The combinatorics of scattering in layered media

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Abstract

Reflection and transmission of waves in piecewise constant layered media are important in various imaging modalities and have been studied extensively. Despite this, no exact time domain formulas for the Green's functions have been established. Indeed, there is an underlying combinatorial obstacle: the analysis of scattering sequences. In the present paper we exploit a representation of scattering sequences in terms of trees to solve completely the inherent combinatorial problem, and thereby derive new, explicit formulas for the reflection and transmission Green's functions.

1 Introduction

The analysis of wave propagation in layered media is a well-developed subject, with applications to acoustic, electromagnetic and seismic imaging; see [2], [4], [1] and the numerous references therein. In the present introduction we describe briefly the physical framework and cite some needed facts. In the next section we explain a fundamental combinatorial problem arising from the given framework—the enumeration of scattering sequences. The main contribution of the present paper is to solve the combinatorial problem completely, thereby producing new, exact formulas for the reflection and transmission Green's functions. Our main results are Theorem 2.1 and Theorem 3.1.

The basic framework is as follows. Let (x, y, z) denote euclidean coordinates for a solid three-dimensional acoustic medium whose physical parameters (density and bulk modulus) vary only in the z-direction. Suppose

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furthermore that these physical parameters are piecewise constant in z, having jumps at the M + 1 locations

$$z_0 < z_1 < \cdots < z_M.$$

Thus the solid contains M homogenous layers, the *n*th layer corresponding to the *z*-interval

$$z_{n-1} < z < z_n;$$

the layers are sandwiched between the two half spaces $z < z_0$ and $z > z_M$. We shall refer to the z-direction as depth, and depict it as increasing downward, as in Figure 1.



Figure 1: A layered medium with M layers, sitting between two half spaces. The depth coordinate z increases downward.

From the perspective of acoustic imaging the problem is to infer the physical parameters for the M layers by probing them with acoustic waves in one of two ways. The first way is to send an acoustic pulse from a fixed depth $z_{-1} < z_0$ toward the interface at z_0 and to record the pulse train reflected back from the M layers as it crosses the original depth z_{-1} . The *reflection problem* is to infer the structure of the M layers from this recorded reflection data. A second experiment is to transmit a pulse from z_{-1} as before, but to record the resulting pulse train that is transmitted across the M layers to some fixed depth $z_{M+1} > z_M$. The *transmission problem* is to

infer the structure of the M layers from this transmitted data, recorded at z_{M+1} . It is assumed for both the reflection and transmission experiments that the initial pulse is a plane wave of the form f(z - ct), where t denotes time and c(z) denotes the speed of sound at depth z. Thus although the physical setting is three-dimensional, by symmetry the analysis reduces to one spatial dimension, the z-direction.

If the initial pulse is idealized to a Dirac delta function initially centred at z_{-1} , so of the form

$$\delta(z-z_{-1}-ct),$$

then the reflection data G(t) and the transmission data H(t) are Green's functions for the governing partial differential equation (see Appendix A), and they have the form

$$G(t) = \sum_{n=1}^{\infty} a_n \,\delta(t - \sigma_n), \qquad (1.1)$$

$$H(t) = \sum_{n=1}^{\infty} b_n \,\delta(t - \sigma_n). \tag{1.2}$$

The numbers a_n and b_n will be referred to as reflection amplitudes and transmission amplitudes, respectively; the numbers σ_n and σ'_n will be referred to as arrival times.

As a consequence of the standard theory, both G and H are completely determined by two vectors:

- 1. the sequence $R = (R_0, \ldots, R_M)$ of reflection coefficients at the layer boundaries; and
- 2. the sequence $\tau' = (\tau_0, \ldots, \tau_{M+1})$ of two-way travel times, where τ_n denotes twice the time it takes a downward-traveling acoustic wave to go from z_{n-1} to z_n .

The travel time τ_{M+1} is obviously irrelevant for the reflection problem, so G is in fact determined by R and $\tau = (\tau_0, \ldots, \tau_M)$. We incorporate this basic fact into our notation, writing

$$G^{(\tau,R)}$$
 and $H^{(\tau',R)}$

to denote the respective reflection and transmission data determined by a given pair (τ', R) .

Different layered media that correspond to the same parameters (τ', R) are for present purposes indistinguishable, and we shall simply refer to the

pair (τ', R) as a medium, letting it be understood that a class of physical systems are thereby represented. (See Appendix A.)

The above facts lead naturally to a basic question: What is the formula for the amplitude coefficients a_n and b_n in terms of (τ', R) ? It turns out that no finite, closed form formula has ever been established—only series expansions that must be estimated when it comes to practical computation. (See, for example, [4, Chapter 3], [1, Chapter 2], [2, Section 2.5]; concerning theoretical developments applied specifically to seismic, see [8], [9], [11],[5]) This is because there is a substantial combinatorial problem blocking the way to an exact formula. The purpose of the present paper is to solve the combinatorial problem directly, and to present the resulting explicit formulas for the reflection and transmission Green's functions G and H in terms of (τ', R) .

