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DOI
10.1098/rspa.2016.0162

Publication date
2016

Document Version
Accepted author manuscript

Published in
Royal Society of London. Proceedings A. Mathematical, Physical and Engineering Sciences

Citation (APA)

Important note
To cite this publication, please use the final published version (if applicable). Please check the document version above.
Unified double- and single-sided homogeneous Green’s function representations

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In wave theory, the homogeneous Green’s function consists of the impulse response to a point source, minus its time-reversal. It can be represented by a closed boundary integral. In many practical situations the closed boundary integral needs to be approximated by an open boundary integral because the medium of interest is often accessible from one side only. The inherent approximations are acceptable as long as the effects of multiple scattering are negligible. However, in case of strongly inhomogeneous media, the effects of multiple scattering can be severe. We derive double- and single-sided homogeneous Green’s function representations. The single-sided representation applies to situations where the medium can be accessed from one side only. It correctly handles multiple scattering. It employs a focusing function instead of the backward propagating Green’s function in the classical (double-sided) representation. When reflection measurements are available at the accessible boundary of the medium, the focusing function can be retrieved from these measurements. Throughout the paper we use a unified notation which applies to acoustic, quantum-mechanical, electromagnetic and elastodynamic waves. We foresee many interesting applications of the unified single-sided homogeneous Green’s function representation in holographic imaging and inverse scattering, time-reversed wave field propagation, and interferometric Green’s function retrieval.
1. Introduction

In wave theory, the homogeneous Green’s function consists of the impulse response to a point source, minus its time-reversal. When there are no losses, the impulse response and its time-reversal obey the same wave equation with a delta-singularity at the position of the point source. When the difference of these wave equations is taken, the delta-singularities cancel each other. Hence, the homogeneous Green’s function obeys a wave equation without a delta-singularity.

The homogeneous Green’s function can be represented by a closed boundary integral. This representation plays an important role in optical, acoustic and seismic holography [1–3], imaging and inverse scattering [4,5], time-reversal acoustics [6] and Green’s function retrieval from ambient noise [7,8]. In many practical situations the closed boundary integral needs to be approximated by an open boundary integral because the medium of interest is often accessible from one side only. This can lead to unacceptable errors, particularly when multiple scattering cannot be ignored. To overcome this problem, we recently formulated a single-sided homogeneous Green’s function representation [9]. This representation was derived for the scalar wave equation. In this paper we use a unified matrix-vector notation for acoustic, quantum-mechanical, electromagnetic and elastodynamic waves. Based on a unified wave equation, we derive double- and single-sided representations for the homogeneous Green’s function. In particular the single-sided homogeneous Green’s function representation has many interesting potential applications in holographic imaging and inverse scattering, time-reversed wave field propagation and interferometric Green’s function retrieval, using scalar or vectorial wave fields.

2. Unified double-sided two-way representation

Throughout this paper, we define a “closed boundary” as two infinite horizontal boundaries, one above and one below the medium of interest. For this configuration we derive in this section a double-sided homogeneous Green’s function representation, expressed as integrals along these two boundaries. We start in section (a) by defining a unified two-way wave equation, which relates the vertical derivative of a wave vector via an operator matrix to the derivatives of the same wave vector in the horizontal plane. In section (b) we discuss two-way reciprocity theorems, using specific symmetry properties of the two-way wave equation. In section (c) we introduce the homogeneous Green’s function of the two-way wave equation and discuss its symmetry properties. Finally, in section (d) we use the two-way reciprocity theorem to derive the double-sided two-way representation of the homogeneous Green’s function.

(a) Two-way wave equation

We define the temporal Fourier transform of a space- and time-dependent quantity \( f(x, t) \) as

\[
 f(x, \omega) = \int_{-\infty}^{\infty} f(x, t) \exp(i\omega t) dt.
\]

(2.1)

Here \( t \) denotes time, \( \omega \) angular frequency, \( i \) is the imaginary unit, and \( x = (x_1, x_2, x_3) \) denotes the Cartesian coordinate vector; the \( x_3 \)-axis is pointing downward. For notational convenience, we use the same symbol (here \( f \)) for quantities in the time domain and in the frequency domain. The starting point for our derivations is a unified wave equation in the space-frequency domain, in matrix-vector form given by

\[
 \partial_3 \mathbf{q} - \mathbf{A} \mathbf{q} = \mathbf{d}.
\]

