Wave-field representations with Green’s functions, propagator matrices and Marchenko-type focusing functions

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Abstract

Classical acoustic wave-field representations consist of volume and boundary integrals, of which the integrands contain specific combinations of Green’s functions, source distributions and wave fields. Using a unified matrix-vector wave equation for different wave phenomena, these representations can be reformulated in terms of Green’s matrices, source vectors and wave-field vectors. The matrix-vector formalism also allows the formulation of representations in which propagator matrices replace the Green’s matrices. These propagator matrices, in turn, can be expressed in terms of Marchenko-type focusing functions. An advantage of the representations with propagator matrices and focusing functions is that the boundary integrals in these representations are limited to a single open boundary. This makes these representations a suitable basis for developing advanced inverse scattering, imaging and monitoring methods for wave fields acquired on a single boundary.
I. INTRODUCTION

The aim of this paper is to give a systematic treatment of different types of wave-field representation (with Green’s functions, propagator matrices and Marchenko-type focusing functions), to discuss their mutual relations, and indicate some new applications.

- Representations with Green’s functions. A Green’s function is the response of a medium to an impulsive point source. It is named after George Green, who, in a privately published essay [1], introduced the use of impulse responses in field representations [2]. Wave-field representations with Green’s functions have been formulated, among others, for optics [3], acoustics [4, 5], elastodynamics [6–9] and electromagnetics [10–12]. They find numerous applications in forward modeling problems [13–15], inverse source problems [12, 16], inverse scattering problems [5, 17–19], imaging [20–25], time-reversal acoustics [26], and Green’s function retrieval from ambient noise [27–29].

- Representations with propagator matrices. In elastodynamic wave theory, a matrix formalism has been introduced to describe the propagation of waves in laterally invariant layered media [30, 31]. This formalism was refined by Gilbert and Backus [32], who coined the name propagator matrix. In essence, a propagator matrix ‘propagates’ a wave field (represented as a vectorial quantity) from one plane in space to another. Using perturbation theory, the connection between wave-field representations with Green’s functions and the propagator matrix formalism was discussed [33]. The propagator matrix has been extended for laterally varying isotropic and anisotropic layered media [34, 35]. Propagation invariants for laterally varying layered media have been introduced and the propagator matrix concept has been proposed for the modeling of reflection and transmission responses [36–39]. The propagator matrix has
also been used in a seismic imaging method that accounts for multiple scattering in a model-driven way [40].

- **Representations with Marchenko-type focusing functions.** Building on a 1D acoustic autofocusing method, it has been shown that the wave field inside a laterally invariant layered medium can be retrieved with the Marchenko method from the single-sided reflection response at the surface of the medium [41–43]. This concept was extended to a 3D Marchenko wave-field retrieval method for laterally varying media [44]. Central in the 3D Marchenko method are wave-field representations containing focusing functions. These representations have found applications in imaging methods [45–47] and inverse source problems [48] that account for multiple scattering in a data-driven way.

The setup of this paper is as follows. In section II we briefly review the matrix-vector wave equation for laterally varying media [34, 35], generalized for different wave phenomena, and we briefly discuss the concept of the Green’s matrix, the propagator matrix and the Marchenko-type focusing function. The symmetry properties of the matrix-vector wave equation allow the formulation of unified matrix-vector wave-field reciprocity theorems [49, 50], which are reviewed in section III. These reciprocity theorems form the basis for a systematic treatment of the different types of wave-field representation mentioned above. Traditionally, a wave-field representation is obtained by replacing one of the states in a reciprocity theorem by a Green’s state. In section IV we follow this approach for the matrix-vector reciprocity theorems. By replacing one of the wave-field vectors by the Green’s matrix (and the source vector by a unit source matrix) we obtain wave-field representations with Green’s matrices. Analogous to this, in section V we replace one of the wave-field vectors in
the reciprocity theorems by the propagator matrix and thus obtain wave-field representations
with propagator matrices. In section VI we discuss a mixed form, obtained by replacing one
of the wave-field vectors by the Green’s matrix and the other by the propagator matrix. In
section VII we discuss the relation between the propagator matrix and the Marchenko-type
focusing functions and use this relation to derive wave-field representations with focusing
functions. We end with conclusions in section VIII.

II. THE UNIFIED MATRIX-VECTOR WAVE EQUATION, THE GREEN’S MA-
TRIX, THE PROPAGATOR MATRIX AND THE FOCUSING FUNCTION

A. The matrix-vector wave equation

We use a unified matrix-vector wave equation as the basis for the derivations in this
paper. In the space-frequency domain it has the following form [32–36]

$$\partial_3 \mathbf{q} - \mathbf{A} \mathbf{q} = \mathbf{d},$$  \hspace{1cm} (1)

with

$$\mathbf{q} = \begin{pmatrix} \mathbf{q}_1 \\ \mathbf{q}_2 \end{pmatrix}, \quad \mathbf{d} = \begin{pmatrix} \mathbf{d}_1 \\ \mathbf{d}_2 \end{pmatrix}, \quad \mathbf{A} = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix}. \hspace{1cm} (2)$$

Here $\mathbf{q}(x, \omega)$ is a space- and frequency-dependent $N \times 1$ wave-field vector, where $x$ denotes
the Cartesian coordinate vector $(x_1, x_2, x_3)$ (with the positive $x_3$-axis pointing downward)
and $\omega$ the angular frequency. The $N/2 \times 1$ sub-vectors $\mathbf{q}_1(x, \omega)$ and $\mathbf{q}_2(x, \omega)$ contain wave-
field quantities, which are specified for different wave phenomena in Table I. Operator $\partial_3$
stands for the differential operator $\partial/\partial x_3$. Matrix $\mathbf{A}(x, \omega)$ is an $N \times N$ operator matrix;
it contains the space- and frequency-dependent anisotropic medium parameters and the horizontal differential operators \( \partial_1 \) and \( \partial_2 \). Definitions of this operator matrix for different wave phenomena can be found in many of the references mentioned in the introduction.

\( N \times 1 \) vector \( \mathbf{d}(\mathbf{x}, \omega) \) contains the space- and frequency-dependent source functions. A comprehensive overview of the operator matrices and source vectors for the wave phenomena considered in Table I (with some minor modifications) is given in reference [51].

For all wave phenomena considered in Table I, operator matrix \( \mathbf{A} \) obeys the following symmetry properties

\[
\mathbf{A}^\dagger \mathbf{N} = - \mathbf{N} \mathbf{A}, \quad (3)
\]

\[
\mathbf{A}^\dagger \mathbf{K} = - \mathbf{K} \bar{\mathbf{A}}, \quad (4)
\]

\[
\mathbf{A}^* \mathbf{J} = \mathbf{J} \bar{\mathbf{A}}, \quad (5)
\]

with

\[
\mathbf{N} = \begin{pmatrix} \mathbf{O} & \mathbf{I} \\ -\mathbf{I} & \mathbf{O} \end{pmatrix}, \quad \mathbf{K} = \begin{pmatrix} \mathbf{O} & \mathbf{I} \\ \mathbf{I} & \mathbf{O} \end{pmatrix}, \quad \mathbf{J} = \begin{pmatrix} \mathbf{I} & \mathbf{O} \\ \mathbf{O} & -\mathbf{I} \end{pmatrix}, \quad (6)
\]

where \( \mathbf{O} \) and \( \mathbf{I} \) are \( N/2 \times N/2 \) zero and identity matrices. Superscript \( t \) denotes transposition (meaning that the matrix is transposed and the operators in the matrix are also transposed, with \( \partial_1^t = -\partial_1 \) and \( \partial_2^t = -\partial_2 \)), \( * \) denotes complex conjugation, and \( \dagger \) transposition and complex conjugation. In general, the medium parameters in \( \mathbf{A} \) are complex-valued and frequency-dependent, accounting for losses. The bar above a quantity means that this quantity is defined in the adjoint medium. Hence, if \( \mathbf{A} \) is defined in a lossy medium, then \( \bar{\mathbf{A}} \) is defined in an effectual medium and vice versa [52] (a wave propagating through an
effectual medium gains energy). For lossless media the bar can be dropped. For all wave
phenomena considered in Table I, the power-flux density \( j \) in the \( x_3 \)-direction is related to
the sub-vectors \( \mathbf{q}_1 \) and \( \mathbf{q}_2 \) according to

\[
 j = \frac{1}{4}(\mathbf{q}_1 \dagger \mathbf{q}_2 + \mathbf{q}_2 \dagger \mathbf{q}_1).
\]  

(7)

As a special case we consider acoustic waves in an inhomogeneous stationary medium,
with complex-valued and frequency-dependent compressibility \( \kappa(x, \omega) \) and mass density
\( \rho_{kl}(x, \omega) \). The latter is defined as a tensor, to account for effective anisotropy, for example
due to fine layering at the micro scale [53]. The mass density tensor is symmetric, that is,
\( \rho_{kl}(x, \omega) = \rho_{lk}(x, \omega) \). We introduce the inverse of the mass density tensor, the specific vol-
ume tensor \( \vartheta_{kl}(x, \omega) \), via

\[
\vartheta_{kl} \rho_{lm} = \delta_{km}.
\]

Einstein’s summation convention holds for repeated
subscripts (unless otherwise noted); Latin subscripts run from 1 to 3 and Greek subscripts
from 1 to 2. For the acoustic situation the vectors and matrix in Eq. (1) are given by

\[
 \mathbf{q} = \begin{pmatrix} p \\ v_3 \end{pmatrix}, \quad \mathbf{d} = \begin{pmatrix} \partial_{33}^{-1} \partial_{3l} f_l \\ \frac{1}{i\omega} \partial_{\alpha}(b_{\alpha\beta} f_{\beta}) + q \end{pmatrix},
\]

(8)

\[
 \mathbf{A} = \begin{pmatrix} -\partial_{33}^{-1} \partial_{3\beta} \partial_{\beta} & i\omega \partial_{33}^{-1} \\ i\omega \kappa - \frac{1}{i\omega} \partial_{\alpha} b_{\alpha\beta} \partial_{\beta} & -\partial_{\alpha} \partial_{\alpha3} \partial_{33}^{-1} \partial_{3\beta} \end{pmatrix},
\]

(9)

with

\[
b_{\alpha\beta} = \partial_{\alpha\beta} - \partial_{\alpha3} \partial_{33}^{-1} \partial_{3\beta},
\]

(10)

where \( i \) is the imaginary unit and \( q(x, \omega) \) and \( f_l(x, \omega) \) are sources in terms of volume-injection
rate density and external force density, respectively.
Finally, for an isotropic medium, using $\vartheta_{kl} = \rho^{-1} \delta_{kl}$ (with $\rho$ the scalar mass density), we obtain for the source vector and operator matrix [54–58]

$$d = \begin{pmatrix} f_3 \\ \frac{1}{i\omega} \partial_\alpha (\frac{1}{\rho} f_\alpha) + q \end{pmatrix}, \quad A = \begin{pmatrix} 0 & i\omega \rho \\ i\omega \kappa - \frac{1}{i\omega} \partial_\alpha \frac{1}{\rho} \partial_\alpha & 0 \end{pmatrix}. \quad (11)$$

B. The Green’s matrix

In the space-time domain, a Green’s function is the response to an impulsive point source, with the impulse defined as $\delta(t)$. The Fourier transform of $\delta(t)$ equals 1, hence, in the space-frequency domain the Green’s function is the response to a point source with unit amplitude for all frequencies. We introduce the $N \times N$ Green’s matrix $G(x, x_A, \omega)$ for an unbounded, arbitrary inhomogeneous, anisotropic medium as the solution of

$$\partial_3 G - AG = I \delta(x - x_A), \quad (12)$$

where $x_A = (x_{1,A}, x_{2,A}, x_{3,A})$ defines the position of the point source and $I$ is an $N \times N$ identity matrix. Here $I$ has a size different from that in Eq. (6). For simplicity we use one notation for differently sized identity matrices (the size always follows from the context). Also for the zero matrix $O$ we use a single notation for differently sized matrices. Similar to operator matrix $A$, the Green’s matrix is partitioned as

$$G(x, x_A, \omega) = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix}(x, x_A, \omega). \quad (13)$$
Equation (12) does not have a unique solution. To specify a unique solution, we demand that the time-domain Green’s function $G(x, x_A, t)$ is causal, hence

$$G(x, x_A, t < 0) = 0.$$  \hspace{1cm} (14)

This condition implies that $G$ is outward propagating for $|x - x_A| \to \infty$.

The simplest representation involving the Green’s matrix is obtained when $q$ and $G$ reside in the same medium throughout space and both are outward propagating for $|x - x_A| \to \infty$. Whereas $q(x, \omega)$ is the response to a source distribution $d(x, \omega)$ (Eq. (1)), $G(x, x_A, \omega)$ is the response to a point source $I\delta(x - x_A)$ for an arbitrary source position $x_A$ (Eq. (12)). Since both equations are linear, a representation for $q(x, \omega)$ follows by applying the superposition principle, according to

$$q(x, \omega) = \int_{\mathbb{R}^3} G(x, x_A, \omega)d(x_A, \omega)d^3x_A,$$ \hspace{1cm} (15)

where $\mathbb{R}$ is the set of real numbers. This representation is a special case of more general representations with Green’s matrices, derived in a more formal way in section IV.

Next, we discuss the $2 \times 2$ acoustic Green’s matrix as a special case of the $N \times N$ Green’s matrix. For this situation $G$ is partitioned as

$$G(x, x_A, \omega) = \begin{pmatrix} G^{p,f} & G^{p,q} \\ G^{v,f} & G^{v,q} \end{pmatrix}(x, x_A, \omega).$$ \hspace{1cm} (16)

Here the first superscript ($p$ or $v$) refers to the observed wave-field quantity at $x$ (acoustic pressure or vertical component of particle velocity), whereas the second superscript ($f$ or $q$) refers to the source type at $x_A$ (vertical component of force or volume injection rate).
unit of a specific element of the Green’s matrix is the ratio of the units of the observed wave-
field quantity at \( \mathbf{x} \) and the source quantity at \( \mathbf{x}_A \). For example, \([G^{p,f}(\mathbf{x}, \mathbf{x}_A, \omega)] = \frac{|p|}{|f|} = \text{m}^{-2}\). For an isotropic medium, all elements can be expressed in terms of the upper-right

\[
G^{\rho,d}(\mathbf{x}, \mathbf{x}_A, \omega) = \frac{1}{i \omega \rho(\mathbf{x}, \omega)} \partial_3 G^{\rho,d}(\mathbf{x}, \mathbf{x}_A, \omega),
\]

(17)

\[
G^{p,f}(\mathbf{x}, \mathbf{x}_A, \omega) = -\frac{1}{i \omega \rho(\mathbf{x}_A, \omega)} \partial_3 G^{p,d}(\mathbf{x}, \mathbf{x}_A, \omega),
\]

(18)

\[
G^{v,f}(\mathbf{x}, \mathbf{x}_A, \omega) = \frac{1}{i \omega \rho(\mathbf{x}, \omega)} \left( \partial_3 G^{p,f}(\mathbf{x}, \mathbf{x}_A, \omega) - \delta(\mathbf{x} - \mathbf{x}_A) \right).
\]

(19)

Here \( \partial_3 \) stands for differentiation with respect to the source coordinate \( x_{3,A} \). Equations

(17) and (19) follow directly from Eqs. (11), (12) and (16). Equation (18) follows from Eq.

