such that each square subscatterer on the bottom level is a wavelength or smaller. If p points per wavelength is the linear density of the mesh, then a bottom level subscatterer is discretized with $p \times p$ points or less. Usually, p is about 10. Obviously, n is about $p\,2^L$; therefore for simplicity, we will assume that a bottom level square is discretized by $p \times p$ mesh with

$$n = p\ 2^L \tag{48}$$

for some small, fixed integer $p > 0$, independent of n. Since a subscatterer on level ℓ is discretized by a $2^{L-\ell}$-by-$2^{L-\ell}$ mesh, the number of points on the boundary of the subscatterer is $4(2^{L-\ell} - 1)$. Hence, when discretized, all matrices for S, E, R, T, S_p, which appear in the merging and splitting formulae, are expected to be of size $O(2^{L-\ell}) \times O(2^{L-\ell})$ on level ℓ.

5.1. **Step 1.** For each subscatterer of the bottom level, calculate scattering matrices S_i by (12) and their perturbations dS_i by (18).

Cost for each subproblem is proportional to that of inverting P, which is $p^2 \times p^2$. Total cost is

$$C_1 = O(p^6)\, 4^L = O(n^2)\, p^4 = O(n^2). \tag{49}$$

5.2. **Step 2.** Merging up: For level $\ell = L, L-1, \ldots, 1$ of the hierarchy, merge 4 child scattering matrices S_i and their perturbation dS_i to the parent scattering matrix S and its perturbation dS, using Theorem 4.2.

Cost for (45) and (46) is proportional to that of the matrix-matrix product, for matrices of size $O(2^{L-\ell}) \times O(2^{L-\ell})$ on level ℓ. There are 4^ℓ matrices to merge with every 4 matrices merging to one on level $\ell - 1$. Total cost on level ℓ is

$$C_{2,\ell} = O(2^{L-\ell})^3\, 4^{\ell-1} = O\big[(2^L)^3\big]/2^\ell = O(n^3)/2^\ell. \tag{50}$$

Total cost of Step 2 over all levels is

$$C_2 = \sum_{\ell=1}^{L} C_{2,\ell} = O(n^3). \tag{51}$$

Remark 8. After Step 2, $O(n^3)$ flops are required to obtain the perturbation dS for the entire scatterer D, as well as the scattering matrix S for D.

To obtain the perturbation $d\beta$ for D, we proceed with the remaining two steps.

5.3. **Step 3.** Splitting down: Having obtained S and dS for subscatterers at all levels, decouple the scattering problem on D into its 4 children by Theorem 4.1, and continue this splitting process recursively down to the bottom level. Input is the incident source α_0 of (3) to D, and its perturbation $d\alpha_0 = 0$. Output is α_i and $d\alpha_i$ to the bottom level subscatterers Ω_i, $i = 1 : 4^L$.

Cost for (41) is proportional to that of matrix-vector product, for matrices of size $O(2^{L-\ell}) \times O(2^{L-\ell})$ on level $\ell = 1 : L$. Total cost on level ℓ is

$$C_{3,\ell} = O(2^{L-\ell})^2\, 4^{\ell-1} = O\big[(2^L)^2\big] = O(n^2). \tag{52}$$

Total cost of Step 3 over all levels is

$$C_3 = \sum_{\ell=1}^{L} C_{3,\ell} = O(n^2)\ L = O(n^2 \log_4 n). \tag{53}$$

5.4. **Step 4.** With α_i and $d\alpha_i$ obtained in Step 3 for each bottom level subscatterer Ω_i, $i = 1 : 4^L$, the separated scattering problems (31) and (32) on Ω_i are solved independently to yield β and $d\beta$ for each Ω_i, which are β and $d\beta$ for the entire scatterer D by (26).

Cost for each subproblem is proportional to that of inverting P, which is $p^2 \times p^2$. Total cost is

$$C_4 = O(p^6)\, 4^L = O(n^2)\, p^4 = O(n^2). \tag{54}$$

Remark 9. Step 3 and 4 compute the perturbation $d\beta$, as well as the scattering solution β, for the entire scatterer D in $O(n^2 \log n)$ flops.

6. **Conclusions.** We have established merging and splitting formulae for the perturbational calculations for the Helmholtz equation in two dimensions. For numerical implementations, a discrete analogue of the merging and splitting formulae is necessary and was developed, and a Fortran code implementing these procedures is available.

The discrete merging and splitting formulae work directly with the mesh points resulting from discretization of the Lippmann-Schwinger integral equation with quadratures. These numerical issues are beyond the scope of this paper and will be presented elsewhere.

The fast algorithm for the perturbational calculations requires $O(n^3)$ steps for an m-by-m wavelength problem. In its implementation, n is usually $10m$ to $20m$, and L is such that $p = 10$ in (48). Then a more careful examination shows that the flops required for Step 1-4 to obtain dS, and to obtain $d\beta$ for n distinct incident waves, will be

$$c_1 \sim 12267n^2 \qquad c_2 \sim (10n)^3$$
$$c_3 < (8n)^3 \qquad c_4 \sim 100n^3,$$

provided that $n \leq 10^6$.

The fast algorithm can be extended to 3D calculations, with a complexity of $O(n^6)$ for a $n \times n \times n$ mesh. This is prohibitively expensive even for a small scattering problem. It appears that the merging and splitting formalism is not apt for improvement on the asymptotic rate of the complexity.

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Received May 2006; 1st revision October 2006; 2nd revision April 2007.

E-mail address: marcos@cimat.mx; yuchen@cims.nyu.edu