(2.2)

Here \( \mathbf{q} = \mathbf{q}(x, \omega) \) is a \( N \times 1 \) vector containing a specific choice of wave field components, \( \mathbf{d} = \mathbf{d}(x, \omega) \) is a \( N \times 1 \) vector containing the source functions, and \( \mathbf{A} = \mathbf{A}(x, \omega) \) is a \( N \times N \) operator matrix containing the medium parameters and the differential operators \( \partial_1 \) and \( \partial_2 \) (\( \partial_k \) for \( k = 1, 2, 3 \) stands for differentiation in the \( x_k \)-direction). The value of \( N \) depends on the type of wave field considered. We call equation (2.2) the “two-way” wave equation because, unlike in the
“one-way” wave equation discussed in section 3, equation (2.2) does not explicitly distinguish between “downward” and “upward” propagation. The wave field vector \( q \) implicitly contains the superposition of downgoing and upgoing waves.

For acoustic waves in fluids we have \( N = 2 \) [10–13], for quantum-mechanical waves \( N = 2 \), for electromagnetic waves in matter \( N = 4 \) [14–16], for elastodynamic waves in solids \( N = 6 \) [17,18], for poroelastic waves in porous solids \( N = 8 \), for coupled elastodynamic and electromagnetic waves in piezo-electric materials \( N = 10 \), and for coupled elastodynamic and electromagnetic waves in porous solids \( N = 12 \) [19]. From here onward we consider lossless media, hence, we exclude the two situations that concern waves in porous solids.

We subdivide the vectors in equation (2.2) into \( N/2 \times 1 \) subvectors and the matrix into \( N/2 \times N/2 \) submatrices, according to

\[
q = \begin{pmatrix} q_1 \\ q_2 \end{pmatrix}, \quad d = \begin{pmatrix} d_1 \\ d_2 \end{pmatrix}, \quad \mathcal{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}.
\]

We illustrate this for acoustic waves and for the Schrödinger equation. The basic acoustic equations are the equation of motion and the deformation equation

\[
\partial_t p + \rho \partial_t v_i = f_i, \quad \partial_t v_i + \kappa \partial_t p = q. \tag{2.4}
\]

Here the wave field components are acoustic pressure \( p = p(x, t) \) and particle velocity \( v_i = v_i(x, t) \), the source functions are external force density \( f_i = f_i(x, t) \) and injection-rate density \( q = q(x, t) \) (not to be confused with the components \( q_1 \) and \( q_2 \) of wave field vector \( q \) in equation (2.3)), the medium parameters are compressibility \( \kappa = \kappa(x) \) and mass density \( \rho = \rho(x) \).

Lower-case Latin subscripts (except \( t \)) run from 1 to 3, whereas lower-case Greek subscripts can take the values 1 and 2 to denote the horizontal components. The summation convention applies to repeated subscripts. We transform equations (2.4) and (2.5) to the space-frequency domain, using equation (2.1). The time derivatives are thus replaced by \(-i\omega\). Next, by eliminating the horizontal components of the particle velocity, \( v_1 \) and \( v_2 \), we obtain

\[
\partial_3 p - i \omega \rho v_3 = f_3, \tag{2.6}
\]

\[
\partial_3 v_3 - i \omega \kappa p + \frac{1}{i \omega} \partial_\alpha \left( \frac{1}{\rho} \partial_\alpha p \right) = q + \frac{1}{i \omega} \partial_\alpha \left( \frac{1}{\rho} f_\alpha \right). \tag{2.7}
\]

with \( p = p(x, \omega) \), etc. Equations (2.6) and (2.7) can be cast in the form of two-way wave equation (2.2) by defining the vectors and operator matrix as follows

\[
q = \begin{pmatrix} p \\ v_3 \end{pmatrix}, \quad d = \begin{pmatrix} f_3 \\ q + \frac{1}{i \omega} \partial_\alpha \left( \frac{1}{\rho} f_\alpha \right) \end{pmatrix}, \quad \mathcal{A} = \begin{pmatrix} 0 & i \omega \rho \\ i \omega \kappa - \frac{1}{i \omega} \partial_\alpha \left( \frac{1}{\rho} \partial_\alpha \right) & 0 \end{pmatrix}. \tag{2.8}
\]