(17) and a source-receiver reciprocity relation, which is derived in section IV A.

We illustrate \( G^{\rho,q} \), decomposed into plane waves, for a horizontally layered lossless

isotropic medium. To this end, we first define the spatial Fourier transform of a space-

and frequency-dependent function \( u(\mathbf{x}, \omega) \) along the horizontal coordinates \( \mathbf{x}_H = (x_1, x_2) \),

according to

\[
\tilde{u}(\mathbf{s}, x_3, \omega) = \int_{\mathbb{R}^2} \exp\{-i\omega \mathbf{s} \cdot \mathbf{x}_H\} u(\mathbf{x}_H, x_3, \omega) d^2 \mathbf{x}_H,
\]

(20)

with \( \mathbf{s} = (s_1, s_2) \), where \( s_1 \) and \( s_2 \) are horizontal slownesses. This transform decomposes

the function \( u(\mathbf{x}, \omega) \) at a given depth level \( x_3 \) into monochromatic plane-wave components.

Next, we define the inverse temporal Fourier transform, per slowness value \( \mathbf{s} \), as

\[
u(\mathbf{s}, x_3, \tau) = \frac{1}{\pi} \Re \int_0^\infty \tilde{u}(\mathbf{s}, x_3, \omega) \exp\{-i \omega \tau\} d\omega,
\]

(21)
where $\Re$ denotes the real part and $\tau$ is the intercept time [59]. We apply these transforms to the Green’s function $G^{p,q}(s_1, x_3, x_{3,0}, \tau)$ and the source function $\delta(x - x_A)$, choosing $x_A = (0, 0, x_{3,0})$ and setting $s_2 = 0$ (the field is cylindrically symmetric in the considered horizontally layered isotropic medium). We thus obtain $G^{p,q}(s_1, x_3, x_{3,0}, \tau)$, which is the plane-wave response (as a function of $x_3$ and $\tau$) to a source function $\delta(x_3 - x_{3,0})\delta(\tau)$.

An example horizontally layered medium is shown in Fig. 1(a). The propagation velocities in the layers are indicated by $c_n$ (with $c = 1/\sqrt{\kappa \rho}$). The depth level of the source is chosen as $x_{3,0} = 0$ m, see Fig. 1(b). The vertical green line in this figure is the line $\tau = 0$, left of which the field is zero due to the causality condition (similar as in Eq. (14)). Figure 1(b)
further shows the numerically modelled Green’s function $G^{p,q}(s_1, x_3, x_{3,0}, \tau)$ as a function of $x_3$ and $\tau$, for a single horizontal slowness $s_1 = 1/3500$ s/m (red and blue arrows indicate downgoing and upgoing waves). This is the wave field that would be measured by a series of acoustic pressure receivers, vertically above and below the volume-injection rate source at $x_{3,0} = 0$ m. Each trace shows $G^{p,q}(s_1, x_3, x_{3,0}, \tau)$ for a specific depth $x_3$ as a function of $\tau$ (actually, at each depth the Green’s function has been convolved with a time-symmetric wavelet, with a central frequency of 50 Hz, to get a nicer display).

The horizontal slowness $s_1$ is related to the propagation angle $\alpha_n$ in layer $n$ via $\sin \alpha_n = s_1 c_n$, hence, in layer 1 (with $c_1 = 1600$ m/s) the propagation angle is $\alpha_1 = 27.2^\circ$. In the thin layer, with $c_3 = 3600$ m/s, we obtain $\sin \alpha_3 = 1.03$, meaning that $\alpha_3$ is complex-valued. This implies that the wave is evanescent in this layer. Since the layer is thin, the wave tunnels through the layer and continues with a lower amplitude as a downgoing wave in the lower half-space.

C. The homogeneous Green’s matrix

For a lossless medium, a homogeneous Green’s function is the superposition of a Green’s function and its complex conjugate (or, in the time domain, its time-reversed version). The superposition is chosen such that the source terms of the two functions cancel each other, hence, a homogeneous Green’s function obeys a wave equation without a source term [19, 20]. Here we extend this concept for the matrix-vector wave equation for a medium with losses.

Let $G(x, x_A, \omega)$ be again the outward propagating solution of Eq. (12) for an unbounded, arbitrary inhomogeneous, anisotropic medium. We introduce the Green’s matrix of the
adjoint medium, \( G(x, x_A, \omega) \), as the outward propagating solution of

\[
\partial_3 \bar{G} - \bar{A} \bar{G} = I \delta(x - x_A). \tag{22}
\]

Pre- and post multiplying all terms by \( J \) and subsequently using Eq. (5) and \( JJ = I \) gives

\[
\partial_3 J \bar{G} - A^* J \bar{G} = I \delta(x - x_A). \tag{23}
\]

Subtracting the complex conjugate of all terms in this equation from the corresponding terms in Eq. (12) yields

\[
\partial_3 G_h - A G_h = 0, \tag{24}
\]

with

\[
G_h(x, x_A, \omega) = G(x, x_A, \omega) - J \bar{G}^*(x, x_A, \omega) J. \tag{25}
\]

Since \( G_h(x, x_A, \omega) \) obeys a wave equation without a source term, we call it the homogeneous Green’s matrix. According to Eqs. (6), (13) and (25), it is partitioned as

\[
G_h(x, x_A, \omega) = \begin{pmatrix}
\{G_{11} - \bar{G}_{11}^*\} & \{G_{12} + \bar{G}_{12}^*\} \\
\{G_{21} + \bar{G}_{21}^*\} & \{G_{22} - \bar{G}_{22}^*\}
\end{pmatrix}(x, x_A, \omega). \tag{26}
\]

D. The propagator matrix

We introduce the \( N \times N \) propagator matrix \( W(x, x_A, \omega) \) for an arbitrary inhomogeneous anisotropic medium as the solution of the unified matrix-vector wave equation (1), but
without the source vector $d$. Hence,

$$\partial_3 W - \mathcal{A}W = 0.$$  \hfill (27)

Similar to operator matrix $\mathcal{A}$ and Green’s matrix $G$, the propagator matrix is partitioned as

$$W(x, x_A, \omega) = \begin{pmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{pmatrix} (x, x_A, \omega).$$  \hfill (28)

Equation (27) does not have a unique solution. To specify a unique solution, we impose the boundary condition

$$W(x, x_A, \omega)|_{x_3 = x_{3,A}} = \mathbf{I} \delta(x_H - x_{H,A}),$$  \hfill (29)

where $x_{H,A}$ denotes the horizontal coordinates of $x_A$, hence, $x_{H,A} = (x_{1,A}, x_{2,A})$. Since Eq. (27) is first order in $\partial_3$, a single boundary condition suffices. Note that $W(x, x_A, \omega)$ only depends on the medium parameters between depth levels $x_{3,A}$ and $x_3$. This is different from the Green’s matrix $G(x, x_A, \omega)$, which, for an arbitrary inhomogeneous medium, depends on the entire medium (this is easily understood from the illustration in Fig. 1(b)).

The simplest representation involving the propagator matrix is obtained when $q$ and $W$ reside in the same medium in the region between $x_{3,A}$ and $x_3$ and both have no sources in this region. Whereas $q(x, \omega)$ obeys no boundary conditions in this region, $W(x, x_A, \omega)$ collapses to $\mathbf{I} \delta(x_H - x_{H,A})$ at depth level $x_{3,A}$ (Eq. (29)). Applying the superposition principle again
yields

\[ q(x, \omega) = \int_{\partial D_A} W(x, x_A, \omega) q(x_A, \omega) d^2 x_A, \quad (30) \]

where \( \partial D_A \) is the horizontal boundary defined as \( x_3 = x_{3,A} \) [32–36]. Note that \( W(x, x_A, \omega) \) ‘propagates’ the field vector \( q \) from depth level \( x_{3,A} \) to \( x_3 \), hence the name ‘propagator matrix’. This representation is a special case of more general representations with propagator matrices, derived in a more formal way in section V.

When we replace \( q(x_A, \omega) \) by a Green’s matrix \( G(x_A, x_B, \omega) \), with \( x_B \) outside the region between \( x_{3,A} \) and \( x_3 \), we obtain

\[ G(x, x_B, \omega) = \int_{\partial D_A} W(x, x_A, \omega) G(x_A, x_B, \omega) d^2 x_A. \quad (31) \]

This is the simplest relation between the Green’s matrix and the propagator matrix. It is a special case of more general representations with Green’s matrices and propagator matrices, derived in a more formal way in section VI A. Alternatively, we may replace \( G(x, x_B, \omega) \) by the homogeneous Green’s matrix \( G_h(x, x_B, \omega) \), where \( x_B \) may be located anywhere, since the homogeneous Green’s function has no source at \( x_B \), hence

\[ G_h(x, x_B, \omega) = \int_{\partial D_A} W(x, x_A, \omega) G_h(x_A, x_B, \omega) d^2 x_A. \quad (32) \]

This relation will be derived in a more formal way in section VI B.

Next, we discuss the \( 2 \times 2 \) acoustic propagator matrix as a special case of the \( N \times N \)
propagator matrix. For this situation \( W \) is partitioned as

\[
W(\mathbf{x}, \mathbf{x}_A, \omega) = \begin{pmatrix}
W^{p,p} & W^{p,v} \\
W^{v,p} & W^{v,v}
\end{pmatrix}(\mathbf{x}, \mathbf{x}_A, \omega).
\] (33)

The first and second superscripts refer to the wave-field quantities at \( \mathbf{x} \) and \( \mathbf{x}_A \), respectively (with superscript \( p \) again standing for acoustic pressure and \( v \) for the vertical component of particle velocity). The unit of a specific element of the propagator matrix is the ratio of the units of the wave-field quantities at \( \mathbf{x} \) and \( \mathbf{x}_A \). For example, \([W^{p,v}(\mathbf{x}, \mathbf{x}_A, \omega)] = [p]/[v] = \text{kg s}^{-1}\text{m}^{-2}\). For an isotropic medium, the elements can be expressed in terms of the upper-right element, as follows

\[
W^{v,v}(\mathbf{x}, \mathbf{x}_A, \omega) = \frac{1}{i\omega \rho(\mathbf{x}, \omega)} \partial_3 W^{p,v}(\mathbf{x}, \mathbf{x}_A, \omega), \tag{34}
\]

\[
W^{p,p}(\mathbf{x}, \mathbf{x}_A, \omega) = -\frac{1}{i\omega \rho(\mathbf{x}_A, \omega)} \partial_{3, A} W^{p,v}(\mathbf{x}, \mathbf{x}_A, \omega), \tag{35}
\]

\[
W^{v,p}(\mathbf{x}, \mathbf{x}_A, \omega) = \frac{1}{i\omega \rho(\mathbf{x}, \omega)} \partial_3 W^{p,p}(\mathbf{x}, \mathbf{x}_A, \omega). \tag{36}
\]

Equations (34) and (36) follow directly from Eqs. (11), (27) and (33). Equation (35) follows from Eqs. (34) and a source-receiver reciprocity relation, which is derived in section VA.

We illustrate the elements \( W^{p,p} \) and \( W^{p,v} \), decomposed into plane waves, for the horizontally layered medium of Fig. 1(a). We choose again \( \mathbf{x}_A = (0, 0, x_{3,0}) \) and set \( s_2 = 0 \). Usually the propagator matrix is considered in the frequency domain, but to facilitate the comparison with the Green’s function in Fig. 1(b), we consider the time-domain functions \( W^{p,p}(s_1, x_3, x_{3,0}, \tau) \) and \( W^{p,v}(s_1, x_3, x_{3,0}, \tau) \) (obtained via the transforms of Eqs. (20) and (21)), again for a single horizontal slowness \( s_1 = 1/3500 \text{ s/m} \), see Figs. 2(a) and 3(a). At \( x_3 = x_{3,0} \) (the horizontal green lines in these figures) the boundary conditions for these
FIG. 2. (color online) (a) Propagator element $W^{p,p}(s_1,x_3,x_3,0,\tau)$ (fixed $s_1$), convolved with a wavelet. (b) Last trace of (a).

FIG. 3. (color online) (a) Propagator element $W^{p,v}(s_1,x_3,x_3,0,\tau)$ (fixed $s_1$), convolved with a wavelet. (b) Last trace of (a).
functions are $W^{p,p}(s_1, x_{3,0}, x_{3,0}, \tau) = \delta(\tau)$ and $W^{p,v}(s_1, x_{3,0}, x_{3,0}, \tau) = 0$, respectively (this follows from applying the transforms of Eqs. (20) and (21) to Eq. (29), with $\mathbf{x}_{H,A} = (0, 0)$).

Following these functions along the depth coordinate, starting at $x_3 = x_{3,0}$, we observe an acausal upgoing wave and a causal downgoing wave until we reach the first interface. Here both events split into upgoing and downgoing waves below the interface. The waves tunnel through the high-velocity layer, split again, and continue with higher amplitudes in the next layer. This illustrates that evanescent waves may lead to unstable behaviour of the propagator matrix and should be handled with care. Note that $W^{p,p}(s_1, x_3, x_{3,0}, \tau)$ and $W^{p,v}(s_1, x_3, x_{3,0}, \tau)$ are symmetric and asymmetric in time, respectively. This is best seen in Figs. 2(b) and 3(b), which show the last trace of both elements. The same holds for elements $W^{v,v}$ and $W^{v,p}$, which are not shown.