2 The combinatorics of reflection

The one-dimensional wave equation for a homogenous medium generates traveling wave solutions; in a layered medium one has to take into account the behaviour of these traveling waves at interfaces between homogenous layers. This behaviour depends on the reflection coefficient R_n associated with the interface at z_n in the following way. When a wave $f(z - z_n - c_n t)$ traveling downward from z_{n-1} toward z_n for t < 0 hits the interface at t = 0, it splits into a reflected wave,

$$R_n f(z - z_n + c_n t)$$

that travels back up toward z_{n-1} , and a transmitted wave

$$\sqrt{1-R_n^2} f(z-z_n-c_{n+1}t)$$

that continues down toward z_{n+1} (at modified speed c_{n+1}). The reflected and transmitted waves then hit the respective interfaces at z_{n-1} and z_{n+1} , generating two new sets of reflected and transmitted waves, and a cascade of successive reflections and transmissions continues indefinitely. The case of an initial wave traveling upward from z_{n+1} toward z_n instead of downward from z_{n-1} is similar, except that the reflection coefficient $-R_n$ applies instead of R_n ; the transmission coefficient $\sqrt{1-R_n^2}$ remains unchanged. We use the notation $T = (T_0, \ldots, T_M)$ for the transmission coefficients that correspond to reflection coefficients $R = (R_0, \ldots, R_M)$ by way of the formula

$$T_n = \sqrt{1 - R_n^2} \qquad (0 \le n \le M).$$

A standard idea is to view $G^{(\tau,R)}(t)$ as the sum total of all possible sequences of successive reflections and transmissions of an initial pulse at z_{-1} that eventually return to z_{-1} . (See [4, Chapter 3] for details.) The idea is worth illustrating further, since it underpins the arguments below. For example, consider an initial downward traveling unit pulse of the form $\delta(z - z_{-1} - c_0 t)$. After $\tau_0/2$ seconds, the initial pulse reaches the interface at z_0 . Part of it is transmitted into the first layer as $T_0\delta(z - z_0 - c_1(t - \frac{\tau_0}{2}))$, which, after another $\tau_1/2$ seconds, reaches the interface z_1 . Part of this pulse is reflected back into first layer as $R_1T_0\delta(z - z_1 + c_1(t - \frac{\tau_0+\tau_1}{2}))$. Traveling back up to z_0 , the latter reaches z_0 after a further $\tau_1/2$ seconds, and is partly transmitted back to z_{-1} as

$$R_1 T_0^2 \delta \left(z - z_0 + c_0 \left(t - \frac{\tau_0 + 2\tau_1}{2} \right) \right), \tag{2.1}$$

arriving at z_{-1} at time $\sigma = \tau_0 + \tau_1$. Thus the part of the initial pulse that traverses the sequence of depths $\mathbf{p} = (z_{-1}, z_0, z_1, z_0, z_{-1})$ returns to z_{-1} with an amplitude $\alpha = R_1 T_0^2$ at arrival time $\sigma = \tau_0 + \tau_1$, thereby contributing a term of the form $\alpha \delta(t - \sigma)$ to $G^{(\tau,R)}(t)$. The sequence \mathbf{p} is called a scattering sequence, and the amplitude α is called the weight of \mathbf{p} . As mentioned earlier, the impulse response itself is a delta train of the form

$$G^{(\tau,R)}(t) = \sum_{n=1}^{\infty} \alpha_n \delta(t - \sigma_n), \qquad (2.2)$$

composed of the cumulative contributions of all possible scattering sequences returning to z_{-1} , with their associated weights and arrival times. In the above example, **p** is the only scattering sequence having arrival time σ . But in general different scattering sequences may arrive simultaneously, so each amplitude α_n occurring in (2.2) is the sum of the weights of all scattering sequences arriving at time σ_n . Given an arrival time σ_n , the essential combinatorial problem, then, is to enumerate all the associated scattering sequences, along with their weights, to derive a formula for α_n .

2.1 Scattering sequences and the Green's function

The first step is to establish some terminology and notation, as follows. A scattering sequence that starts and ends at z_{-1} is represented by a path in the graph

$$Z_{-1}$$
 Z_0 Z_1 Z_2 Z_3 Z_4 ... Z_{M-1} Z_M (2.3)

Formally, given an integer $M \ge 1$, let S_M denote the set of all sequences of the form

$$\mathsf{p} = (\mathsf{p}_0, \mathsf{p}_1, \dots, \mathsf{p}_L)$$

such that $L \geq 2$ and:

 $\forall n$

$$\mathbf{p}_0 = \mathbf{p}_L = z_{-1} \text{ and } \mathbf{p}_n \in \{z_1, \dots, z_M\} \text{ if } 1 \le n \le L - 1;$$
 (2.4a)

with
$$0 \le n \le L - 1$$
, $\exists j \text{ with } -1 \le j \le M - 1 \text{ such that}$
 $\{\mathbf{p}_n, \mathbf{p}_{n+1}\} = \{z_j, z_{j+1}\}.$ (2.4b)

The elements of S_M will be referred to as scattering sequences. Condition (2.4a) says a scattering sequence starts and ends at z_{-1} , and condition (2.4b) (which refers to *un*ordered pairs) says that adjacent terms in a scattering sequence are adjacent vertices in the graph (2.3).

For example, for $0 \leq n \leq M$, the shortest scattering sequence that reaches z_n is

$$(z_{-1}, z_0, z_1, \dots, z_{n-1}, z_n, z_{n-1}, \dots, z_1, z_0, z_{-1});$$
 (2.5)

this is called a primary scattering sequence. A scattering sequence reaching maximum depth z_n that is not shortest possible is called a multiple scattering sequence.