Schrödinger’s wave equation for a particle with mass \( m \) in a potential \( V = V(x) \) is given by

\[
i \hbar \partial_t \Psi = -\frac{\hbar^2}{2m} \partial_x^2 \Psi + V \Psi, \tag{2.9}
\]

where \( \Psi = \Psi(x, t) \) is the wave function and \( \hbar = h/2\pi \), with \( h \) Planck’s constant. We transform this equation to the space-frequency domain, replace \( \partial_t \) by \(-i\omega\), and separate the vertical derivatives (\( \partial_\alpha \partial_3 \)) from the horizontal derivatives (\( \partial_\alpha \partial_\alpha \)). This gives

\[
\frac{2\hbar}{im} \partial_\alpha \partial_3 \Psi - 4i \left( \omega - \frac{V}{\hbar} \right) \Psi + \frac{2\hbar}{im} \partial_\alpha \partial_\alpha \Psi = 0, \tag{2.10}
\]

with \( \Psi = \Psi(x, \omega) \). This equation, together with the trivial equation \( \partial_3 \Psi = \frac{im}{2\hbar} \left( \frac{2\hbar}{im} \partial_3 \Psi \right) \), can be cast in the form of two-way wave equation (2.2), with

\[
q = \begin{pmatrix} \Psi \\ 0 \end{pmatrix}, \quad d = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad \mathcal{A} = \begin{pmatrix} 0 & \frac{im}{2\hbar} \\ 4i \left( \omega - \frac{V}{\hbar} \right) & 0 \end{pmatrix}. \tag{2.11}
\]
The vectors and matrices for the electromagnetic and elastodynamic situation can be found in several of the aforementioned references. Details of the definitions vary from author to author. In this paper we employ the definitions of Appendix C in reference [22], albeit that here we only consider real-valued medium parameters (because we consider lossless media) and we replace $-j$ by $i$ (to be consistent with the use of $i$ in Schrödinger’s equation).

For all considered cases, matrix $\mathbf{A}$ obeys the following symmetry properties
\[ N\mathbf{A}^t N = \mathbf{A}, \quad K\mathbf{A}^\dagger K = -\mathbf{A}, \quad (2.12) \]
where
\[ N = \begin{pmatrix} O & I \\ -I & O \end{pmatrix}, \quad K = \begin{pmatrix} O & I \\ I & O \end{pmatrix}, \quad (2.13) \]
with $I$ and $O$ being identity and zero matrices of appropriate size. Superscript $t$ denotes the transposed operator and $\dagger$ the adjoint (the complex conjugate transposed). Here transposed and adjoint operators are introduced via their integral properties
\[ \int_{\hat{A}} (U^f)g \, d^2x = \int_{\hat{A}} f^t(U^t)g \, d^2x \quad \text{and} \quad \int_{\hat{A}} (U^f)g^\dagger \, d^2x = \int_{\hat{A}} f^t(U^t)g^\dagger \, d^2x, \quad (2.14) \]
where $\hat{A}$ denotes an infinite horizontal integration boundary at arbitrary depth ($x_3 =$ constant), $f = f(x)$ and $g = g(x)$ are vector functions with “sufficient decay” at infinity, $f^t$ is the transposed vector, $f^\dagger$ is the complex conjugate transposed vector, and $U$ is an operator matrix containing the differential operators $\partial_1$ and $\partial_2$. Equation (2.14) implies that $U^t$ involves transposition of the matrix and transposition of the operators contained in the matrix, with $\hat{\partial}_1^t = -\partial_1$ and $\hat{\partial}_2^t = -\partial_2$. Other relevant implications are $U^t = (U^*)^t$ (where the asterisk denotes complex conjugation) and $(UV)^t = V^tU^t$ (where $V$ is also an operator matrix).