E. The Marchenko-type focusing function

For an arbitrary inhomogeneous anisotropic medium, the time-domain version of boundary condition (29) reads

$$W(x, x_A, t)|_{x_3=x_{3,A}} = \mathbf{I} \delta(x_H - x_{H,A}) \delta(t).$$

(37)

This boundary condition has a similar form as the focusing condition for the focusing functions appearing in the multidimensional Marchenko method [44]. In section VII A we discuss the general relations between the propagator matrix and the Marchenko-type focusing functions. Here we present a short preview of these relations by considering the acoustic propagator matrix in the horizontally layered lossless isotropic medium of Fig. 1(a). We combine the elements $W^{p,p}$ and $W^{p,v}$, decomposed into plane waves (Figs. 2 and 3), as
follows [60]

\[ F^p(s_1, x_3, x_{3,0}, \tau) = W^{p,p}(s_1, x_3, x_{3,0}, \tau) - \frac{s_{3,0}}{\rho_0} W^{p,v}(s_1, x_3, x_{3,0}, \tau), \]  

(38)

where the vertical slowness \( s_{3,0} \) is defined as

\[ s_{3,0} = \sqrt{1/c_0^2 - s_1^2}, \]  

(39)

with \( c_0 \) and \( \rho_0 \) being the propagation velocity and mass density of the upper half-space \( x_3 \leq x_{3,0} \). Due to the symmetric form of \( W^{p,p} \) and the asymmetric form of \( W^{p,v} \), half of the events double in amplitude and the other half of the events cancel. The result is shown in Fig. 4. For the interpretation of this focusing function we start at the bottom of Fig. 4(a). The blue arrows indicate upgoing waves, which are tuned such that, after interaction with the tunneling waves in the thin layer and the downgoing wave just above the thin layer (indicated by a red arrow), they continue as a single upgoing wave, which finally focuses at depth level \( x_{3,0} \) as a temporal delta function \( \delta(\tau) \) and continues as an upgoing wave into the homogeneous upper half-space.

Note that, although we interpret the focusing function here in terms of upgoing and downgoing waves, it is derived from the propagator matrix (which does not rely on up/down decomposition) and the vertical slowness \( s_{3,0} \) and mass density \( \rho_0 \) of the upper half-space. Moreover, the focusing function is defined in the actual medium rather than in a truncated version of the actual medium, as is usually the case for Marchenko-type focusing functions [44]. Hence, the only assumption is that a real-valued vertical slowness \( s_{3,0} \) exists in the upper half-space. Other than that, the focusing function \( F^p(s_1, x_3, x_{3,0}, \tau) \), as defined in Eq. (38), does not require a truncated medium, does not rely on up/down decomposition.
FIG. 4. (color online) (a) Focusing function $F^p(s_1, x_3, x_3, 0, \tau)$ (fixed $s_1$), convolved with a wavelet. (b) Last trace of (a).

inside the medium, and does (at least in principle) not break down when waves become evanescent inside the medium. These properties also hold for the more general version of the Marchenko-type focusing functions defined in section VII.

III. UNIFIED MATRIX-VECTOR WAVE-FIELD RECIPROCITY THEOREMS

As the basis for the derivation of the general representations with Green’s matrices (section IV), propagator matrices (section V), or a combination thereof (section VI), we introduce unified matrix-vector wave-field reciprocity theorems. In general, a wave-field reciprocity theorem interrelates two wave states (sources, wave fields and medium parameters) in the same spatial domain [12]. Reciprocity theorems have been formulated for acoustic [4], electromagnetic [61], elastodynamic [62, 63], poroelastodynamic [64], piezoelectric [65, 66] and seismoelectric waves [67]. The matrix-vector equation discussed in section II allows a
unified formulation of the reciprocity theorems for these different wave phenomena [49, 50], which extends the theory of propagation invariants [36–39]. Using the symmetry properties of operator matrix $\mathcal{A}$, formulated in Eqs. (3) and (4), the following matrix-vector reciprocity theorems can be derived [49, 50]

$$\int_{D} (d_A^t \mathcal{N}q_B + q_A^t \mathcal{N}d_B) d^3x = \int_{\partial D_0 \cup \partial D_M} q_A^t \mathcal{N}q_B n_3 d^2x + \int_{D} q_A^t \mathcal{N}(\mathcal{A}_A - \mathcal{A}_B)q_B d^3x \quad (40)$$

and

$$\int_{D} (d_A^t \mathcal{K}q_B + q_A^t \mathcal{K}d_B) d^3x = \int_{\partial D_0 \cup \partial D_M} q_A^t \mathcal{K}q_B n_3 d^2x + \int_{D} q_A^t \mathcal{K}(\bar{\mathcal{A}}_A - \mathcal{A}_B)q_B d^3x. \quad (41)$$

Here $D$ denotes a domain enclosed by two infinite horizontal boundaries $\partial D_0$ and $\partial D_M$ at depth levels $x_{3,0}$ and $x_{3,M}$ with outward pointing normals $n_3 = -1$ and $n_3 = 1$, respectively, see Fig. 5. Subscripts $A$ and $B$ refer to two independent states. These theorems hold for lossless media and for media with losses [51]. Equation (40) is a convolution-type reciprocity theorem, since products like $q_A^t \mathcal{N}q_B$ in the frequency domain correspond to convolutions in the time domain (like in reference [63]). Equation (41) is a correlation-type reciprocity theorem, since products like $q_A^t \mathcal{K}q_B$ in the frequency domain correspond to correlations in the time domain (like in reference [18]).

A special case is obtained when the sources, wave fields and medium parameters are identical in both states. We may then drop the subscripts $A$ and $B$ and Eq. (41) simplifies to

$$\int_{D} \frac{1}{4} (d^t \mathcal{K}q + q^t \mathcal{K}d) d^3x = \int_{\partial D_0 \cup \partial D_M} \frac{1}{4} q^t \mathcal{K}q n_3 d^2x + \int_{D} \frac{1}{4} q^t \mathcal{K}(\bar{\mathcal{A}} - \mathcal{A})q d^3x. \quad (42)$$

Since $\frac{1}{4} q^t \mathcal{K}q = \frac{1}{4} (q_1^t q_2 + q_2^t q_1) = j$ (see Eq. (7)), Eq. (42) formulates the unified power
balance. The term on the left-hand side is the power generated by the sources in \( \mathbb{D} \). The first term on the right-hand side is the power flux through the boundary \( \partial \mathbb{D}_0 \cup \partial \mathbb{D}_M \) (i.e., the power leaving the domain \( \mathbb{D} \)) and the second term on the right-hand side is the dissipated power in \( \mathbb{D} \).

IV. REPRESENTATIONS WITH GREEN’S MATRICES

A wave-field representation is obtained by replacing one of the states in a reciprocity theorem by a Green’s state [6–9]. In this section we follow this approach to derive wave-field representations with Green’s matrices from the matrix-vector reciprocity theorems discussed in section III.

A. Symmetry property of the Green’s matrix

Before we derive wave-field representations, we first derive a symmetry property of the Green’s matrix. To this end, we replace both wave-field vectors \( \mathbf{q}_A \) and \( \mathbf{q}_B \) in reciprocity theorem (40) by Green’s matrices \( \mathbf{G}(\mathbf{x}, \mathbf{x}_A, \omega) \) and \( \mathbf{G}(\mathbf{x}, \mathbf{x}_B, \omega) \), respectively. Accordingly, we replace the source vectors \( \mathbf{d}_A \) and \( \mathbf{d}_B \) by \( \mathbf{I} \delta(\mathbf{x} - \mathbf{x}_A) \) and \( \mathbf{I} \delta(\mathbf{x} - \mathbf{x}_B) \), respectively, with
\( x_A \) and \( x_B \) denoting the source positions, see Figure 5. Furthermore, we replace \( \mathbb{D} \) by \( \mathbb{R}^3 \), so that the boundary integral in Eq. (40) vanishes (Sommerfeld radiation condition). Both Green’s matrices are defined in the same medium, hence, \( \mathcal{A}_A = \mathcal{A}_B \). This implies that the second integral on the right-hand side of Eq. (40) also vanishes. From the remaining integral we thus obtain the following symmetry property of the Green’s matrix

\[
G^t(x_B, x_A, \omega)N = -NG(x_A, x_B, \omega).
\]  

(43)

The Green’s matrix on the left-hand side is the response to a source at \( x_A \), observed by a receiver at \( x_B \). Similarly, the Green’s matrix on the right-hand side is the response to a source at \( x_B \), observed by a receiver at \( x_A \). Hence, Eq. (43) is a unified source-receiver reciprocity relation.

Using this relation and \( JN = -NJ \), we find for the homogeneous Green’s matrix defined in Eq. (25)

\[
G^t_h(x_B, x_A, \omega)N = -NG_h(x_A, x_B, \omega).
\]

(44)

B. Representations of the convolution type with the Green’s matrix

We derive a representation of the convolution type for the actual wave-field vector \( q(x, \omega) \), emitted by the actual source distribution \( d(x, \omega) \) in the actual medium; the operator matrix in the actual medium is defined as \( \mathcal{A}(x, \omega) \). We let state \( B \) in reciprocity theorem (40) be this actual state, hence, we drop subscript \( B \) from \( q_B \), \( d_B \) and \( \mathcal{A}_B \). For state \( A \) we choose the Green’s state. Hence, we replace \( q_A(x, \omega) \) in reciprocity theorem (40) by \( G(x, x_A, \omega) \) and \( d_A(x, \omega) \) by \( \delta(x - x_A) \). We keep the subscript \( A \) in \( \mathcal{A}_A(x, \omega) \), to account for the fact
that in general this operator matrix is defined in a medium that may be different from the actual medium. We thus obtain

$$\chi_D(x_A)Nq(x_A, \omega) = \int_D G_t(x, x_A, \omega)Nd(x, \omega)d^3x + \int_{\partial D_0 \cup \partial D_M} G_t(x, x_A, \omega)Nq(x, \omega)n_3d^2x$$

$$+ \int_D G_t(x, x_A, \omega)N(A - A)q(x, \omega)d^3x,$$

(45)

where \(\chi_D(x)\) is the characteristic function for domain \(D\), defined as

$$\chi_D(x) = \begin{cases} 1, & \text{for } x \text{ inside } D, \\ \frac{1}{2}, & \text{for } x \text{ on } \partial D_0 \cup \partial D_M, \\ 0, & \text{for } x \text{ outside } D. \end{cases}$$

(46)

Using the symmetry property of the Green’s matrix, formulated by Eq. (43), we obtain

$$\chi_D(x_A)q(x_A, \omega) = \int_D G(x_A, x, \omega)d(x, \omega)d^3x - \int_{\partial D_0 \cup \partial D_M} G(x_A, x, \omega)q(x, \omega)n_3d^2x$$

$$- \int_D G(x_A, x, \omega)\{A_A - A\}q(x, \omega)d^3x.$$

(47)

This is the unified wave-field representation of the convolution type with the Green’s matrix. The left-hand side is the wave-field vector \(q\) at a specific point \(x_A\), multiplied with the characteristic function. According to the right-hand side, this field consists of a contribution from the source distribution in \(D\) (the first integral), a contribution from the wave field on the boundary of \(D\) (the second integral), and a contribution caused by the contrasts between the operator matrices in the Green’s and the actual state (the third integral).

Note that Eq. (15) follows as a special case of Eq. (47) if we choose the same medium parameters in both states and replace \(D\) by \(\mathbb{R}^3\) (except that the roles of \(x\) and \(x_A\) are
interchanged since we used the symmetry property of Eq. (43) in the derivation of Eq. (47)).

Next we consider another special case. We choose again the same medium parameters in both states, but this time we replace $D$ by the entire half-space below $\partial D_0$, which we choose to be source-free in the actual state. Assuming $\mathbf{x}_A$ lies in the lower half-space, we thus obtain

$$q(\mathbf{x}_A, \omega) = \int_{\partial D_0} G(\mathbf{x}_A, \mathbf{x}, \omega) q(\mathbf{x}, \omega) d^2 \mathbf{x}, \quad \text{for } x_{3,A} > x_{3,0}. \quad (48)$$

Using Eqs. (8), (16) and (18) for the isotropic acoustic situation, Eq. (48) yields for the upper element of $q(\mathbf{x}_A, \omega)$

$$p(\mathbf{x}_A, \omega) = \int_{\partial D_0} \left( -\frac{1}{i\omega \rho(\mathbf{x}, \omega)} \{ \partial_3 G^{p,q}(\mathbf{x}_A, \mathbf{x}, \omega) \} p(\mathbf{x}, \omega) + G^{p,q}(\mathbf{x}_A, \mathbf{x}, \omega) v_3(\mathbf{x}, \omega) \right) d^2 \mathbf{x}, \quad (49)$$

which is the well-known acoustic Kirchhoff-Helmholtz integral. Hence, the representation of Eq. (48) is the unified Kirchhoff-Helmholtz integral. It can be used for forward wave-field extrapolation of the wave-field vector $q(\mathbf{x}, \omega)$ from $\partial D_0$ to any point $\mathbf{x}_A$ below $\partial D_0$.

Note that the Green’s matrix $G(\mathbf{x}_A, \mathbf{x}, \omega)$ depends on the medium parameters of the entire half-space below $\partial D_0$. In section V B we derive a relation similar to Eq. (48), but with the Green’s matrix replaced by the propagator matrix, which depends only on the medium parameters between $x_{3,0}$ and $x_{3,A}$.

Finally, we replace $q(\mathbf{x}, \omega)$ by $G(\mathbf{x}, \mathbf{x}_B, \omega)$ in Eq. (48). Since we assumed that the lower half-space is source-free for $q$, we choose $\mathbf{x}_B$ in the upper half-space. We thus obtain

$$G(\mathbf{x}_A, \mathbf{x}_B, \omega) = \int_{\partial D_0} G(\mathbf{x}_A, \mathbf{x}, \omega) G(\mathbf{x}, \mathbf{x}_B, \omega) d^2 \mathbf{x}, \quad \text{for } x_{3,A} > x_{3,0} > x_{3,B}. \quad (50)$$
This expression shows that the Green’s matrix can be composed from a cascade of Green’s matrices, assuming a specific order of the depth levels at which the Green’s sources and receivers are situated. In section VB we derive a similar relation for propagator matrices, for an arbitrary order of depth levels.

Equation (50) can be seen as a generalization of the representation that underlies Green’s function retrieval by cross-convolution (where \( G(x_A, x_B, \omega) \) is the unknown [68]) or by multidimensional deconvolution (where \( G(x_A, x, \omega) \) is the unknown [69]).

C. Representations of the correlation type with the Green’s matrix

We derive a representation of the correlation type for the actual wave-field vector \( q(x, \omega) \), emitted by the actual source distribution \( d(x, \omega) \) in the actual medium. Similar as in section IVB, we let state \( B \) be this actual state, and state \( A \) the Green’s state. Hence, making the same substitutions as in section IVB, this time in reciprocity theorem (41), using Eq. (43) and \( N^{-1} K = -J \), yields

\[
\chi_D(x_A) q(x_A, \omega) = \int_D J G^*(x_A, x, \omega) J d(x, \omega) d^3x - \int_{\partial D_D \cup \partial D_M} J G^*(x_A, x, \omega) J q(x, \omega) n_3 d^2x - \int_D J G^*(x_A, x, \omega) J \{ \mathcal{A}_A - \mathcal{A} \} q(x, \omega) d^3x.
\]

(51)

This is the unified wave-field representation of the correlation type with the Green’s matrix.