2.1.1 The weight of a scattering sequence

The weight $w(\mathbf{p})$ corresponding to a scattering sequence

$$\mathsf{p} = (\mathsf{p}_0, \mathsf{p}_1, \dots, \mathsf{p}_L)$$

in an *M*-layer medium (τ, R) is defined as follows. For each *n* in the range $1 \le n \le L - 1$, and given that $\mathbf{p}_n = z_j$, define

$$w_n = \begin{cases} R_j & \text{if } \mathsf{p}_{n-1} = \mathsf{p}_{n+1} = z_{j-1} \\ -R_j & \text{if } \mathsf{p}_{n-1} = \mathsf{p}_{n+1} = z_{j+1} \\ \sqrt{1 - R_j^2} & \text{otherwise} \end{cases}$$
(2.6)

The three possibilities correspond respectively to: reflection inside the *j*th layer at z_j ; reflection inside the (j+1)st layer at z_j ; and transmission between the *j*th and (j + 1)st layers. Finally, set

$$w(\mathbf{p}) = \prod_{n=1}^{L-1} w_n$$

Thus the part of an initial unit impulse that traverses p returns to z_{-1} with amplitude w(p).

2.2 Transit count and branch count vectors

We define two maps,

$$\kappa, \beta: \mathsf{S}_M \to \mathbb{Z}^{M+1}$$

that associate integer vectors to a given scattering sequence.

A scattering sequence $\mathbf{p} \in S_M$ may be represented graphically as in Figure 2; Stanley [10] calls such a representation a Dyck path.



Figure 2: The Dyck path for a scattering sequence p, with the horizontal coordinate now representing time, which increases to the right.



Figure 3: The intervals I_j^2 , in red. There are five intervals, two of which have positive length, so $k_2 = 5$ and $b_2 = 2$.

Given the Dyck path for a scattering sequence $\mathbf{p} \in S_M$, let t denote the horizontal coordinate and (as usual) let z denote the vertical coordinate. Let U denote the portion of the t, z-plane on or above the Dyck path and at or below $z = z_{-1}$ —the shaded region in Figure 3. For each n in the range $0 \le n \le M$, consider the horizontal line L_n at depth z_n . The intersection $L_n \cap U$ consists of a disjoint union of closed intervals I_j^n , where $1 \le j \le k_n$; see Figure 3. The intervals of I_j^n are of two types: degenerate intervals consisting of a single points; and non-degenerate intervals having positive length. Letting k_n denote the total number of intervals I_j^n , and letting b_n denote the number of non-degenerate intervals, set

$$\kappa(\mathbf{p}) = k = (k_0, \dots, k_M)$$
 and $\beta(\mathbf{p}) = b = (b_0, \dots, b_M)$.

Observe that the entry k_n of the vector $k = \kappa(\mathbf{p})$ counts the number of times the Dyck path crosses back and forth across the *n*th layer $z_{n-1} < z < z_n$; the vector k is therefore called the transit count vector for \mathbf{p} . The vector $b = \beta(\mathbf{p})$ is called the branch count vector, for reasons that will be apparent in Section 2.3.

2.2.1 The set of transit count vectors

The range of κ is contained in the set

$$\mathfrak{L}_{M} = \{ (k_{0}, k_{1}, \dots, k_{M}) \in \mathbb{N}^{M+1} \mid k_{0} = 1 \& \forall n \leq M-1, \, k_{n} = 0 \Rightarrow k_{n+1} = 0 \}.$$
(2.7)

Conversely, for any given $k \in \mathfrak{L}_M$, it is straightforward to construct a realizing scattering sequence. Thus \mathfrak{L}_M is precisely the range $\kappa(\mathsf{S}_M)$ of the mapping $\kappa: \mathsf{S}_M \to \mathbb{Z}^{M+1}$.

2.2.2 Arrival times

The arrival time of \mathbf{p} , expressed in terms of the transit count vector $k = \kappa(\mathbf{p})$, is simply

$$\langle k,\tau\rangle = k_0\tau_0 + k_1\tau_1 + \dots + k_M\tau_M.$$

Therefore $G^{(\tau,R)}(t)$ may be written as

$$G^{(\tau,R)}(t) = \sum_{k \in \mathfrak{L}_M} a(R,k)\delta(t - \langle k, \tau \rangle), \qquad (2.8)$$

where the amplitudes a(R, k) are given by the formula

$$a(R,k) = \sum_{\substack{\mathbf{p} \in \mathsf{S}_M \text{ such that} \\ \kappa(\mathbf{p}) = k}} w(\mathbf{p}). \tag{2.9}$$

Note that the weight $w(\mathbf{p})$ of a scattering sequence depends only on R, and not on τ ; the next step is to find an explicit formula for a(R, k). This is greatly facilitated by introducing another representation for scattering sequences, in terms of trees.

2.3 The tree representation of a scattering sequence

A tree is a connected cycle-free graph. The vertices of a tree are divided into three anatomical types, as follows: the root is a single, specially designated vertex; a non-root that belongs to just one edge is called a leaf; all other non-root vertices are called branch points. Vertices in a tree have a height, determined by their distance (in the sense of shortest path) to the root. See Figure 4.



Figure 4: A tree, with the leaves coloured green. The root is at the bottom, and horizontal lines indicate the various heights of vertices.

The association between a scattering sequence and a tree is well-known (see [10, Exercise 6.19]) and arises, for instance, in the analysis of Brownian excursions and superprocesses (see [7, Section 1.1]). The tree representing a scattering sequence $\mathbf{p} \in \mathbf{S}_M$ may be obtained simply by collapsing its Dyck path, as follows. Recall the intervals I_j^n used to define $\kappa(\mathbf{p})$ and $\beta(\mathbf{p})$ above; for present purposes let I_1^{-1} denote the intersection of $z = z_{-1}$ with U. To collapse the Dyck path, contract each of the intervals I_j^n to a point, keeping the distances between intervals unchanged, and interpolate this horizontal contraction linearly on each depth interval $z_{n-1} < z < z_n$. This operation transforms the original Dyck path into a tree (in fact it is an isotopy between the region U and the resulting tree). See Figure 5. Note that the degenerate intervals I_j^n (coloured green for emphasis) end up as leaves, while non-degenerate intervals are contracted to branch points of the tree—except for I_1^{-1} , which is contracted to the root.