For all considered cases the submatrices of $\mathbf{A}$ are either real-valued or imaginary-valued, according to
\[ \Im \mathbf{A}_{11} = \Im \mathbf{A}_{22} = \Re \mathbf{A}_{12} = \Re \mathbf{A}_{21} = O, \quad (2.15) \]
where $\Re$ and $\Im$ denote the real and imaginary part, respectively. From this equation and the structure of matrix $\mathbf{A}$ defined in equation (2.3) we find the following additional symmetry property
\[ J\mathbf{A}^* J = \mathbf{A}, \quad \text{with} \quad J = \begin{pmatrix} I \\ O \\ -I \end{pmatrix}. \quad (2.16) \]

The wave vector $\mathbf{q}$ for all considered cases is scaled such that the power-flux density in the $x_3$-direction (or, for quantum-mechanical waves, the probability current density) is given by
\[ J(x, \omega) = \frac{1}{4} \mathbf{q}^t \mathbf{K} \mathbf{q} = \frac{1}{4} \{ \mathbf{q}_1^t \mathbf{q}_2 + \mathbf{q}_2^t \mathbf{q}_1 \}. \quad (2.17) \]

Finally, Table 1 summarises properties of matrices $N$, $K$, and $J$ that are frequently used throughout this paper without always explicitly mentioning this.

<table>
<thead>
<tr>
<th>Matrix</th>
<th>Inversion/Transposition</th>
<th>Mutual relations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N$</td>
<td>$N^{-1} = N^t = -N$</td>
<td>$N = JK = -KJ$</td>
</tr>
<tr>
<td>$K$</td>
<td>$K^{-1} = K^t = K$</td>
<td>$K = JN = -NJ$</td>
</tr>
<tr>
<td>$J$</td>
<td>$J^{-1} = J^t = J$</td>
<td>$J = NK = -KN$</td>
</tr>
</tbody>
</table>
(b) Two-way reciprocity theorems

We consider two wave field states $A$ and $B$, characterised by independent wave vectors $q_A(x, \omega)$ and $q_B(x, \omega)$, obeying wave equation (2.2) with independent source vectors $d_A(x, \omega)$ and $d_B(x, \omega)$ and operator matrices $A_A(x, \omega)$ and $A_B(x, \omega)$, respectively. The subscripts of the operator matrices refer to possibly different medium parameters (or quantum-mechanical potentials) in states $A$ and $B$. We consider a spatial domain $D$ enclosed by two infinite horizontal boundaries $\partial D_0$ and $\partial D_1$ (with $\partial D_1$ below $\partial D_0$), together denoted by $\partial D$. In this domain we define the interaction quantities $\partial_1\{q_A \cdot Nq_B\}$ and $\partial_2\{q_A \cdot Kq_B\}$. Applying the product rule for differentiation, using wave equation (2.2) in both states, integrating the result over domain $D$, applying the theorem of Gauss, and using the symmetry relations of equation (2.12) for operator matrices $D$ and operator matrices $A$, we obtain the following two-way reciprocity theorems [23,24]

$$\int_D (d_A^t Nq_B + q_A^t Nd_B) d^3x = \int_{\partial D} q_A^t Nq_B n_3 d^2x - \int_D q_A^t (A_B - A_A) q_B d^3x$$

(2.18)

and

$$\int_D (d_A^t Kq_B + q_A^t Kd_B) d^3x = \int_{\partial D} q_A^t Kq_B n_3 d^2x - \int_D q_A^t (A_B - A_A) q_B d^3x.$$  

(2.19)

Here $n_3$ is the vertical component of the outward pointing normal vector on $\partial D$, with $n_3 = -1$ at the upper boundary $\partial D_0$ and $n_3 = +1$ at the lower boundary $\partial D_1$. Equation (2.18) is a convolution-type reciprocity theorem [25,26] because products like $q_A^t Nq_B$ in the frequency domain correspond to convolutions in the time domain. Similarly, equation (2.19) is a correlation-type reciprocity theorem [27] because products like $q_A^t Kq_B$ in the frequency domain correspond to correlations in the time domain. Note that when there are no sources in $D$ and the medium parameters in $\mathbb{D}$ are equal in both states, then only the boundary integrals remain. These are then so-called two-way propagation invariants, which have been extensively used in the analysis of symmetry properties of reflection and transmission responses and for the design of efficient numerical modelling schemes [28–31].