As a special case we derive a representation for the homogeneous Green’s matrix \( G_h \). To this end, for state \( B \) we choose the Green’s matrix in the actual medium, hence, we replace \( q(x, \omega) \) by \( G(x, x_B, \omega) \), and \( d(x, \omega) \) by \( \mathbf{I} \delta(x - x_B) \). For state \( A \) we replace the Green’s matrix by that in the adjoint of the actual medium, hence, we replace \( G(x_A, x, \omega) \) by \( \bar{G}(x_A, x, \omega) \), and \( \mathcal{A}_A \) by \( \bar{A} \). With this choice the contrast operator \( \bar{A}_A - \mathcal{A} = \bar{A} - \mathcal{A} \) vanishes. Making
these substitutions in Eq. (51), taking $x_A$ and $x_B$ both inside $D$, using Eq. (25), we obtain

$$G_h(x_A, x_B, \omega) = -\int_{\partial D_0 \cup \partial D_M} J G^*(x_A, x, \omega) J G(x, x_B, \omega) n_3 d^2 x,$$

for $x_{3,M} > x_{3 \{A,B\}} > x_{3,0}$.  \hspace{1cm} (52)

This is the unified homogeneous Green’s matrix representation. It finds applications in optical, acoustic and seismic holography [20, 25], inverse source problems [16], inverse scattering methods [19] and Green’s function retrieval by cross-correlation [27–29, 70, 71]. A disadvantage is that the integral is taken along two boundaries $\partial D_0$ and $\partial D_M$, whereas in many practical situations, measurements are only available on a single boundary. Using the propagator matrix, in section VI B we present a single-sided unified homogeneous Green’s function representation.

Finally, using Eqs. (16), (17) and (18) for the isotropic acoustic situation, Eq. (52) yields for the upper-right element of $G_h(x_A, x_B, \omega)$

$$G_{h}^{p,q}(x_A, x_B, \omega) = -\frac{1}{i \omega} \int_{\partial D_0 \cup \partial D_M} \left( \frac{1}{\rho(x, \omega)} \left\{ \partial_3 \bar{G}^{p,q}(x_A, x, \omega) \right\} \bar{G}^{p,q}(x, x_B, \omega) 
- \frac{1}{\rho(x, \omega)} \left( \bar{G}^{p,q}(x_A, x, \omega) \right) \partial_3 \bar{G}^{p,q}(x, x_B, \omega) \right) n_3 d^2 x,$$

with

$$G_{h}^{p,q}(x_A, x_B, \omega) = G^{p,q}(x_A, x_B, \omega) + \left\{ \bar{G}^{p,q}(x_A, x_B, \omega) \right\}^*,$$  \hspace{1cm} (54)

according to Eqs. (16) and (26). For a lossless constant density medium, using $G^{p,q}(x, x_B, \omega) = -i \omega \rho G(x, x_B, \omega)$, Eq. (53) is the well-known scalar homogeneous Green’s function representation [19, 20], applied to the configuration of Fig. 5.
V. REPRESENTATIONS WITH PROPAGATOR MATRICES

We follow a similar approach as in section IV to derive wave-field representations. However, this time we replace one of the states in the reciprocity theorems by a propagator state (instead of a Green’s state). Hence, this leads to wave-field representations with propagator matrices.

A. Symmetry properties of the propagator matrix

We start with deriving symmetry properties of the propagator matrix. To this end, we replace both wave-field vectors $q_A$ and $q_B$ in reciprocity theorem (40) by propagator matrices $W(x, x_A, \omega)$ and $W(x, x_B, \omega)$, respectively. We define horizontal boundaries $\partial D_A$ and $\partial D_B$, containing the points $x_A$ and $x_B$, respectively, see Fig. 5. We replace $\partial D_0$ and $\partial D_M$ in Eq. (40) by these boundaries (and $\mathcal{D}$ by the region enclosed by these boundaries).

Note that boundary condition (29) implies $W(x, x_A, \omega) = I\delta(x_H - x_{H,A})$ for $x$ at $\partial D_A$ and $W(x, x_B, \omega) = I\delta(x_H - x_{H,B})$ for $x$ at $\partial D_B$. The propagators obey wave equation (27) without sources, hence, we set $d_A$ and $d_B$ to $O$. This implies that the integral on the left-hand side of Eq. (40) vanishes. Both propagator matrices are defined in the same medium, hence, $\mathcal{A}_A = \mathcal{A}_B$. This implies that the second integral on the right-hand side vanishes.

Evaluating the remaining integral along the boundary $\partial D_A \cup \partial D_B$ yields (irrespective of the arrangement of $\partial D_A$ and $\partial D_B$)

$$W^i(x_B, x_A, \omega)N = NW(x_A, x_B, \omega). \quad (55)$$

This is the first unified symmetry relation for the propagator matrix.

A second symmetry relation can be derived from reciprocity theorem (41). To this end
we replace \( q_A \) and \( q_B \) by \( \mathbf{W}(x, x_A, \omega) \) and \( \mathbf{W}(x, x_B, \omega) \), respectively. We replace \( \partial \mathcal{D}_0 \cup \partial \mathcal{D}_M \) in Eq. (41) by \( \partial \mathcal{D}_A \cup \partial \mathcal{D}_B \) (and \( \mathcal{D} \) by the enclosed region). We set \( d_A \) and \( d_B \) to \( O \), hence, the integral on the left-hand side vanishes. The propagator matrices are defined in mutually adjoint media, hence, \( \mathcal{A}_A = \mathcal{A}_B \). This implies that the second integral on the right-hand side of Eq. (41) vanishes. From the remaining integral we thus obtain

\[
\mathbf{W}^+(x_B, x_A, \omega) \mathbf{K} = \mathbf{K} \mathbf{W}(x_A, x_B, \omega). \tag{56}
\]

From Eqs. (55) and (56), using \( \mathbf{K} \mathbf{N}^{-1} = \mathbf{J} \), we find

\[
\mathbf{W}^*(x_B, x_A, \omega) \mathbf{J} = \mathbf{J} \mathbf{W}(x_B, x_A, \omega). \tag{57}
\]

Note that in this last equation \( x_B \) and \( x_A \) appear in the same order on the left- and right-hand sides.

**B. Representations of the convolution type with the propagator matrix**

We derive a representation of the convolution type for the actual wave-field vector \( q(x, \omega) \), emitted by the actual source distribution \( d(x, \omega) \) in the actual medium; the operator matrix in the actual medium is defined as \( \mathcal{A}(x, \omega) \). We let state \( B \) in reciprocity theorem (40) be
this actual state, hence, we drop subscript $B$ from $q_B$, $d_B$ and $A_B$. For state $A$ we choose the propagator state. Hence, we replace $q_A(x, \omega)$ in reciprocity theorem (40) by $W(x, x_A, \omega)$ and $d_A(x, \omega)$ by $O$. We keep the subscript $A$ in $A_A(x, \omega)$, to account for the fact that in general this operator matrix is defined in a medium that may be different from the actual medium. We replace $\partial \mathbb{D}_0 \cup \partial \mathbb{D}_M$ in reciprocity theorem (40) by $\partial \mathbb{D}_0 \cup \partial \mathbb{D}_A$, where $\partial \mathbb{D}_A$ is the boundary containing $x_A$. Here and in the following, $\partial \mathbb{D}_A$ is below $\partial \mathbb{D}_0$, hence $x_{3,A} > x_{3,0}$.

The domain enclosed by this boundary is called $\mathbb{D}_A$, see Fig. 6. Unlike in the classical, decomposition-based derivations of the Marchenko method [44, 72], the domain $\mathbb{D}_A$ does not define a truncated medium; in general the medium below $\partial \mathbb{D}_A$ is inhomogeneous. Applying the mentioned substitutions in Eq. (40), using boundary condition (29) and symmetry relation (55) (with $x_B$ replaced by $x$) yields

$$q(x_A, \omega) = \int_{\mathbb{D}_A} W(x_A, x, \omega) d(x, \omega) d^3x + \int_{\partial \mathbb{D}_0} W(x_A, x, \omega) q(x, \omega) d^2x$$

$$- \int_{\mathbb{D}_A} W(x_A, x, \omega) \{A_A - A\} q(x, \omega) d^3x.$$  

(58)

This is the unified wave-field representation of the convolution type with the propagator matrix. Note the analogy with the representation of the convolution type with the Green's matrix, Eq. (47). An important difference is that the boundary integral in Eq. (58) is single-sided.

We consider a special case by choosing the same medium parameters in $\mathbb{D}_A$ in both states, and choosing $\mathbb{D}_A$ to be source-free. We thus obtain

$$q(x_A, \omega) = \int_{\partial \mathbb{D}_0} W(x_A, x, \omega) q(x, \omega) d^2x.$$  

(59)

This is the special case that was already presented in Eq. (30) (except that the roles of $x$
and \( x_A \) are interchanged since we used the symmetry property of Eq. (55) in the derivation of Eq. (58)).

Note the analogy of Eq. (59) with Eq. (48), which contains a Green’s matrix instead of the propagator matrix. The propagator matrix in Eq. (59) depends only on the medium parameters between \( x_{3,0} \) and \( x_{3,A} \). Equation (59) is used in section VII as the basis for deriving Marchenko-type representations.

Next, we consider again Eq. (58), in which we replace \( q(x, \omega) \) by \( W(x, x_B, \omega) \), and hence \( d(x, \omega) \) by \( O \) and \( A \) by \( A_A \). This implies that the first and the third integral on the right-hand side vanish. Moreover, we replace \( \partial D_0 \) by \( \partial D_C \) at a newly chosen depth level \( x_{3,C} \), see Fig. 6. This yields

\[
W(x_A, x_B, \omega) = \int_{\partial D_C} W(x_A, x, \omega) W(x, x_B, \omega)d^2x. \tag{60}
\]

This expression shows that the propagator matrix can be composed from a cascade of propagator matrices \([32–36]\). It is similar to Eq. (50) with the cascade of Green’s matrices, but unlike in Eq. (50), where \( x_{3,A} > x_{3,0} > x_{3,B} \), the arrangement of \( x_{3,A}, x_{3,B} \) and \( x_{3,C} \) in Eq. (60) is arbitrary (since there are no sources in both states).

Finally, we replace \( x_B \) in Eq. (60) by \( x'_{A} = (x'_{H,A}, x_{3,A}) \). Applying boundary condition (29) to the left-hand side, we obtain

\[
I\delta(x_{H,A} - x'_{H,A}) = \int_{\partial D_C} W(x_A, x, \omega) W(x, x'_{A}, \omega)d^2x. \tag{61}
\]

This equation defines \( W(x_A, x, \omega) \) as the inverse of \( W(x, x_A, \omega) \) \([32–36]\).
C. Representations of the correlation type with the propagator matrix

We aim to derive a representation of the correlation type for the actual wave-field vector \( q(x, \omega) \), emitted by the actual source distribution \( d(x, \omega) \) in the actual medium. Similar as in section V B, we let state \( B \) be this actual state. For state \( A \) we choose the adjoint propagator state. Hence, we replace \( q_A(x, \omega), A_A(x, \omega) \) and \( d_A(x, \omega) \) by \( W(x, x_A, \omega), A_A(x, \omega) \) and \( O \), respectively. Furthermore, we replace \( \partial D_0 \cup \partial D_M \) again by \( \partial D_0 \cup \partial D_A \). Applying these substitutions in reciprocity theorem (41), using boundary condition (29) and symmetry relation (56) (with \( x_B \) replaced by \( x \)) yields again Eq. (58). Hence, due to the additional symmetry property of the propagator matrix (Eq. (56)), the correlation-type reciprocity theorem does not lead to a new representation.

VI. REPRESENTATIONS WITH GREEN’S MATRICES AND PROPAGATOR MATRICES

We follow a similar approach as in sections IV and V to derive wave-field representations. However, this time we replace one of the states in the reciprocity theorem of the convolution type by a Green’s state and the other by a propagator state. This leads to wave-field representations with Green’s matrices and propagator matrices.

A. Single-sided Green’s matrix representation

In reciprocity theorem (40) we choose for state \( A \) the propagator state and for state \( B \) the Green’s state. Hence, in state \( A \) we replace \( q_A(x, \omega) \) and \( d_A(x, \omega) \) by \( W(x, x_A, \omega) \) and \( O \), respectively. In state \( B \) we replace \( q_B(x, \omega) \) and \( d_B(x, \omega) \) by \( G(x, x_B, \omega) \) and \( I\delta(x - x_B) \), respectively. The medium parameters in states \( A \) and \( B \) may be different, hence, we keep
the subscripts in $A_A(x, \omega)$ and $A_B(x, \omega)$. Last but not least, we replace $\partial D_0 \cup \partial D_M$ by $\partial D_0 \cup \partial D_A$ and $D$ by the enclosed region $D_A$, see Fig. 6. With these substitutions, using boundary condition (29) and symmetry relation (55), reciprocity theorem (40) yields

$$G(x_A, x_B, \omega) - \chi_{D_A}(x_B)W(x_A, x_B, \omega) =$$

$$\int_{\partial D_0} W(x_A, x, \omega)G(x, x_B, \omega)d^2x - \int_{D_A} W(x_A, x, \omega)\{A_A - A_B\}G(x, x_B, \omega)d^3x, \quad (62)$$

where $\chi_{D_A}(x)$ is the characteristic function for domain $D_A$, defined similarly as $\chi_{D}(x)$ in equation (46). Equation (62) is a representation for $G - W$ (when $x_B$ is inside $D_A$) in terms of integrals containing $G$ and $W$. When $G$ and $W$ are defined in the same medium, this representation simplifies to

$$G(x_A, x_B, \omega) - \chi_{D_A}(x_B)W(x_A, x_B, \omega) = \int_{\partial D_0} W(x_A, x, \omega)G(x, x_B, \omega)d^2x. \quad (63)$$

Finally, when $x_B$ (the position of the source of the Green’s function) lies outside $D_A$ (i.e., above $\partial D_0$ or below $\partial D_A$), then the latter expression simplifies to

$$G(x_A, x_B, \omega) = \int_{\partial D_0} W(x_A, x, \omega)G(x, x_B, \omega)d^2x, \quad \text{for } x_{3,B} < x_{3,0} \text{ or } x_{3,B} > x_{3,A}. \quad (64)$$

This is a single-sided representation of the Green’s matrix that uses the propagator matrix. This special case was already presented in Eq. (31) (except that the roles of $x$ and $x_A$ are interchanged since we used the symmetry property of Eq. (55) in the derivation of Eq. (64)). Note the analogy of Eq. (64) with Eq. (50), which contains a Green’s matrix instead of the propagator matrix. The propagator matrix in Eq. (64) depends only on the medium parameters between $x_{3,0}$ and $x_{3,A}$. Moreover, unlike the representation of Eq. (50), which only holds for $x_{3,B} < x_{3,0}$, Eq. (64) also holds for $x_{3,B} > x_{3,A}$.
B. Single-sided homogeneous Green’s matrix representation

We follow the same procedure as in section VI A, except in state $B$ we choose the homogeneous Green’s function, hence, we replace $q_B(x, \omega)$ and $d_B(x, \omega)$ in reciprocity theorem (40) by $G_h(x, x_B, \omega)$ and $O$, respectively. We thus obtain

$$G_h(x_A, x_B, \omega) = \int_{\partial D_0} W(x_A, x, \omega) G_h(x, x_B, \omega) d^2 x$$

$$- \int_{D_A} W(x_A, x, \omega) \{ \mathcal{A}_A - \mathcal{A}_B \} G_h(x, x_B, \omega) d^3 x. \quad (65)$$

When $G_h$ and $W$ are defined in the same medium, this representation simplifies to

$$G_h(x_A, x_B, \omega) = \int_{\partial D_0} W(x_A, x, \omega) G_h(x, x_B, \omega) d^2 x. \quad (66)$$

This is a single-sided representation of the homogeneous Green’s matrix that uses the propagator matrix. This special case was already presented in Eq. (32) (except that the roles of $x$ and $x_A$ are interchanged since we used the symmetry property of Eq. (55) in the derivation of Eq. (66)). Note that, unlike the Green’s matrix representation of Eq. (64), the homogeneous Green’s matrix representation of Eq. (66) has no restrictions for the position of $x_B$ (since there is no source at $x_B$).