Conversely, given a tree, one may recover the original scattering sequence by tracing the outline of the tree, from the root (keeping the tree on the left), and recording the depths of the vertices in the order that they are passed.



Figure 5: The collapsing of a Dyck path (a) to a tree (f) (depicted upside down), an operation which is reversible.

Observe that the vectors $(k, b) = (\kappa(\mathbf{p}), \beta(\mathbf{p}))$ have a simple interpretation in terms of the tree representing $\mathbf{p} \in S_M$. For each $0 \le n \le M$, k_n is the number of vertices at depth z_n , and b_n is the number of branch points at z_n . (This is the reason for calling b the branch count vector for \mathbf{p} .) There are some evident constraints on these quantities. Note first that $b_M = 0$. Furthermore, for $0 \le n \le M - 1$,

$$\min\{1, k_{n+1}\} \le b_n \le k_{n+1} \quad (0 \le n \le M - 1), \tag{2.10}$$

since each vertex at z_{n+1} is connected by an edge to a unique branch point at z_n . It is convenient to refer to the left shift \tilde{k} of $k = \kappa(\mathbf{p})$; that is,

$$\tilde{k} = (k_1, k_2, \dots, k_M, 0) \in \mathbb{Z}^{M+1}.$$
 (2.11)

In terms of this notation, the constraints (2.10) become

$$\min\{1, \tilde{k}_n\} \le b_n \le \min\{k_n, \tilde{k}_n\} \quad (0 \le n \le M).$$
(2.12)

An easy application of the tree representation is to determine the possible values of $b = \beta(\mathbf{p})$ for each given $k = \kappa(\mathbf{p})$, or in other words, to determine the set

$$V(k) = \beta(\kappa^{-1}(k)).$$
(2.13)

In fact V(k) is determined precisely by (2.12).

Proposition 2.1 Given $k \in \mathfrak{L}_M$,

$$V(k) = \left\{ b \, \big| \min\{\mathbb{1}, \tilde{k}\} \le b \le \min\{k, \tilde{k}\} \right\};$$

equivalently, V(k) may be expressed as a Cartesian product of sets,

$$V(k) = V_0 \times V_1 \times \cdots \times V_M,$$

where $V_n = \{\min\{1, \tilde{k}_n\}, \min\{1, \tilde{k}_n\} + 1, \dots, \min\{k_n, \tilde{k}_n\}\} \quad (0 \le n \le M).$

Here $\mathbb{1} \in \mathbb{Z}^{M+1}$ is the vector whose entries are all 1. The minimum is to be interpreted entrywise, meaning that for $x, y \in \mathbb{R}^{M+1}$,

 $\min\{x, y\} = \left(\min\{x_0, y_0\}, \min\{x_1, y_1\}, \dots, \min\{x_M, y_M\}\right) \in \mathbb{R}^{M+1}.$

Proof. The constraints (2.12) imply that $V(k) \subset V_0 \times \cdots \times V_M$. It remains to show that any $b \in V_0 \times \cdots \times V_M$ belongs to V(k), which entails showing that there exists a scattering sequence **p** such that $(\kappa(\mathbf{p}), \beta(\mathbf{p})) = (k, b)$. It suffices to construct a tree representing such a **p**, as follows. Given $b \in V_0 \times \cdots \times V_M$, place k_n vertices, consisting of b_n branch points and $k_n - b_n$ leaves (in any order), at depth z_n , for $0 \leq n \leq M$, and place a root at z_{-1} (considered as a branch point). Let N denote the largest index such that $k_N \neq 0$. For $0 \leq n \leq N$,

$$1 \le b_{n-1} \le \min\{k_{n-1}, k_n\},\$$

so there exists a surjection f_n from the k_n vertices at z_n onto the b_{n-1} branch points at z_{n-1} . The tree representing **p** is completed by drawing an edge from each vertex v at z_n to $f_n(v)$.

2.3.1 A formula for the weight

The tree representation facilitates deriving a simple formula for the weights. The following lemma uses multi-index notation, whereby given a vector $s = (s_0, s_1, \ldots, s_M)$ and an integer vector $d = (d_0, \ldots, d_M)$,

$$s^d = \prod_{n=0}^M s_n^{d_n}.$$

Lemma 2.2 Let $\mathbf{p} \in S_M$ be a scattering sequence in an M-layer medium (τ, R) , and set $(k, b) = (\kappa(\mathbf{p}), \beta(\mathbf{p}))$. Then

$$w(\mathbf{p}) = (-R)^{k-b} R^{k-b} T^{2b}.$$

Proof. Consider the tree representing p. Observe that each instance of $w_n = R_j$ in (2.6) corresponds to a unique leaf at z_j (see Figure 5). Since there are $k_n - b_n$ leaves at z_n this results in a total contribution of R^{k-b} .

Let v be a branch point at z_j having d_v edges to vertices at z_{j+1} . Observe that precisely $d_v - 1$ of these edges correspond to an instance of $w_n = -R_j$ in (2.6), and every occurrence of $w_n = -R_j$ arises this way. The sum total of numbers $d_v - 1$ over branch points v at z_j is simply $k_{n+1} - b_n = \tilde{k}_n - b_n$, making for a total contribution over all depths of $(-R)^{\tilde{k}-b}$.