(c) Two-way homogeneous Green’s function

We introduce the two-way Green’s function $G(x, x_B, \omega)$ as a $N \times N$ matrix obeying wave equation (2.2), with the source vector replaced by a diagonal point-source matrix, according to

$$\partial_t G - A_G = \delta(x - x_B),$$

(2.20)

where $x_B$ denotes the position of the point source of the Green’s function. As boundary condition we impose the physical radiation condition of outgoing waves at infinity, which corresponds to causality in the time domain, i.e., $G(x, x_B, t) = O$ for $t < 0$. In other words, $G(x, x_B, \omega)$ is the forward propagating Green’s function. Analogous to matrix $A$, we subdivide the Green’s matrix into $N/2 \times N/2$ submatrices, according to

$$G(x, x_B, \omega) = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix} (x, x_B, \omega).$$

(2.21)

The first subscript refers to the type of two-way wave field ($q_1$ or $q_2$) observed at $x$; the second subscript refers to the type of source ($d_1$ or $d_2$) at $x_B$. For example, for the acoustic situation we have

$$G(x, x_B, \omega) = \begin{pmatrix} G_{p,f} & G_{p,q} \\ G_{v,f} & G_{v,q} \end{pmatrix} (x, x_B, \omega),$$

(2.22)

where subscripts $p$ and $v$ stand for the observed wave quantities acoustic pressure ($p$) and particle velocity ($v$) at $x$, and subscripts $f$ and $q$ stand for the source types external force ($f$) and volume-injection rate ($q$) at $x_B$.

The two-way homogeneous Green’s function $G_{ij}(x, x_B, \omega)$ is introduced as a solution of wave equation (2.20), but without the delta singularity on the right-hand side. We therefore search for
a second solution of wave equation (2.20) (with the singularity), which will be subtracted from \( G(x, x_B, \omega) \) to form the homogeneous Green’s function. To find this second solution, take the complex conjugate of wave equation (2.20), and pre- and post-multiply all terms by \( J \). This gives

\[
\partial_t (JG^* J) - JA^* G^* J = JJ \delta(x - x_B). \tag{2.23}
\]

Using the property \( JJ = I \), this can be rewritten as

\[
\partial_t (JG^* J) - JA^* JG^* J = I \delta(x - x_B), \tag{2.24}
\]
or, using equation (2.16),

\[
\partial_t (JG^* J) - JG(JG^* J) = I \delta(x - x_B). \tag{2.25}
\]

Hence, \( JG^* (x, x_B, \omega) J \) is a second solution of wave equation (2.20). Subtracting wave equations (2.20) and (2.25), we obtain

\[
\partial_t G_h(x, x_B, \omega) - \mathcal{A} G_h(x, x_B, \omega) = 0, \tag{2.26}
\]
with the two-way homogeneous Green’s function \( G_h(x, x_B, \omega) \) defined as

\[
G_h(x, x_B, \omega) = G(x, x_B, \omega) - JG^* (x, x_B, \omega)J. \tag{2.27}
\]

Note that \( JG^* (x, x_B, \omega)J \) obeys the non-physical radiation condition of incoming waves at infinity, which corresponds to acausality in the time domain, i.e., \( JG(x, x_B, -t)J = 0 \) for \( t > 0 \).

In other words, \( JG^* (x, x_B, \omega)J \) is the backward propagating Green’s function. Using equation (2.21) and the definition of \( J \) in equation (2.16), equation (2.27) can be written as

\[
G_h(x, x_B, \omega) = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix} \begin{pmatrix} G_{11} + G_{12} \\ G_{21} + G_{22} \end{pmatrix} (x, x_B, \omega) = 2 \begin{pmatrix} \mathcal{I}G_{11} & \mathcal{I}G_{12} \\ \mathcal{I}G_{21} & \mathcal{I}G_{22} \end{pmatrix} (x, x_B, \omega). \tag{2.28}
\]

We conclude this section by deriving a reciprocity relation for the Green’s function. To this end we use the convolution-type reciprocity theorem (equation 2.18). For state \( A \) we replace the wave vector \( q_A(x, \omega) \) by matrix \( G(x, x_A, \omega) \) and the source vector \( d_A(x, \omega) \) by \( I \delta(x - x_A) \), which defines the source of the Green’s function at \( x_A \). Similarly, for state \( B \) we replace \( q_B(x, \omega) \) by \( G(x, x_B, \omega) \) and \( d_B(x, \omega) \) by \( I \delta(x - x_B) \). We choose \( x_A \) and \( x_B \) both in \( \mathbb{D} \). We take the medium parameters the same for both states, hence, the last integral in equation (2.18) vanishes. The boundary integral in equation (2.18) vanishes on account of the Sommerfeld radiation condition of outgoing waves at infinity. Using the silt-property of the Dirac delta function, the remaining integral in equation (2.18) gives

\[
NG(x_A, x_B, \omega) + G^T(x_B, x_A, \omega)N = 0, \tag{2.29}
\]
or, using \( N^{-1} = -N \),

\[
NG^T(x_B, x_A, \omega)N = G(x_A, x_B, \omega). \tag{2.30}
\]