Equation (66) is the single-sided counterpart of the unified homogeneous Green’s matrix representation of Eq. (52). Whereas in Eq. (52) the integral is taken along two boundaries $\partial D_0$ and $\partial D_M$, in Eq. (66) the integral is taken only along $\partial D_0$. This is an important advantage for practical situations, where measurements are often available only on a single boundary. In section VIC we indicate how Eq. (66) can be used in a process called source and receiver redatuming.
Finally, using Eqs. (16), (17), (26), (33) and (35) for the isotropic acoustic situation, assuming real-valued \( \rho(x) \), Eq. (66) yields for the upper-right element of \( G_h(x_A, x_B, \omega) \)

\[
G_{p,q}^{h}(x_A, x_B, \omega) = -\frac{1}{i\omega} \int_{\partial D_0} \frac{1}{\rho(x)} \left( \{ \partial_3 W^{p,v}(x_A, x, \omega) \} G_{h}^{p,q}(x, x_B, \omega) \\
- W^{p,v}(x_A, x, \omega) \partial_3 G_{h}^{p,q}(x, x_B, \omega) \right) \, d^2x,
\]

with \( G_{h}^{p,q}(x_A, x_B, \omega) \) defined in Eq. (54).

C. Source and receiver redatuming

Redatuming is the process of moving sources and/or receivers from the acquisition boundary to positions inside the medium [22, 57, 73, 74]. Traditionally this is done with Kirchhoff-Helmholtz integrals with Green’s functions defined in a smooth background medium, thus ignoring multiple scattering. Here we derive a unified redatuming method that accounts for multiple scattering, using the single-sided homogeneous Green’s matrix representation of section VI B as the starting point.

Let \( x_S \) and \( x_R \) denote source and receiver coordinates, respectively, at the acquisition boundary \( \partial D_0 \). Then the Green’s matrix \( G(x_R, x_S, \omega) \) represents the medium’s response, measured with sources and receivers at the surface, see Fig. 7(a). Assuming the medium is lossless, the homogeneous Green’s matrix \( G_h(x_R, x_S, \omega) \) is obtained from this Green’s matrix via Eq. (25).

First we discuss a method for source redatuming. We rename some variables in Eq. (66) \((x_B \rightarrow x_R, x_A \rightarrow x_B, x \rightarrow x_S)\) and transpose all matrices, which gives

\[
G_h^T(x_B, x_R, \omega) = \int_{\partial D_0} G_h^T(x_S, x_R, \omega) W^T(x_B, x_S, \omega) \, d^2x_S.
\]
FIG. 7. Illustration of source and receiver redatuming. All responses in this figure are represented by simple rays, but in reality these are multi-component wave fields, including primaries, multiples, converted, refracted and evanescent waves. (a) The response $G(x_R, x_S, \omega)$ at the surface. The homogeneous Green’s matrix $G_h(x_R, x_S, \omega)$ is obtained from this response with Eq. (25). (b) Source redatuming. Using Eq. (69), the homogeneous Green’s matrix $G_h(x_R, x_B, \omega)$ is obtained for a virtual source at $x_B$. (c) Receiver redatuming. Using Eq. (70), the homogeneous Green’s matrix $G_h(x_A, x_B, \omega)$ is obtained for a virtual receiver at $x_A$.

Using Eqs. (44) and (55) we obtain

$$G_h(x_R, x_B, \omega) = \int_{\partial D_0} G_h(x_R, x_S, \omega) W(x_S, x_B, \omega) d^2 x_S. \quad (69)$$

The latter expression describes redatuming of the sources from $x_S$ at the acquisition bound-
ary to a virtual-source position $x_B$ inside the medium, see Fig. 7(b).

Next, we discuss receiver redatuming. We replace $x$ by $x_R$ in Eq. (66), which gives

$$G_h(x_A, x_B, \omega) = \int_{\partial D_0} W(x_A, x_R, \omega) G_h(x_R, x_B, \omega) d^2 x_R. \quad (70)$$

This expression describes redatuming of the receivers from $x_R$ at the acquisition boundary to a virtual-receiver position $x_A$ inside the medium, see Fig. 7(c). The Green’s matrix under the integral is the output of the source redatuming method, described by Eq. (69).

Combining Eq. (69) with Eq. (70) gives the following expression for combined source and receiver redatuming

$$G_h(x_A, x_B, \omega) = \int_{\partial D_0} \int_{\partial D_0} W(x_A, x_R, \omega) G_h(x_R, x_S, \omega) W(x_S, x_B, \omega) d^2 x_S d^2 x_R. \quad (71)$$

This expression redatums the actual sources and receivers from the acquisition boundary $\partial D_0$ to virtual sources and receivers inside the medium. Since it takes multiple scattering into account, it generalizes classical source and receiver redatuming [22, 57, 73, 74]. Equation (71) resembles expressions for source-receiver interferometry [75, 76], but with the integrals along a closed boundary replaced by integrals along the open acquisition boundary $\partial D_0$, and with two of the Green’s functions replaced by propagator matrices. When the medium is known, these matrices can be numerically modelled. Alternatively, the propagator matrices can be expressed in terms of focusing functions which, at least for the acoustic situation, can be retrieved via the Marchenko method from the reflection response at the acquisition boundary. In the next section we introduce relations between the propagator matrix and focusing functions (section VII A) and derive Marchenko-type representations which relate the focusing functions to the reflection response at the acquisition boundary (section VII B).
VII. REPRESENTATIONS WITH FOCUSING FUNCTIONS

A. Relation between propagator matrix and focusing functions

In section II E we indicated that there is a relation between the propagator matrix and the Marchenko-type focusing functions. Here we derive this relation for the propagator matrix of the unified matrix-vector wave equation, assuming the medium is lossless. Our starting point is Eq. (59), which is repeated here for convenience

\[ q(x_A, \omega) = \int_{\partial D_0} W(x_A, x, \omega)q(x, \omega)d^2x, \]  

with boundary condition

\[ W(x_A, x, \omega)|_{x_3, A = x_3, 0} = I\delta(x_{H, A} - x_H), \]  

for \( x \) at \( \partial D_0 \). From here onward we assume that the half-space above \( \partial D_0 \) (including \( \partial D_0 \)) is homogeneous and isotropic; the medium below \( \partial D_0 \) is arbitrary inhomogeneous, anisotropic and source-free, and \( x_A \) is chosen at or below \( \partial D_0 \) (hence \( x_{3, A} \geq x_{3, 0} \)).

Without loss of generality, we can decompose \( q(x, \omega) \) in the upper half-space into down- and upgoing plane waves. To this end, we defined the spatial Fourier transform \( \tilde{u}(s, x_3, \omega) \) of a space- and frequency-dependent function \( u(x, \omega) \) in Eq. (20). For a function of two space variables, \( u(x_A, x, \omega) \), we define the spatial Fourier transform along the horizontal components of the second space variable as

\[ \tilde{u}(x_A, s, x_3, \omega) = \int_{\mathbb{R}^2} u(x_A, x_H, x_3, \omega) \exp\{i\omega s \cdot x_H\}d^2x_H. \]
Using these definitions and Parseval’s theorem, we rewrite Eq. (72) as

\[ q(x_A, \omega) = \frac{\omega^2}{4\pi^2} \int_{\mathbb{R}^2} \tilde{W}(x_A, s, x_{3,0}, \omega) \tilde{q}(s, x_{3,0}, \omega) d^2s, \]  

(75)

with boundary condition

\[ \tilde{W}(x_A, s, x_{3,0}, \omega)|_{x_3 = x_{3,0}} = I \exp\{i\omega s \cdot x_{H,A}\}. \]  

(76)

In the upper half-space we relate the wave-field vector \( \tilde{q} \) to downgoing and upgoing wave-field vectors \( \tilde{p}^+ \) and \( \tilde{p}^- \), respectively, via

\[ \tilde{q} = \begin{pmatrix} \tilde{q}_1 \\ \tilde{q}_2 \end{pmatrix} = \begin{pmatrix} L_1^+ & L_1^- \\ \tilde{L}_2^+ & \tilde{L}_2^- \end{pmatrix} \begin{pmatrix} \tilde{p}^+ \\ \tilde{p}^- \end{pmatrix}, \quad \text{for} \quad x_3 \leq x_{3,0} \]  

(77)

[55–57, 77]. Next, we renormalize the downgoing and upgoing wave-field vectors. To this end, we define the downgoing and upgoing parts of \( \tilde{q}_1 \) as

\[ \tilde{q}_1^\pm = L_1^\pm \tilde{p}^\pm \]  

(78)

and rewrite Eq. (77) as

\[ \tilde{q} = \begin{pmatrix} \tilde{q}_1 \\ \tilde{q}_2 \end{pmatrix} = \begin{pmatrix} I & I \\ \tilde{D}_1^+ & \tilde{D}_1^- \end{pmatrix} \begin{pmatrix} \tilde{q}_1^+ \\ \tilde{q}_1^- \end{pmatrix}, \quad \text{for} \quad x_3 \leq x_{3,0}, \]  

(79)

with

\[ \tilde{D}_1^+ = \tilde{L}_2^+ (\tilde{L}_1^+)^{-1}. \]  

(80)
In Appendix A we give explicit expressions for $\tilde{D}_1^\pm$ for the acoustic, electromagnetic and elastodynamic situation. Substitution of Eq. (79) into Eq. (75) gives

$$q(x_A, \omega) = \frac{\omega^2}{4\pi^2} \int_{\mathbb{R}^2} \tilde{Y}_1(x_A, s, x_{3,0}, \omega) \tilde{b}_1(s, x_{3,0}, \omega) d^2s,$$

(81)

with

$$\tilde{Y}_1(x_A, s, x_{3,0}, \omega) = \tilde{W}(x_A, s, x_{3,0}, \omega) \tilde{D}_1(s).$$

(82)

Let $\tilde{F}_1(x_A, s, x_{3,0}, \omega)$ be the upper-right $N/2 \times N/2$ matrix of block matrix $\tilde{Y}_1(x_A, s, x_{3,0}, \omega)$. According to Eqs. (28), (82) and the definition of $\tilde{D}_1(s)$ in Eq. (79), it is defined as

$$\tilde{F}_1(x_A, s, x_{3,0}, \omega) = (\tilde{W}_{11} + \tilde{W}_{12} \tilde{D}_1^{-1})(x_A, s, x_{3,0}, \omega).$$

(83)

This is a generalization of the definition of the acoustic focusing function for a horizontally layered medium, defined in Eq. (38). From Eqs. (28) and (76) it follows that $\tilde{F}_1(x_A, s, x_{3,0}, \omega)$ obeys the boundary condition

$$\tilde{F}_1(x_A, s, x_{3,0}, \omega)|_{x_{3,0} = x_{3,0}} = I \exp\{i \omega s \cdot x_{H,A}\},$$

(84)

or, applying an inverse spatial and temporal Fourier transform,

$$F_1(x_A, x, t)|_{x_{3,0} = x_{3,0}} = I \delta(x_{H,A} - x_H) \delta(t),$$

(85)

for $x$ at $\partial D_0$. Hence, $F_1(x_A, x, t)$ is indeed a focusing function (with $x_A$ being a variable and $x$ being the focal point at $\partial D_0$).