Finally, each instance of transmission from the *j*th layer to the (j + 1)st layer in **p** corresponds to a vertex in the tree representing **p** which is not a leaf, i.e., to a branch point at z_j ; and, since the path **p** starts and ends at z_{-1} every such transmission has a corresponding return transmission in the opposite direction, from the (j + 1)st layer to the *j*th layer. There are b_j branch points at z_j , and each of these corresponds to two transmissions across the boundary at z_j , making for a total contribution to $w(\mathbf{p})$ of T^{2b} . Since every w_n is covered by one of the above cases, the lemma follows.

2.4 The Green's function

A formula for the coefficients a(R, k) in (2.8), defined as the summation (2.9), is now within easy reach. Recall that the binomial coefficient $\binom{x}{y}$ for a pair of non-negative integer vectors $x, y \in \mathbb{Z}^{M+1}$, with $y \leq x$, is to be interpreted as

$$\binom{x}{y} = \prod_{n=0}^{M} \binom{x_n}{y_n}.$$

(The inequality $y \leq x$ means that x - y has non-negative entries.)

Lemma 2.3 Let $k \in \mathfrak{L}_M$ and let $\min\{\mathfrak{l}, \tilde{k}\} \leq b \leq \min\{k, \tilde{k}\}$. Then

$$\# \left\{ \mathbf{p} \in \mathsf{S}_M \, | \, (\kappa(\mathbf{p}), \beta(\mathbf{p})) = (k, b) \right\} = \binom{k}{b} \binom{\tilde{k} - u}{b - u}.$$

Proof. To count the number of scattering sequences having a given transit count vector, it suffices to count the number of corresponding trees—which is straightforward. Consider first the arrangement of vertices in a tree for which $(\kappa(\mathbf{p}), \beta(\mathbf{p})) = (k, b)$. At each depth z_n , there are k_n vertices of which b_n are branch points and $k_n - b_n$ are leaves. There are $\binom{k_n}{b_n}$ ways of arranging these from left to right, making for a total of

$$\binom{k}{b} = \prod_{j=0}^{M} \binom{k_n}{b_n}$$
(2.14)

possible vertex arrangements. (There is only one way to place the root at z_{-1} , which may be ignored.)

For each vertex arrangement there are various possible edge arrangements, as follows. Each of the $k_{n+1} = \tilde{k}_n$ vertices at z_{n+1} must be connected by an edge to one of the b_n branch points at z_n , respecting the vertex ordering (so that edges don't cross). This is equivalent to choosing a b_n -part ordered partition of the integer \tilde{k}_n . If $\tilde{k}_n \ge 1$, there are $\begin{pmatrix} \tilde{k}_n - 1 \\ b_n - 1 \end{pmatrix}$ possible choices; and if $\tilde{k}_n = 0$ then $b_n = 0$ and there is $1 = \begin{pmatrix} \tilde{k}_n \\ b_n \end{pmatrix}$ (empty) arrangement. Letting N denote the largest index for which $\tilde{k}_N \neq 0$, the total number of edge arrangements is

$$\begin{pmatrix} \tilde{k} - u \\ b - u \end{pmatrix} = \prod_{n=0}^{N} \begin{pmatrix} \tilde{k}_n - 1 \\ b_n - 1 \end{pmatrix}.$$
 (2.15)

Combining (2.14) and (2.15) yields a total tree count of

$$\# \{ \mathbf{p} \in \mathsf{S}_M \,|\, (\kappa(\mathbf{p}), \beta(\mathbf{p})) = (k, b) \} = \binom{k}{b} \binom{\tilde{k} - u}{b - u},$$

completing the proof.

Combining the foregoing lemmas gives a formula for the reflection Green's function, as follows.

Theorem 2.1 Let (τ, R) be an *M*-layer medium for some integer $M \ge 1$. Then

$$G^{(\tau,R)}(t) = \sum_{k \in \mathfrak{L}_M} a(R,k)\delta(t - \langle k, \tau \rangle)$$

where for each $k \in \mathfrak{L}_M$, the amplitude a(R,k) is given by the following formula. Setting $u = \min\{\mathbb{1}, \tilde{k}\},$

$$a(R,k) = \sum_{b \in V(k)} \binom{k}{b} \binom{k-u}{b-u} (-R)^{\tilde{k}-b} R^{k-b} T^{2b}, \qquad (2.16)$$

where V(k) denotes the set of $b \in \mathbb{Z}^{M+1}$ such that $u \leq b \leq \min\{k, \tilde{k}\}$.

Proof. The total amplitude resulting from scattering sequences having a given transit count vector $k \in \mathfrak{L}_M$ is

$$a(R,k) = \sum_{\substack{ \mathsf{p} \in \mathsf{S}_M \text{ such that} \\ \kappa(\mathsf{p}) = k}} w(\mathsf{p}).$$

By Proposition 2.1 and Lemma 2.2 the above sum may be rearranged as

$$\begin{aligned} a(R,k) &= \sum_{b \in V(k)} \sum_{\substack{\mathbf{p} \in \mathsf{S}_M \text{ such that} \\ (\kappa(\mathbf{p}),\beta(\mathbf{p})) = (k,b)}} w(\mathbf{p}) \\ &= \sum_{b \in V(k)} \left(\#\{\mathbf{p} \in \mathsf{S}_M \mid (\kappa(\mathbf{p}),\beta(\mathbf{p})) = (k,b)\} \right) (-R)^{\tilde{k}-b} R^{k-b} T^{2b}. \end{aligned}$$

Applying Lemma 2.3 then gives the stated formula.