Using \( JN = -NJ \) it follows that the same relation holds for the two-way homogeneous Green’s function defined in equation (2.27), i.e.,

\[
NG^T_h(x_B, x_A, \omega)N = G_h(x_A, x_B, \omega). \tag{2.31}
\]

(d) Double-sided two-way homogeneous Green’s function representation

We use the correlation-type reciprocity theorem (equation 2.19) to derive a representation for the two-way homogeneous Green’s function \( G_h(x_A, x_B, \omega) \). For states \( A \) and \( B \) we make the same replacements as above. Taking also the medium parameters again the same in both states, the last
Figure 1. Visualisation of the double-sided two-way homogeneous Green’s function representation (equation 2.33). Note that the “rays” in this and following figures (except Figure 4) represent the full responses between the source and receiver points, including multiple scattering and, in the elastodynamic situation, wave conversion. The arrows indicate that $G(x, x_B, \omega)$ is forward propagating (from $x_B$ to $x$), $KG(x, x_A, \omega)K$ is backward propagating (from $x$ to $x_A$), and $G_h(x_A, x_B, \omega)$ is a superposition of forward and backward propagating Green’s functions (between $x_B$ and $x_A$).

The integral in equation (2.19) vanishes. The remaining two integrals yield

$$KG(x_A, x_B, \omega) + G \dagger (x_B, x_A, \omega)K = \int \mathcal{B}_D \mathcal{D}_1 G \dagger (x, x_A, \omega)KG(x, x_B, \omega)n_3 d^2x.$$  \hspace{2cm} (2.32)

Note that the integral along the boundaries $\partial D_0$ and $\partial D_1$ does not vanish because the back-propagating Green’s function $G \dagger (x, x_A, \omega)$ obeys the non-physical radiation condition of incoming waves at infinity. Pre-multiplying all terms by $K$, using $KK = I$ and equations (2.30) and (2.27), gives

$$G_h(x_A, x_B, \omega) = \int \mathcal{B}_D \mathcal{D}_1 KG \dagger (x, x_A, \omega)KG(x, x_B, \omega)n_3 d^2x.$$  \hspace{2cm} (2.33)

This is the double-sided two-way homogeneous Green’s function representation, which is illustrated in Figure 1. It states that the two-way homogeneous Green’s function $G_h(x_A, x_B, \omega)$, with $x_A$ and $x_B$ both in $\mathcal{D}$, can be obtained from measurements at the boundary $\partial \mathcal{D}$. We have explicitly expressed the boundary $\partial \mathcal{D}$ as $\partial D_0 \cup \partial D_1$, to emphasise the fact that measurements should be carried out at two boundaries. Hence, application of equation (2.33) requires that the medium is accessible from two sides. Section 4 is dedicated to finding an alternative representation in terms of an integral along a single boundary, which is applicable for situations in which the medium is accessible from one side only.

We conclude this section by considering a special case. First, note that for the upper-right submatrix of $G_h(x_A, x_B, \omega)$, which we will call $G_h,12(x_A, x_B, \omega)$, equation (2.33) becomes

$$G_h,12(x_A, x_B, \omega) = \int \mathcal{B}_D \mathcal{D}_1 \left(G_{12} \dagger (x, x_A, \omega)G_{22}(x, x_B, \omega) + G_{22} \dagger (x, x_A, \omega)G_{12}(x, x_B, \omega)\right)n_3 d^2x,$$  \hspace{2cm} (2.34)

with $G_{h,12}(x_A, x_B, \omega) = 2R\{G_{12}(x_A, x_B, \omega)\}$, see equation (2.28). For the acoustic Green’s matrix, defined in equation (2.22), we replace $G_{12}(x, x_B, \omega)$ by $G_{p,q}(x, x_B, \omega) \equiv G(x, x_B, \omega)$ and $G_{22}(x, x_B, \omega)$ by $G_{v,q}(x, x_B, \omega) = (i\omega \rho)^{-1}\partial_3G_{p,q}(x, x_B, \omega)$ (and similar replacements for $G_{12}(x, x_A, \omega)$ etc.). Equation (2.34) thus becomes