To analyse the upper-left $N/2 \times N/2$ matrix of block matrix $\tilde{Y}_1(x_A, s, x_{3,0}, \omega)$, we first
establish some symmetry properties. The symmetry of $\tilde{W}$ follows from the Fourier transform of Eq. (57) for the lossless situation, hence

$$\tilde{W}(x_A, s, x_{3,0}, \omega) = J \tilde{W}^*(x_A, -s, x_{3,0}, \omega)J.$$  (86)

For the sub-matrices of $\tilde{W}$ this implies

$$\tilde{W}_{\alpha\beta}(x_A, s, x_{3,0}, \omega) = J_{\alpha\alpha} \tilde{W}_{\alpha\beta}^*(x_A, -s, x_{3,0}, \omega)J_{\beta\beta}$$  (87)

(no summation convention) with $J_{11} = -J_{22} = I$. The symmetry of $\tilde{D}^\pm_1$ follows from its explicit definitions in Appendix A. In all cases, the following symmetry holds

$$\tilde{D}^+_1(s) = -\tilde{D}^-_1(-s).$$  (88)

When we ignore evanescent waves at and above $\partial D_0$, then $\tilde{D}^+_1(s)$ is real-valued, see Appendix A. Hence, given that $\tilde{F}_1(x_A, s, x_{3,0}, \omega)$ is the upper-right $N/2 \times N/2$ matrix of $\tilde{Y}_1(x_A, s, x_{3,0}, \omega)$, we derive from Eqs. (28), (82), (87) and (88) and the structure of $\tilde{D}_1$ indicated in Eq. (79), that the upper-left $N/2 \times N/2$ matrix is equal to $\tilde{F}_1^*(x_A, -s, x_{3,0}, \omega)$. Using this in Eq. (81) we obtain for the upper $N/2 \times 1$ vector of $q(x_A, \omega)$

$$q_1(x_A, \omega) = \frac{\omega^2}{4\pi^2} \int_{\mathbb{R}^2} \tilde{F}_1^*(x_A, -s, x_{3,0}, \omega)q_1^+(s, x_{3,0}, \omega)d^2s$$

$$+ \frac{\omega^2}{4\pi^2} \int_{\mathbb{R}^2} \tilde{F}_1(x_A, s, x_{3,0}, \omega)q_1^-(s, x_{3,0}, \omega)d^2s.$$  (89)

Applying Parseval’s theorem again, we obtain

$$q_1(x_A, \omega) = \int_{\partial D_0} F_1^*(x_A, x, \omega)q_1^+(x, \omega)d^2x + \int_{\partial D_0} F_1(x_A, x, \omega)q_1^-(x, \omega)d^2x.$$  (90)
This relation has previously been derived via another route for the situations of acoustic waves \((q_1 = p)\) and elastodynamic waves \((q_1 = v)\) [78], but without explicitly defining the focusing function \(F_1(x_A, x, \omega)\). Here we have an explicit expression for the Fourier transform of this focusing function (Eq. (83)). In section VII B we use Eq. (90) as the basis for deriving Marchenko-type Green’s matrix representations.

Next, we derive a representation similar to Eq. (90) for \(q_2(x_A, \omega)\). To this end, we define the downgoing and upgoing parts of \(\tilde{q}_2\) as

\[
\tilde{q}_2^\pm = \tilde{L}_2^\pm \tilde{p}^\pm
\]

and rewrite Eq. (77), analogous to Eq. (79), as

\[
\tilde{q} = \begin{pmatrix}
\tilde{q}_1 \\
\tilde{q}_2
\end{pmatrix} = \begin{pmatrix}
\tilde{D}_2^+ & \tilde{D}_2^- \\
I & I
\end{pmatrix} \begin{pmatrix}
\tilde{q}_2^+ \\
\tilde{q}_2^-
\end{pmatrix}, \quad \text{for } x_3 \leq x_{3,0},
\]

with

\[
\tilde{D}_2^\pm = \tilde{L}_1^\pm (\tilde{L}_2^\pm)^{-1} = (\tilde{D}_1^\pm)^{-1}.
\]

Substitution of Eq. (92) into Eq. (75) gives

\[
q(x_A, \omega) = \frac{\omega^2}{4\pi^2} \int_{\mathbb{R}^2} \tilde{Y}_2(x_A, s, x_{3,0}, \omega) \tilde{b}_2(s, x_{3,0}, \omega) d^2s,
\]

with

\[
\tilde{Y}_2(x_A, s, x_{3,0}, \omega) = \tilde{W}(x_A, s, x_{3,0}, \omega) \tilde{D}_2(s).
\]
Let \( \tilde{F}_2(x_A, s, x_3, \omega) \) be the lower-right \( N/2 \times N/2 \) matrix of block-matrix \( \tilde{Y}_2(x_A, s, x_3, \omega) \).

According to Eqs. (28), (95) and the definition of \( \tilde{D}_2(s) \) in Eq. (92), it is defined as

\[
\tilde{F}_2(x_A, s, x_3, \omega) = (\tilde{W}_21 \tilde{D}_2^- + \tilde{W}_22)(x_A, s, x_3, \omega).
\]  \hspace{1cm} (96)

\( \tilde{F}_2 \) is a focusing function, with similar focusing properties as \( \tilde{F}_1 \), expressed in equations (84) and (85).

To analyse the lower-left \( N/2 \times N/2 \) matrix of block matrix \( \tilde{Y}_2(x_A, s, x_3, \omega) \), we first derive from Eqs. (88) and (93)

\[
\tilde{D}_2^+(s) = -\tilde{D}_2^-(s).
\]  \hspace{1cm} (97)

When we ignore evanescent waves at and above \( \partial D_0 \), then \( \tilde{D}_2^+(s) \) is real-valued. Hence, given that \( \tilde{F}_2(x_A, s, x_3, \omega) \) is the lower-right \( N/2 \times N/2 \) matrix of \( \tilde{Y}_2(x_A, s, x_3, \omega) \), we derive from Eqs. (28), (87), (95) and (97) and the structure of \( \tilde{D}_2 \) indicated in Eq. (92), that the lower-left \( N/2 \times N/2 \) matrix is equal to \( \tilde{F}_2(x_A, -s, x_3, \omega) \). Using this in Eq. (94) we obtain for the lower \( N/2 \times 1 \) vector of \( q(x_A, \omega) \)

\[
q_2(x_A, \omega) = \frac{\omega^2}{4\pi^2} \int_{\mathbb{R}^2} \tilde{F}_2^*(x_A, -s, x_3, \omega)\tilde{q}_2^+(s, x_3, \omega) d^2s + \frac{\omega^2}{4\pi^2} \int_{\mathbb{R}^2} \tilde{F}_2(x_A, s, x_3, \omega)\tilde{q}_2^-(s, x_3, \omega) d^2s.
\]  \hspace{1cm} (98)

Applying Parseval’s theorem again, we obtain

\[
q_2(x_A, \omega) = \int_{\partial D_0} F_2^*(x_A, x, \omega)q_2^+(x, \omega) d^2x + \int_{\partial D_0} F_2(x_A, x, \omega)q_2^-(x, \omega) d^2x.
\]  \hspace{1cm} (99)

From Eqs. (78), (80) and (91) we obtain \( \tilde{q}_2^\pm = \tilde{D}_1^\pm q_1^\pm \). Substituting this into Eq. (98)
we obtain a representation for \( q_2(x_A, \omega) \) in terms of \( \tilde{q}_1^+ \) and \( \tilde{q}_1^- \). Combining this with Eq. (89) into a single equation, we obtain Eq. (81), with (using Eq. (88))

\[
\tilde{Y}_1(x_A, s, x_{3,0}, \omega) = \begin{pmatrix}
\tilde{F}^*_1(x_A, -s, x_{3,0}, \omega) & \tilde{F}_1(x_A, s, x_{3,0}, \omega) \\
-\tilde{F}^*_2(x_A, -s, x_{3,0}, \omega)D_1^-(s) & \tilde{F}_2(x_A, s, x_{3,0}, \omega)D_1^-(s)
\end{pmatrix}.
\tag{100}
\]

Once \( \tilde{Y}_1 \) is known, the propagator matrix \( \tilde{W} \) follows from inverting Eq. (82), according to

\[
\tilde{W}(x_A, s, x_{3,0}, \omega) = \tilde{Y}_1(x_A, s, x_{3,0}, \omega)\{\tilde{D}_1(s)\}^{-1}.
\tag{101}
\]

Equations (100) and (101), with \( \tilde{D}_1(s) \) defined in Eq. (79), express the propagator matrix explicitly in terms of focusing functions.

For the acoustic situation, using Eq. (A16), Eqs. (83) and (96) become

\[
\tilde{F}^p(x_A, s, x_{3,0}, \omega) = \left( \tilde{W}^{p,p} - \frac{s_{3,0}}{\rho_0} \tilde{W}^{p,v} \right)(x_A, s, x_{3,0}, \omega),
\tag{102}
\]

\[
\tilde{F}^v(x_A, s, x_{3,0}, \omega) = \left( -\frac{\rho_0}{s_{3,0}} \tilde{W}^{v,p} + \tilde{W}^{v,v} \right)(x_A, s, x_{3,0}, \omega),
\tag{103}
\]

with \( s_3 \) defined in Eq. (A15). Equation (100) yields for the acoustic situation

\[
\tilde{Y}_1(x_A, s, x_{3,0}, \omega) = \begin{pmatrix}
\{\tilde{F}^p(x_A, -s, x_{3,0}, \omega)\}^* & \tilde{F}^p(x_A, s, x_{3,0}, \omega) \\
\frac{s_{3,0}}{\rho_0} \{\tilde{F}^v(x_A, -s, x_{3,0}, \omega)\}^* & -\frac{s_{3,0}}{\rho_0} \tilde{F}^v(x_A, s, x_{3,0}, \omega)
\end{pmatrix}.
\tag{104}
\]

Using this in Eq. (101), together with

\[
\{\tilde{D}_1(s)\}^{-1} = \begin{pmatrix}
\frac{1}{2} & \frac{\rho_0}{2s_{3,0}} \\
\frac{1}{2} & -\frac{\rho_0}{2s_{3,0}}
\end{pmatrix},
\tag{105}
\]

we obtain an explicit expression for \( \tilde{W}(x_A, s, x_{3,0}, \omega) \) in terms of acoustic focusing functions.
Transforming this to the space-frequency domain, replacing \( s_{3,0} \) by \( \frac{i}{\omega} H_1 \) (where \( H_1 \) is the square-root of the Helmholtz operator \( \omega^2/c_0^2 + \partial_\alpha \partial_\alpha \) in the homogeneous upper half-space [54, 56, 57]), yields [60]

\[
W(x_A, x, \omega) = \left( \begin{array}{c}
\Re\{F^p(x_A, x, \omega)\} \\
-i\omega\rho_0 H_1^{-1}(x, \omega) \Im\{F^p(x_A, x, \omega)\} \\
\frac{1}{i\omega\rho_0} H_1(x, \omega) \Im\{F^v(x_A, x, \omega)\} \\
\Re\{F^v(x_A, x, \omega)\}
\end{array} \right), \tag{106}
\]

for \( x \) at \( \partial \mathbb{D}_0 \), where \( \Im \) denotes the imaginary part.

### B. Marchenko-type Green’s matrix representations with focusing functions

We use Eqs. (90) and (99) as the starting point for deriving two Marchenko-type Green’s function representations. We follow a similar procedure as reference [78, Appendix B], generalized for the different wave phenomena considered in this paper. We replace the \( N/2 \times 1 \) vector \( q_1(x, \omega) \) by a modified version \( \Gamma_{12}(x, x_S, \omega) \) of the \( N/2 \times N/2 \) Green’s matrix \( G_{12}(x, x_S, \omega) \). Here \( G_{12}(x, x_S, \omega) \) stands for the \( q_1 \)-type field observed at \( x \), in response to a unit \( d_2 \)-type source at \( x_S \). We choose \( x_S = (x_H, x_3, S) \) in the upper half-space, at a vanishing distance \( \epsilon \) above \( \partial \mathbb{D}_0 \), hence, \( x_3, S = x_3, 0 - \epsilon \). Our aim is to modify this Green’s matrix such that for \( x \) at \( \partial \mathbb{D}_0 \) (i.e., just below the source) its downgoing part simplifies to

\[
\Gamma^+_{12}(x, x_S, \omega)\big|_{x_3=x_3,0} = I\delta(x_H - x_{H, S}). \tag{107}
\]
First we derive the properties of the downgoing part of $G_{12}(x, x_S, \omega)$ for $x$ at $\partial D_0$. To this end, consider the inverse of Eq. (79), which reads

$$
\begin{pmatrix}
\tilde{q}_1^+ \\
\tilde{q}_1^-
\end{pmatrix} = \begin{pmatrix}
- (\tilde{\Delta}_1)^{-1} \tilde{D}_1^- & (\tilde{\Delta}_1)^{-1} \\
(\tilde{\Delta}_1)^{-1} \tilde{D}_1^+ & - (\tilde{\Delta}_1)^{-1}
\end{pmatrix} \begin{pmatrix}
\tilde{q}_1 \\
\tilde{q}_2
\end{pmatrix},
$$

(108)

for $x_3 \leq x_{3,0}$, with

$$
\tilde{\Delta}_1 = \tilde{D}_1^+ - \tilde{D}_1^-.
$$

(109)

The upper-right $N/2 \times N/2$ matrix $(\tilde{\Delta}_1)^{-1}$ transforms $\tilde{q}_2$ into a downgoing field vector $\tilde{q}_1^+$. In a similar way, this matrix transforms a unit $d_2$-type source in a homogeneous half-space into the downgoing part of the Green’s matrix $\tilde{G}_{12}$ just below this source, according to

$$
\lim_{x_3 \downarrow x_{3}, S} \tilde{G}^+_{12}(s, x_3, 0, x_S, \omega) = \{\tilde{\Delta}_1(s)\}^{-1}.
$$

(110)

Explicit expressions for $(\tilde{\Delta}_1)^{-1}$ are given in Appendix A. In Eq. (110) the source is located at $(0, x_{3, S})$. Next, we consider $G_{12}(x, x_S, \omega)$ for a laterally shifted source position $(x_{H,S}, x_{3,S})$. Applying a spatial Fourier transform along the horizontal source coordinate $x_{H,S}$, using Eq. (74) with $x_H$ replaced by $x_{H,S}$, yields $\tilde{G}_{12}(x, s, x_{3,S}, \omega)$. For the downgoing part just below the source we obtain a phase-shifted version of the Green’s function of Eq. (110), according to

$$
\lim_{x_3 \downarrow x_{3}, S} \tilde{G}^+_{12}(x, s, x_{3,S}, \omega) = \{\tilde{\Delta}_1(s)\}^{-1} \exp\{i\omega s \cdot x_H\}.
$$

(111)
This suggests to define the modified Green's matrix as

$$\tilde{\Gamma}_{12}(x, s, x, S, \omega) = \tilde{G}_{12}(x, s, x, S, \omega) \tilde{\Delta}_1(s), \quad (112)$$

such that

$$\lim_{x_3 \downarrow x_3} \tilde{\Gamma}_{12}^+(x, s, x, S, \omega) = I \exp\{i\omega s \cdot \chi_H\}. \quad (113)$$