Note that since each transmission coefficient $T_n = \sqrt{1 - R_n^2}$ occurs to an even power in (2.16), the amplitude a(R, k) is a polynomial in the variables R_0, \ldots, R_M of precise degree

$$\langle k+\tilde{k},\mathbb{1}\rangle.$$

Note further that this polynomial depends only on the R_n corresponding to the support of the vector k: if $k_n = 0$, then a(R, k) does not depend on R_n . Because the amplitudes are polynomial functions of the reflection coefficients, Theorem 2.1 is straightforward to code. This makes it possible to compute $G^{(\tau,R)}(t)$ exactly up to some cutoff time T > 0, and to do so very efficiently—see Section 4.

The simplest possible transit count vectors are those that correspond to primary scattering sequences (2.5); given $n \ge 1$, write k^n for the primary transit count vector defined as

$$k_j^n = \begin{cases} 1 & \text{if } 0 \le j \le n \\ 0 & \text{if } n < j \end{cases}$$

17 May 2013

The formula for the corresponding amplitude is easy to work out directly. It is the only explicit example we found in the existing literature, appearing in the early work of Kunetz [6]. Observe that $V(k^n) = \{k^{n-1}\}$ is a singleton, so that the general formula (2.16) reduces just to

$$a(R,k^{n}) = (-R)^{0} R^{k^{n} - k^{n-1}} T^{2k^{n-1}} = R_{n} \prod_{j=0}^{n-1} (1 - R_{j}^{2}),$$

which is exactly Kunetz's formula.

3 The combinatorics of transmission

The case of transmission is in many ways similar to that of reflection. We therefore give a much more compressed presentation, emphasizing only those points where there is a substantial difference.

3.1 Scattering sequences and weights

In the case of transmission, a scattering sequence is a path in the graph

$$z_{-1} \quad z_0 \quad z_1 \quad z_2 \quad z_3 \quad z_4 \quad \dots \quad z_{M-1} \quad z_M \quad z_{M+1} \quad (3.1)$$

that starts at z_{-1} and ends at z_{M+1} . (See Figure 1.) Formally, given an integer $M \ge 1$, let S'_M denote the set of all sequences of the form

$$\mathsf{p} = (\mathsf{p}_0, \mathsf{p}_1, \dots, \mathsf{p}_L)$$

such that:

$$p_{0} = z_{-1}, p_{L} = z_{M+1} \text{ and } p_{n} \in \{z_{1}, \dots, z_{M}\} \text{ if } 1 \le n \le L - 1; \quad (3.2a)$$

$$\forall n \text{ with } 0 \le n \le L - 1, \quad \exists j \text{ with } -1 \le j \le M \text{ such that} \\ \{p_{n}, p_{n+1}\} = \{z_{j}, z_{j+1}\}. \quad (3.2b)$$

The elements of S'_M will be referred to as scattering sequences (or *transmission* scattering sequences for emphasis).

The weight of a scattering sequence in S'_M is computed exactly as for a scattering sequence in S_M ; see Section 2.1.1.



Figure 6: The scattering path for a transmission scattering sequence. As with a Dyck path, the horizontal coordinate represents time, increasing to the right.

3.2 Trees and transit count vectors

Figure 6 depicts what we call a *scattering* path, the analogue of a Dyck path for a transmission scattering sequence.

Note that there are subpaths of a transmission scattering path that themselves are Dyck paths. We call these Dyck subpaths. Collapsing the Dyck subpaths turns the scattering path into a tree, which has some additional structure. There is a distinguished leaf, the single leaf of maximum height (corresponding to z_{M+1}), which we call the *tip*. The subpath leading directly from the root to the tip will be referred to as the *trunk*. See Figure 7.

Collapsing of Dyck paths is reversible, so there is a one-to-one correspondence between scattering paths and trees; the latter serve as a convenient representation for the purpose of counting. Since every tree that corresponds to a scattering sequence has a trunk (including the root and the tip of the tree), it simplifies the combinatorial analysis to focus only on the remaining part of the tree. As in Section 2, we define two maps,

$$\kappa', \beta': \mathsf{S}'_M \to \mathbb{Z}^{M+1}$$

that associate integer vectors to a given transmission scattering sequence



Figure 7: The scattering path with Dyck subpaths filled in, and it's associated tree (depicted upside down, with the root at the top) obtained by collapsing the Dyck subpaths. The tip is coloured yellow; the other leaves are green.

 $\mathbf{p} \in \mathbf{S}'_M$. For each *n* in the range $0 \le n \le M$, define k_n to be the number of nodes at height z_n not on the trunk. (Since there is precisely one node at each level belonging to the trunk, k_n is one less than the total number of nodes at height z_n .) Set

$$\kappa'(\mathbf{p}) = (k_0, k_1, \dots, k_M).$$

Note that with this definition $k_0 = 0$; the other k_n can take any non-negative integer value. Define m_n to be the number of branch points at z_n not on the trunk, and set

$$\beta'(\mathsf{p}) = (m_0, \ldots, m_M).$$

As before, we call $k = (k_0, \ldots, k_M)$ a transit count vector and $m = (m_0, \ldots, m_M)$ a branch count vector, and we define \tilde{k} to be the left shift of k:

$$\tilde{k} = (k_1, k_2, \dots, k_M, 0).$$

Observe that for each n,

$$0 \le m_n \le \min\{k_n, \tilde{k}_n\}. \tag{3.3}$$

Furthermore, letting \mathbb{Z}_+ denote the nonnegative integers, the following result is straightforward (we write 0 for both the number and the zero vector).