Transforming this back to the space domain yields indeed Eq. (107). Next, we define the reflection response $R_{12}(x, x, S, \omega)$ of the medium below $\partial \mathbb{D}_0$ as the upgoing part of the modified Green's function $\Gamma_{12}(x, x, S, \omega)$, for $x$ at $\partial \mathbb{D}_0$, hence

$$R_{12}(x, x, S, \omega) = \Gamma_{12}^-(x, x, S, \omega). \quad (114)$$

Substituting $q_1(x, \omega) = \Gamma_{12}(x, x, x, \omega)$ and $q_{1, 1}^+(x, \omega) = \Gamma_{12}^+(x, x, x, \omega)$ into Eq. (90), using Eqs. (107) and (114), gives

$$\Gamma_{12}(x, x, x, \omega) = \int_{\partial \mathbb{D}_0} F_1(x, x, \omega) R_{12}(x, x, x, \omega) d^2x + F_{1, 1}^+(x, x, x, \omega), \quad (115)$$

for $x_{3, A} \geq x_{3, 0}$. This is the first Marchenko-type representation. In a similar way, we derive a second Marchenko-type representation, for a modified version $\Gamma_{22}(x, x, \omega)$ of the Green's matrix $G_{22}(x, x, \omega)$. We derive the properties of the downgoing part of $G_{22}(x, x, \omega)$ for $x$ at $\partial \mathbb{D}_0$. Consider the inverse of Eq. (92), which reads

$$ \begin{pmatrix} \tilde{q}_2^+ \\ \tilde{q}_2^- \end{pmatrix} = \begin{pmatrix} (\tilde{\Delta}_2)^{-1} & -(\tilde{\Delta}_2)^{-1} \tilde{D}_2^- \\ -(\tilde{\Delta}_2)^{-1} & (\tilde{\Delta}_2)^{-1} \tilde{D}_2^+ \end{pmatrix} \begin{pmatrix} \tilde{q}_1 \\ \tilde{q}_2 \end{pmatrix}, \quad (116)$$
for $x_3 \leq x_{3,0}$, with

$$\tilde{\Delta}_2 = \tilde{D}_2^+ - \tilde{D}_2^-.$$  \hfill (117)

The upper-right $N/2 \times N/2$ matrix $-(\tilde{\Delta}_2)^{-1}\tilde{D}_2^-$ transforms $\tilde{q}_2$ into a downgoing field vector $\tilde{q}_2^+$. In a similar way, this matrix transforms a unit $d_2$-type source in a homogeneous half-space into the downgoing part of the Green’s matrix $\tilde{G}_{22}$ just below this source, according to

$$\lim_{x_3 \downarrow x_{3,S}} \tilde{G}_{22}^+(s, x_3, 0, x_{3,S}, \omega) = -(\tilde{\Delta}_2(s))^{-1}\tilde{D}_2^- (s).$$  \hfill (118)

Explicit expressions for $-(\tilde{\Delta}_2)^{-1}\tilde{D}_2^-$ are given in Appendix A. Similar steps as below Eq. (110) lead to

$$\lim_{x_3 \downarrow x_{3,S}} \tilde{G}_{22}^+(x, s, x_3, s, x_{3,S}, \omega) = -(\tilde{\Delta}_2(s))^{-1}\tilde{D}_2^- (s) \exp\{i\omega s \cdot x_H\}.$$  \hfill (119)

This suggests to define the modified Green’s matrix as

$$\tilde{\Gamma}_{22}(x, s, x_{3,S}, \omega) = -\tilde{G}_{22}(x, s, x_{3,S}, \omega)\{\tilde{D}_2^- (s)\}^{-1}\tilde{\Delta}_2(s),$$  \hfill (120)

such that

$$\Gamma_{22}^+(x, x_S, \omega)|_{x_3 = x_{3,0}} = \mathbf{I} \delta(x_H - x_{H,S}).$$  \hfill (121)

We define the reflection response $R_{22}(x, x_S, \omega)$ as

$$R_{22}(x, x_S, \omega) = \Gamma_{22}^-(x, x_S, \omega)$$  \hfill (122)
for $x$ at $\partial \mathbb{D}_0$. Substituting $q_2(x_A, \omega) = \Gamma_{22}(x_A, x_S, \omega)$ and $q_2^\pm(x, \omega) = \Gamma_{22}^\pm(x, x_S, \omega)$ into Eq. (99), using Eqs. (121) and (122), gives

$$\Gamma_{22}(x_A, x_S, \omega) = \int_{\partial \mathbb{D}_0} F_2(x_A, x, \omega) R_{22}(x, x_S, \omega) d^2 x + F_2^\pm(x_A, x_S, \omega), \quad (123)$$

for $x_{3,A} \geq x_{3,0}$. This is the second Marchenko-type representation.

For the acoustic case, using Eqs. (A16) and (A17), Eqs. (112) and (120) become

$$\tilde{\Gamma}_{12}(x, s, x_{3,S}, \omega) = \frac{2s_{3,0}}{\rho_0} \tilde{G}^{q,q}(x, s, x_{3,S}, \omega), \quad (124)$$

$$\tilde{\Gamma}_{22}(x, s, x_{3,S}, \omega) = 2 \tilde{G}^{v,q}(x, s, x_{3,S}, \omega), \quad (125)$$

or, in the space-frequency domain (using Eq. (18)),

$$\Gamma_{12}(x, x_S, \omega) = 2G^{p,f}(x, x_S, \omega), \quad (126)$$

$$\Gamma_{22}(x, x_S, \omega) = 2G^{v,q}(x, x_S, \omega). \quad (127)$$

For this situation, $R_{12}(x, x_S, \omega)$ and $R_{22}(x, x_S, \omega)$ in the representations of Eqs. (115) and (123) are the upgoing parts of $2G^{p,f}(x, x_S, \omega)$ and $2G^{v,q}(x, x_S, \omega)$, respectively, for $x$ at $\partial \mathbb{D}_0$.

Note that, according to Eq. (43), $G^{v,q}(x, x_S, \omega) = -G^{p,f}(x_S, x, \omega)$.

In their general form, the representations of Eqs. (115) and (123) are generalizations of previously derived representations for the 3D Marchenko method for acoustic [72, 79, 80] and elastodynamic wave fields [81, 82] (but note that the subscripts 1 and 2 of the focusing functions have a different meaning than in those papers; here they refer to the wave-field components $q_1$ and $q_2$). In most previous work on the 3D Marchenko method, one of
the underlying assumptions is that the wave field can be decomposed into downgoing and upgoing waves in the interior of the medium. Only recently several authors proposed to avoid decomposition inside the medium [78, 83, 84]. The representations discussed in this section expand on this. In these representations, decomposition into downgoing and upgoing waves and negligence of evanescent waves occurs only in the upper half-space. However, inside the medium no wave-field decomposition takes place. Moreover, evanescent waves inside the medium (for example in high-velocity layers) are accounted for by the representations of Eqs. (115) and (123). These representations, transformed to the time domain, form the basis for the development of Marchenko schemes, aiming at resolving the focusing functions $F_1$ and $F_2$ from the reflection responses $R_{12}$ and $R_{22}$ at the acquisition boundary $\partial D_0$.

Such schemes have been successfully developed for precritical acoustic data [45–47, 85–88]. For more complex situations, research on retrieving the focusing functions from reflection responses is ongoing (for example [89]). Once the focusing functions are found, they can be used to define the propagator matrix via Eqs. (100) and (101), which can subsequently be used in the representations of sections V and VI.

VIII. CONCLUSIONS

We have discussed different types of wave-field representation in a systematic way. Classical wave-field representations contain Green’s functions. Starting with a unified matrix-vector wave equation, we have formulated wave-field representations with Green’s matrices, analogous to the classical representations. For example, the classical Kirchhoff-Helmholtz integral follows as a special case of the unified representation with the Green’s matrix. Another special case is the classical homogeneous Green’s function representation.

Using the same matrix-vector formalism, we formulated wave-field representations with
propagator matrices. Unlike a Green’s matrix, a propagator matrix depends only on the
medium parameters between the two depth levels for which this matrix is defined. The
representations with the propagator matrices have a similar form as those with the Green’s
matrices. An important difference is that the boundary integrals in the representations with
the propagator matrices are single-sided.

We also formulated representations containing a mix of Green’s matrices and propagator
matrices. A special case is the single-sided homogeneous Green’s function representation, as
the counterpart of the classical closed-boundary homogeneous Green’s function representa-
tion.

We have shown that the propagator matrix is related to Marchenko-type focusing func-
tions. We have used this relation to reformulate the representations with the propagator
matrix into representations with focusing functions. For the acoustic situation, these focus-
ing functions can be retrieved from the single-sided reflection response of the medium by
applying the Marchenko method. For more complex situations, research on retrieving these
focusing functions from the reflection response is ongoing. Once the focusing functions are
known, they can be used to construct the propagator matrix. Subsequently, the propagator
matrix can be used in the representations to obtain the wave field inside the medium which,
in turn, can be used for example for imaging or monitoring. Unlike earlier imaging methods
that use the propagator matrix, this is a data-driven approach (since the propagator matrix
is retrieved from the reflection response) and hence it does not require a detailed model of
the medium.
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Appendix A: Explicit expressions for some matrices in the homogeneous isotropic upper half-space

We derive explicit expressions for $\tilde{D}^\pm_1$, $(\tilde{\Delta}_1)^{-1}$ and $-(\tilde{\Delta}_2)^{-1}\tilde{D}^-_2$ in the homogeneous isotropic upper half-space $x_3 \leq x_{3,0}$ for the acoustic, electromagnetic and elastodynamic situation.

Unified expressions in horizontal slowness domain

For the lossless homogeneous isotropic upper half-space $x_3 \leq x_{3,0}$, we transform the unified matrix-vector wave equation (1) to the horizontal slowness domain, using the spatial Fourier transform of Eq. (20). This yields

$$\partial_3 \tilde{q} - \tilde{A} \tilde{q} = \tilde{d},$$  \hspace{1cm} (A1)

with

$$\tilde{q} = \begin{pmatrix} \tilde{q}_1 \\ \tilde{q}_2 \end{pmatrix}, \quad \tilde{d} = \begin{pmatrix} \tilde{d}_1 \\ \tilde{d}_2 \end{pmatrix}, \quad \tilde{A} = \begin{pmatrix} \tilde{A}_{11} & \tilde{A}_{12} \\ \tilde{A}_{21} & \tilde{A}_{22} \end{pmatrix}.$$  \hspace{1cm} (A2)
The symmetry property defined by Eq. (3) transforms to

\[
\{\tilde{A}(-s,\omega)\}^t N = -N\tilde{A}(s,\omega)\. \tag{A3}
\]

We decompose matrix \(\tilde{A}\) as follows [55, 57, 77]

\[
\tilde{A} = \tilde{L}\tilde{\Lambda}\tilde{L}^{-1}, \tag{A4}
\]

with

\[
\tilde{L} = \begin{pmatrix} \tilde{L}_1^+ & \tilde{L}_1^- \\ \tilde{L}_2^+ & \tilde{L}_2^- \end{pmatrix}, \quad \tilde{\Lambda} = \begin{pmatrix} \tilde{\Lambda}^+ & \mathbf{O} \\ \mathbf{O} & \tilde{\Lambda}^- \end{pmatrix}. \tag{A5}
\]

With a proper scaling of the columns of matrix \(\tilde{L}\), these matrices obey the following symmetry properties

\[
\{\tilde{L}(-s)\}^t N = -N\{\tilde{L}(s)\}^{-1}. \tag{A6}
\]
\[
\{\tilde{A}(-s,\omega)\}^t N = -N\tilde{A}(s,\omega). \tag{A7}
\]

Substitution of Eq. (A4) into Eq. (A1) and premultiplying all terms with \(\tilde{L}^{-1}\) yields

\[
\partial_t \tilde{p} - \tilde{\Lambda}\tilde{p} = \tilde{L}^{-1}d, \tag{A8}
\]

with

\[
\tilde{p} = \tilde{L}^{-1}\tilde{q} = \begin{pmatrix} \tilde{p}^+ \\ \tilde{p}^- \end{pmatrix}. \tag{A9}
\]
where $\tilde{p}^+$ and $\tilde{p}^-$ are wave-field vectors containing downgoing (+) and upgoing (−) waves, respectively. Following Eqs. (80), (93), (109) and (117) we define

$$
\tilde{D}_1^\pm(s) = \tilde{L}_2^\pm(\tilde{L}_1^\pm)^{-1}, \quad \{\tilde{\Delta}_1(s)\}^{-1} = (\tilde{D}_1^+ - \tilde{D}_1^-)^{-1}, \quad (A10)
$$

$$
\tilde{D}_2^\pm(s) = \tilde{L}_1^\pm(\tilde{L}_2^\pm)^{-1}, \quad \{\tilde{\Delta}_2(s)\}^{-1} = (\tilde{D}_2^+ - \tilde{D}_2^-)^{-1}. \quad (A11)
$$

**Acoustic wave equation**

For the acoustic wave equation the $1 \times 1$ sub-matrices of $\tilde{A}$ are

$$
\tilde{A}_{12} = i\omega \rho, \quad \tilde{A}_{21} = i\omega (\kappa - s_r^2/\rho), \quad \tilde{A}_{11} = \tilde{A}_{22} = 0, \quad (A12)
$$

with radial slowness $s_r$ defined as

$$
s_r^2 = s_\alpha s_\alpha = s_1^2 + s_2^2. \quad (A13)
$$

Here $\kappa$ and $\rho$ are the compressibility and mass density of the homogeneous upper half-space.

For convenience, here and in the remainder of this appendix we do not use subscripts 0 to indicate parameters of the upper half-space. The $1 \times 1$ sub-matrices of $\tilde{L}$ and $\tilde{A}$ are

$$
\tilde{L}_1^\pm = \left(\frac{\rho}{2s_3}\right)^{1/2}, \quad \tilde{L}_2^\pm = \pm\left(\frac{s_3}{2\rho}\right)^{1/2}, \quad \tilde{A}^\pm = \pm i\omega s_3, \quad (A14)
$$

with the vertical slowness $s_3$ defined as

$$
s_3 = \begin{cases} 
\sqrt{1/c^2 - s_r^2}, & \text{for } s_r^2 \leq 1/c^2, \\
i\sqrt{s_r^2 - 1/c^2}, & \text{for } s_r^2 > 1/c^2,
\end{cases} \quad (A15)
$$
with propagation velocity \( c \) defined as \( c = 1/\sqrt{\kappa \rho} \). The two expressions in Eq. (A15) represent propagating and evanescent waves, respectively. Upon substitution of Eq. (A14) into Eqs. (A10) and (A11) we obtain

\[
\tilde{D}_1^\pm(s) = \pm \frac{s_3}{\rho}, \quad \{\tilde{\Delta}_1(s)\}^{-1} = \frac{\rho}{2s_3}, \quad (A16)
\]
\[
\tilde{D}_2^\pm(s) = \pm \frac{\rho}{s_3}, \quad -\{\tilde{\Delta}_2(s)\}^{-1}\tilde{D}_2^-(s) = \frac{1}{2}. \quad (A17)
\]

**Electromagnetic wave equation**

For the electromagnetic wave equation the \( 2 \times 2 \) sub-matrices of \( \tilde{A} \) are

\[
\tilde{A}_{12} = i\omega \begin{pmatrix} \mu - \frac{s_1^2}{\varepsilon} & -\frac{s_1s_2}{\varepsilon} \\ -\frac{s_1s_2}{\varepsilon} & \mu - \frac{s_2^2}{\varepsilon} \end{pmatrix}, \quad \tilde{A}_{21} = i\omega \begin{pmatrix} \varepsilon - \frac{s_2^2}{\mu} & \frac{s_1s_2}{\mu} \\ \frac{s_1s_2}{\mu} & \varepsilon - \frac{s_1^2}{\mu} \end{pmatrix}, \quad (A18)
\]
\[
\tilde{A}_{11} = \tilde{A}_{22} = 0. \quad (A19)
\]

Here \( \varepsilon \) and \( \mu \) are the permittivity and permeability of the upper half-space. The \( 2 \times 2 \) sub-matrices of \( \tilde{L} \) and \( \tilde{\Lambda} \) are

\[
\tilde{L}_1^\pm = \frac{i}{\sqrt{2s_r}} \begin{pmatrix} s_1 \left( \frac{s_3}{s_3} \right)^{1/2} & -s_2 \left( \frac{s_3}{s_3} \right)^{1/2} \\ s_2 \left( \frac{s_3}{s_3} \right)^{1/2} & s_1 \left( \frac{s_3}{s_3} \right)^{1/2} \end{pmatrix}, \quad (A20)
\]
\[
\tilde{L}_2^\pm = \pm \frac{i}{\sqrt{2s_r}} \begin{pmatrix} s_1 \left( \frac{s_3}{s_3} \right)^{1/2} & -s_2 \left( \frac{s_3}{s_3} \right)^{1/2} \\ s_2 \left( \frac{s_3}{s_3} \right)^{1/2} & s_1 \left( \frac{s_3}{s_3} \right)^{1/2} \end{pmatrix}, \quad (A21)
\]
\[
\tilde{\Lambda}^\pm = \pm i\omega \begin{pmatrix} s_3 & 0 \\ 0 & s_3 \end{pmatrix}, \quad (A22)
\]
with \( s_r \) and \( s_3 \) defined in Eqs. (A13) and (A15), respectively, but this time with propagation velocity \( c = 1/\sqrt{\varepsilon \mu} \). Upon substitution of Eqs. (A20) and (A21) into Eqs. (A10) and (A11) we obtain

\[
\tilde{D}_1^\pm(s) = \pm \frac{1}{\mu s_3} \begin{pmatrix}
-c_0^{-2} - s_2^2 & s_1 s_2 \\
s_1 s_2 & -c_0^{-2} - s_1^2
\end{pmatrix},
\]  
\( (A23) \)

\[
\{\tilde{\Delta}_1(s)\}^{-1} = \frac{1}{2\varepsilon s_3} \begin{pmatrix}
c_0^{-2} - s_1^2 & -s_1 s_2 \\
-s_1 s_2 & c_0^{-2} - s_2^2
\end{pmatrix},
\]  
\( (A24) \)

\[
\tilde{D}_2^\pm(s) = \pm \frac{1}{\varepsilon s_3} \begin{pmatrix}
c_0^{-2} - s_1^2 & -s_1 s_2 \\
-s_1 s_2 & c_0^{-2} - s_2^2
\end{pmatrix},
\]  
\( (A25) \)

\[
-(\tilde{\Delta}_2)^{-1}\tilde{D}_2^- = \begin{pmatrix}
\frac{1}{2} & 0 \\
0 & \frac{1}{2}
\end{pmatrix}.
\]  
\( (A26) \)

**Elastodynamic wave equation**

For the elastodynamic wave equation the \( 3 \times 3 \) sub-matrices of \( \tilde{A} \) are

\[
\tilde{A}_{11} = i\omega \begin{pmatrix}
0 & 0 & -s_1 \\
0 & 0 & -s_2 \\
-\frac{\lambda}{\lambda + 2\mu} s_1 & -\frac{\lambda}{\lambda + 2\mu} s_2 & 0
\end{pmatrix},
\]  
\( (A27) \)

\[
\tilde{A}_{12} = i\omega \begin{pmatrix}
\frac{1}{\mu} & 0 & 0 \\
0 & \frac{1}{\mu} & 0 \\
0 & 0 & \frac{1}{\lambda + 2\mu}
\end{pmatrix}.
\]  
\( (A28) \)
\[ \hat{A}_{21} = i\omega \begin{pmatrix} \rho - \nu_1 s_1^2 - \mu s_2^2 & -(\nu_2 + \mu)s_1 s_2 & 0 \\ -(\nu_2 + \mu)s_1 s_2 & \rho - \mu s_1^2 - \nu_1 s_2^2 & 0 \\ 0 & 0 & \rho \end{pmatrix}, \quad (A29) \]

\[ \hat{A}_{22} = (\hat{A}_{11})^t, \quad (A30) \]

with

\[ \nu_1 = 4\mu \left( \frac{\lambda + \mu}{\lambda + 2\mu} \right), \quad \nu_2 = 2\mu \left( \frac{\lambda}{\lambda + 2\mu} \right), \quad (A31) \]

where \( \lambda \) and \( \mu \) are the Lamé parameters and \( \rho \) the mass density of the upper half-space.

The \( 3 \times 3 \) sub-matrices of \( \tilde{L} \) and \( \tilde{\Lambda} \) are

\[ \tilde{L}_{1\pm} = \frac{1}{(2\rho)^{1/2}} \begin{pmatrix} \frac{s_1}{(s_3^P)^{1/2}} & -\frac{s_1(s_3^S)^{1/2}}{s_r} & -\frac{s_2}{c_s s_r (s_3^S)^{1/2}} \\ \frac{s_2}{(s_3^P)^{1/2}} & -\frac{s_2(s_3^S)^{1/2}}{s_r} & \frac{s_1}{c_s s_r (s_3^S)^{1/2}} \\ \pm(s_3^P)^{1/2} & \pm \frac{s_r}{(s_3^S)^{1/2}} & 0 \end{pmatrix}, \quad (A32) \]

\[ \tilde{L}_{2\pm} = \left( \frac{\rho}{2} \right)^{1/2} \frac{s_r^2}{c_s^2} \begin{pmatrix} \pm 2s_1(s_3^P)^{1/2} & \mp \frac{s_1(c_s^2 - 2s_2^2)}{s_r (s_3^S)^{1/2}} & \mp \frac{s_2(s_3^S)^{1/2}}{c_s s_r} \\ \pm 2s_2(s_3^P)^{1/2} & \mp \frac{s_2(c_s^2 - 2s_2^2)}{s_r (s_3^S)^{1/2}} & \mp \frac{s_1(s_3^S)^{1/2}}{c_s s_r} \\ \frac{(c_s^2 - 2s_2^2)}{(s_3^S)^{1/2}} & 2s_r(s_3^S)^{1/2} & 0 \end{pmatrix}, \quad (A33) \]

\[ \tilde{\Lambda}_{\pm} = \pm i\omega \begin{pmatrix} s_3^P & 0 & 0 \\ 0 & s_3^S & 0 \\ 0 & 0 & s_3^S \end{pmatrix}, \quad (A34) \]
with $s_r$ defined in Eq. (A13), and the vertical slownesses $s_3^P$ and $s_3^S$ defined as
\[
\frac{s_{3,P,S}^2}{s_3^2} = \begin{cases} 
\sqrt{\frac{1}{c_{P,S}^2} - s_r^2}, & \text{for } s_r^2 \leq \frac{1}{c_{P,S}^2}, \\
i\sqrt{s_r^2 - \frac{1}{c_{P,S}^2}}, & \text{for } s_r^2 > \frac{1}{c_{P,S}^2}.
\end{cases}
\] (A35)

Here $c_P$ and $c_S$ are the $P$- and $S$-wave velocities of the upper half-space, defined as $c_P = \sqrt{(\lambda + 2\mu)/\rho}$ and $c_S = \sqrt{\mu/\rho}$, respectively. Upon substitution of Eqs. (A32) and (A33) into Eqs. (A10) and (A11) we obtain
\[
\tilde{D}_{1}(s) = \frac{\rho c_S^2}{s_3^2 s_3^P + s_r^2} \begin{pmatrix} 
\pm((c_S^{-2} - s_2^2)s_3^P + s_2^2 s_3^S) & \pm s_1 s_2 (s_3^P - s_3^S) & -s_1 (c_S^{-2} - 2S) \\
\pm s_1 s_2 (s_3^P - s_3^S) & \pm((c_S^{-2} - s_1^2)s_3^P + s_1^2 s_3^S) & -s_2 (c_S^{-2} - 2S) \\
s_1 (c_S^{-2} - 2S) & s_2 (c_S^{-2} - 2S) & \pm s_3^2 (c_S^{-2} - 2S)
\end{pmatrix},
\] (A36)
\[
\{\tilde{\Delta}_{1}(s)\}^{-1} = \frac{1}{2\rho} \begin{pmatrix} 
\frac{s_2^2}{s_3^2} + \left(\frac{1}{c_3^2} - s_1^2\right) \frac{1}{s_3^2} & \frac{1}{s_3^2} - \frac{1}{s_3^P} & s_1 s_2 & 0 \\
\frac{1}{s_3^2} - \frac{1}{s_3^S} & s_1 s_2 & \frac{s_2^2}{s_3^2} + \left(\frac{1}{c_3^2} - s_2^2\right) \frac{1}{s_3^2} & 0 \\
0 & 0 & s_3^P + \frac{s_2^2}{s_3^2}
\end{pmatrix},
\] (A37)
\[
-\{\tilde{\Delta}_{2}(s)\}^{-1} \tilde{D}_{2}^{-1}(s) = \begin{pmatrix} 
\frac{1}{2} & 0 & \frac{s_1 (s_3^2 - \frac{1}{2})}{s_3^2} \\
0 & \frac{1}{2} & \frac{s_2 (s_3^2 - \frac{1}{2})}{s_3^2} \\
-\frac{s_1 (s_3^2 - \frac{1}{2})}{s_3^2} & -\frac{s_2 (s_3^2 - \frac{1}{2})}{s_3^2} & \frac{1}{2}
\end{pmatrix}.
\] (A38)

with $S = s_3^P s_3^S + s_r^2$. 

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TABLE I. Wave-field sub-vectors $q_1(x, \omega)$ and $q_2(x, \omega)$ for different wave phenomena. For acoustic waves in stationary fluids, $p$ and $v_3$ stand for the acoustic pressure and the vertical component of the particle velocity, respectively. For electromagnetic waves, $E_\alpha$ and $H_\alpha$ ($\alpha = 1, 2$) are the horizontal components of the electric and magnetic field strength, respectively. For elastodynamic waves, $v_k$ and $\tau_{k3}$ ($k = 1, 2, 3$) are the particle velocity and traction components, respectively. The same quantities appear in the vectors for the other wave phenomena, where, for poroelastodynamic and seismoelectric waves, the quantities are averaged in the bulk, fluid or solid, as indicated by the superscripts $b$, $f$ and $s$, respectively. Finally, $\phi$ denotes the porosity.

<table>
<thead>
<tr>
<th></th>
<th>$N$</th>
<th>$q_1$</th>
<th>$q_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acoustic</td>
<td>2</td>
<td>$p$</td>
<td>$v_3$</td>
</tr>
<tr>
<td>Electromagnetic</td>
<td>4</td>
<td>$E_0 = \begin{pmatrix} E_1 \ E_2 \end{pmatrix}$</td>
<td>$H_0 = \begin{pmatrix} H_2 \ -H_1 \end{pmatrix}$</td>
</tr>
<tr>
<td>Elastodynamic</td>
<td>6</td>
<td>$v = \begin{pmatrix} v_1 \ v_2 \ v_3 \end{pmatrix}$</td>
<td>$-\tau_3 = \begin{pmatrix} \tau_{13} \ \tau_{23} \ \tau_{33} \end{pmatrix}$</td>
</tr>
<tr>
<td>Poroelastodynamic</td>
<td>8</td>
<td>$\begin{pmatrix} v^s \ \phi(v^f_3 - v^s_3) \end{pmatrix}$</td>
<td>$-\tau^b_3$ $\begin{pmatrix} \tau^b_3 \ p^f \end{pmatrix}$</td>
</tr>
<tr>
<td>Piezoelectric</td>
<td>10</td>
<td>$\begin{pmatrix} v^s \ H_0 \end{pmatrix}$</td>
<td>$-\tau_3$ $\begin{pmatrix} \tau_3 \ E_0 \end{pmatrix}$</td>
</tr>
<tr>
<td>Seismoelectric</td>
<td>12</td>
<td>$\begin{pmatrix} v^s \ \phi(v^f_3 - v^s_3) \ H_0 \end{pmatrix}$</td>
<td>$-\tau^b_3$ $\begin{pmatrix} \tau^b_3 \ p^f \end{pmatrix}$</td>
</tr>
</tbody>
</table>
Captions

FIG 1: (color online) (a) Horizontally layered medium. (b) Green’s function $G^{p,q}(s_1,x_3,x_3,0,\tau)$ (fixed $s_1$), convolved with a wavelet.

FIG 2: (color online) (a) Propagator element $W^{p,p}(s_1,x_3,x_3,0,\tau)$ (fixed $s_1$), convolved with a wavelet. (b) Last trace of (a).

FIG 3: (color online) (a) Propagator element $W^{p,v}(s_1,x_3,x_3,0,\tau)$ (fixed $s_1$), convolved with a wavelet. (b) Last trace of (a).

FIG 4: (color online) (a) Focusing function $F^p(s_1,x_3,x_3,0,\tau)$ (fixed $s_1$), convolved with a wavelet. (b) Last trace of (a).

FIG 5: Configuration for the matrix-vector reciprocity theorems, Eqs. (40) and (41) and for the representations with Green’s matrices.

FIG 6: Configuration for the representations with propagator matrices.

FIG 7: Illustration of source and receiver redatuming. All responses in this figure are represented by simple rays, but in reality these are multi-component wave fields, including primaries, multiples, converted, refracted and evanescent waves. (a) The response $G(x_R,x_S,\omega)$ at the surface. The homogeneous Green’s matrix $G_h(x_R,x_S,\omega)$ is obtained from this re-
spose with Eq. (25). (b) Source redatuming. Using Eq. (69), the homogeneous Green’s matrix $G_h(x_R, x_B, \omega)$ is obtained for a virtual source at $x_B$. (c) Receiver redatuming. Using Eq. (70), the homogeneous Green’s matrix $G_h(x_A, x_B, \omega)$ is obtained for a virtual receiver at $x_A$. 