Proposition 3.1 Given any $k \in \{0\} \times \mathbb{Z}^M_+$ and any $0 \le m \le \min\{k, \tilde{k}\}$, there exists a transmission scattering sequence $p \in S'_M$ such that

$$(\kappa'(\mathbf{p}), \beta'(\mathbf{p})) = (k, m).$$

The following is the analogue of Lemma 2.2 for transmission scattering sequences.

Lemma 3.2 Let $\mathbf{p} \in S'_M$ be a transmission scattering sequence in an *M*-layer medium (τ', R) , and set $(k, m) = (\kappa'(\mathbf{p}), \beta'(\mathbf{p}))$. Then

$$w(\mathbf{p}) = (-R)^{\tilde{k}-m} R^{k-m} T^{2m+1}.$$

Proof. Consider the tree representing **p**. Observe that each instance of $w_n = R_j$ in (2.6) corresponds to a unique leaf at z_j (see the right-hand part of Figure 7). Since there are $k_n - m_n$ leaves at z_n this results in a total contribution of R^{k-m} .

Let v be a branch point at z_j (possibly on the trunk) having d_v edges to vertices at z_{j+1} . Observe that precisely $d_v - 1$ of these edges correspond to an instance of $w_n = -R_j$ in (2.6), and every occurrence of $w_n = -R_j$ arises this way. The sum total of numbers $d_v - 1$ over branch points v at z_j is simply $(k_{n+1} + 1) - (m_n + 1) = \tilde{k}_n - m_n$, making for a total contribution over all depths of $(-R)^{\tilde{k}-m}$.

Finally, each instance of transmission from the *j*th layer to the (j + 1)st layer in **p** corresponds to a vertex in the tree representing **p** which is not a leaf, i.e., to a branch point at z_j . Each branch point not on the trunk corresponds to two transmissions across the boundary at z_j (as for a Dyck path), making for a total contribution to $w(\mathbf{p})$ of T^{2m} . Each branch point on the trunk corresponds to a single upward transmission, making for a total contribution of $T^{\mathbb{1}}$. Since every w_n is covered by one of the above cases, the lemma follows.

3.3 The transmission Green's function

The analogue of Lemma 2.3 for transmission scattering sequences is slightly simpler, as follows.

Lemma 3.3 Let $k \in \{0\} \times \mathbb{Z}^M_+$ and let $0 \le m \le \min\{k, \tilde{k}\}$. Then

$$\#\left\{\mathbf{p}\in \mathsf{S}'_{M}\,|\,(\kappa'(\mathbf{p}),\beta'(\mathbf{p}))=(k,m)\right\}=\binom{k}{m}\binom{\tilde{k}}{m}.$$

Proof. To count the number of scattering sequences having a given transit count vector, it suffices to count the number of corresponding trees, as before. Consider first the arrangement of vertices in a tree for which $(\kappa'(\mathbf{p}), \beta'(\mathbf{p})) = (k, m)$. To begin with, there is the trunk, which has fixed structure. At each depth z_n , there are k_n vertices off the trunk, of which m_n are branch points and $k_n - m_n$ are leaves. There are $\binom{k_n}{m_n}$ ways of arranging these from left to right, making for a total of

$$\binom{k}{m} = \prod_{j=0}^{M} \binom{k_n}{m_n}$$
(3.4)

possible vertex arrangements.

For each vertex arrangement there are various possible edge arrangements, as follows. Each of the $k_{n+1} = \tilde{k}_n$ vertices at z_{n+1} must be connected by an edge to one of the $m_n + 1$ branch points at z_n (including the branch point on the trunk), respecting the vertex ordering (so that edges don't cross). This is equivalent to choosing a $m_n + 1$ -part ordered partition of the integer \tilde{k}_n , where the last part—corresponding to the trunk branch point can be empty. There are $\binom{\tilde{k}_n}{m_n+1-1}$ possible choices. Letting N denote the largest index for which $\tilde{k}_N \neq 0$, the total number of edge arrangements is

$$\binom{\tilde{k}}{m} = \prod_{n=0}^{N} \binom{\tilde{k}_n}{m_n}.$$
(3.5)

Combining (3.4) and (3.5) yields a total tree count of

$$\# \{ \mathbf{p} \in \mathsf{S}_M \,|\, (\kappa(\mathbf{p}), \beta(\mathbf{p})) = (k, m) \} = \binom{k}{m} \binom{\tilde{k}}{m}$$

as was to be shown.

Theorem 3.1 Let (τ', R) correspond to an *M*-layer medium for some integer $M \ge 1$, and write $|\tau'| = \tau_0 + \cdots + \tau_{M+1}$. Then

$$H^{(\tau',R)}(t) = \sum_{k \in \{0\} \times \mathbb{Z}_+^M} b(R,k) \,\delta\big(t - \frac{1}{2} |\tau'| - \langle k, \tau \rangle\big)$$

where for each $k \in \{0\} \times \mathbb{Z}^M_+$, the amplitude b(R, k) is given by the formula

$$b(R,k) = \sum_{0 \le m \le \min\{k,\tilde{k}\}} \binom{k}{m} \binom{\tilde{k}}{m} (-R)^{\tilde{k}-m} R^{k-m} T^{2m+1}.$$
(3.6)

Proof. Given τ' , observe that the arrival time for a transmission scattering sequence $\mathbf{p} \in S'_M$ having $\kappa'(\mathbf{p}) = k$ is precisely

$$\frac{1}{2}|\tau'| + \langle k, \tau \rangle$$

17 May 2013

The theorem then follows from Lemmas 3.2 and 3.3.

Note that the factor T^{1} occurring in the formula for the transmission amplitude b(R,k) has the form

$$T^{\mathbb{1}} = \sqrt{1 - R_0^2} \sqrt{1 - R_1^2} \cdots \sqrt{1 - R_M^2},$$

which is not a polynomial in the reflection coefficients (R_0, \ldots, R_M) . So it turns out that $b(R, k)/T^{1}$ is a polynomial in the reflection coefficients, while b(R, k) itself is not. (Recall that by contrast reflection amplitudes a(R, k)are polynomial functions of the reflection coefficients.)



4 An example

Figure 8: The exact reflection Green's function (a) for the example (4.1), and the underlying reflection coefficients plotted against two-way travel time (b). The exact transmission Green's function (c) is plotted on a smaller amplitude scale, with the same reflection coefficients plotted against one-way travel time (d).

The formulas presented in Theorems 2.1 and 3.1 make it easy to compute the reflection and transmission Green's functions exactly up to a finite cutoff time T > 0. We illustrate this in the present situation by working out a

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numerical example. Consider the pair (τ, R) representing an M = 10 layer medium, with the following values.

n	Two-way travel time from $z \rightarrow to z$	$ au_n$	R_n	
	$\lim z_{-1} \text{ to } z_n$			
0	0.432779	0.432779	-0.821708	
1	0.459894	0.0271153	-0.950247	
2	1.1509	0.69101	-0.634818	
3	1.51027	0.35937	0.497529	
4	2.16748	0.657201	-0.66719	(4
5	2.58797	0.420491	0.338592	
6	3.04205	0.454083	0.447163	
7	3.95335	0.911298	0.567927	
8	4.20316	0.249813	-0.256277	
9	4.34889	0.145731	0.630965	
10	4.38014	0.0312502	-0.346928	

Setting $\tau_{M+1} = 0$, which corresponds to measuring the transmission response exactly at z_M , formulas for $G^{(\tau,R)}$ and $H^{(\tau',R)}$ given in Theorems 2.1 and 3.1 were coded up in Mathematica. The resulting functions were computed up to a cutoff time of 5.38 seconds for reflection and 3.69 seconds for transmission. (The respective computations took 3.37 seconds and 17.35 seconds on a 1.8 GHz i7 processor.) The computed pulse trains are depicted in Figure 8. The reflected pulse train has 19 242 terms, and the transmitted one has 35 059 terms; the majority of these are of an amplitude which is too small to be visible in the plots.

This example illustrates that Theorems 2.1 and 3.1, while derived by combinatorial methods not usually associated with the analysis of PDEs, offer a computationally tractable representation of reflected and transmitted waves. This provides a new tool for application to the various imaging modalities where one-dimensional models are important.

A Appendix: The underlying PDE

Let u(t, z) denote the velocity (in the z-direction) of a material particle at depth z and time t, and let p(t, z) denote the pressure. The medium evolves

according to the coupled one-dimensional equations

$$\rho \frac{\partial u}{\partial t} + \frac{\partial p}{\partial z} = 0 \tag{A.1a}$$

$$\frac{1}{K}\frac{\partial p}{\partial t} + \frac{\partial u}{\partial z} = 0. \tag{A.1b}$$

where $\rho(z)$ is the material density at depth z and K(z) is the bulk modulus. For the sake of definiteness we focus on the velocity field u(t, z), although the results can just as easily be formulated in terms of p(t, z). The initial conditions corresponding to a plane wave unit impulse propagating downward from z_{-1} are

$$u(0,z) = \delta(z - z_{-1})$$

$$p(0,z) = \sqrt{K(z_{-1})\rho(z_{-1})} \,\delta(z - z_{-1}).$$
(A.2)

Letting G(t) denote the (velocity) impulse response at z_{-1} , we have that

$$G(t) = u(t, z_{-1})$$
 (t > 0), (A.3)

the solution at depth z_{-1} to the system (A.1a,A.1b,A.2). Similarly, the impulse response at z_{M+1} is

$$H(t) = u(t, z_{M+1})$$
 (t > 0), (A.4)

the solution at depth z_{M+1} to the system (A.1a,A.1b,A.2).

The following facts are derived in [4, Chapter 3], [3, Section 2] and elsewhere. For $1 \leq n \leq M$, let τ_n denote the two-way travel time (for a traveling wave) across the *n*th layer of the above *M*-layer medium, and let τ_0 denote the two-way travel time from depth z_{-1} to z_0 . For $0 \leq n \leq M$, let R_n denote the reflection coefficient at depth z_n relative to a wave traveling toward the interface from above. Letting K_n and ρ_n denote the density and bulk modulus inside the *n*th layer—with K_{-1} , ρ_{-1} and K_{M+1} , ρ_{M+1} denoting the respective values at z_{-1} and any point z_{M+1} below z_M —the travel times and reflection coefficients are given by the formulas

$$\tau_n = \frac{2(z_n - z_{n-1})}{\sqrt{K_n/\rho_n}} \quad \text{and} \quad R_n = \frac{\sqrt{K_n\rho_n} - \sqrt{K_{n+1}\rho_{n+1}}}{\sqrt{K_n\rho_n} + \sqrt{K_{n+1}\rho_{n+1}}}, \tag{A.5}$$

for $0 \le n \le M$. Note that $-1 < R_n < 1$ by virtue of (A.5).

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