$$G_h(x_A, x_B, \omega) = \frac{1}{i\omega \rho(x)} \left(G^\ast(x, x_A, \omega)\partial_3G(x, x_B, \omega) - \partial_3G^\ast(x, x_A, \omega)G(x, x_B, \omega)\right)n_3 d^2x,$$  \hspace{2cm} (2.35)
with the acoustic homogeneous Green's function $G_h(x_A, x_B; \omega)$ defined as

$$G_h(x_A, x_B, \omega) = G(x_A, x_B, \omega) + G^*(x_A, x_B, \omega) = 2R\{G(x_A, x_B, \omega)\}. \tag{2.36}$$

Equation (2.35) is the scalar homogeneous Green's function representation used in reference [9]. Note that the source of $G(x, x_B, \omega)$ is a unit point source of volume-injection rate density (hence, $q(x, \omega) = \delta(x - x_B)$). On the other hand, the Green’s function is often defined as the response to a unit source in the Helmholtz equation (for a medium with constant mass density $\rho$). Let us call this response $G(x, x_B, \omega)$. The relation between these two forms of the Green’s function is $G(x, x_B, \omega) = -i\omega/\rho G(x, x_B, \omega)$. Substituting this into equation (2.35) we obtain

$$G_h(x_A, x_B, \omega) = \int_{\partial\Omega} \left( \hat{G}^*(x, x_A, \omega) \partial_B \hat{G}(x, x_B, \omega) - \partial_B \hat{G}^*(x, x_A, \omega) \hat{G}(x, x_B, \omega) \right) n_B d^2x, \tag{2.37}$$

with

$$G_h(x_A, x_B, \omega) = G(x_A, x_B, \omega) - G^*(x_A, x_B, \omega) = 2i\Omega\{G(x_A, x_B, \omega)\}. \tag{2.38}$$

Equation (2.37) is the classical scalar homogeneous Green's function representation [1,5].

### 3. Unified double-sided one-way representation

In this section we follow a similar path as in section 2, except that the “two-way” wave fields will be replaced by “one-way” (downgoing and upgoing) wave fields. In section (a) we define downgoing and upgoing wavefields and introduce a unified one-way wave equation which governs the coupled propagation of these fields. In section (b) we discuss one-way reciprocity theorems, using specific symmetries of the one-way wave equation. In section (c) we introduce the homogeneous Green’s function of the one-way wave equation and discuss its symmetry properties. In section (d) we use the one-way reciprocity theorem to derive the double-sided one-way representation of the homogeneous Green’s function.

#### (a) One-way wave equation

We introduce a $N \times 1$ wave vector $p$ and a $N \times 1$ source vector $s$, according to

$$p = \begin{pmatrix} p^+ \\ p^- \end{pmatrix}, \quad s = \begin{pmatrix} s^+ \\ s^- \end{pmatrix}. \tag{3.1}$$

Note that we use different symbols for the vectors than in section 2, to distinguish clearly between two-way and one-way quantities (also note that vector $p$ should not be confused with the acoustic pressure $p$ in section 2). Here $p^+ = p^+(x, \omega)$ and $p^- = p^-(x, \omega)$ represent the downgoing (+) and upgoing (−) wavefield, respectively (recall that the $x_3$-axis is pointing downward). Similarly, $s^+ = s^+(x, \omega)$ and $s^- = s^-(x, \omega)$ represent the source functions for downgoing and upgoing waves, respectively. We formally relate the vectors $p$ and $s$ to the vectors $q$ and $d$ in equation (2.2) as follows,

$$q = \mathcal{L}p, \quad d = \mathcal{L}s, \tag{3.2}$$

where $N \times N$ matrix $\mathcal{L} = \mathcal{L}(x, \omega)$ is an operator matrix, containing pseudo-differential operators (such as the square-root Helmholtz operator) [10,12,13,24,32–36]. Substituting these expressions into equation (2.2) and pre-multiplying all terms by $\mathcal{L}^{-1}$ gives, after some straightforward manipulations,

$$\partial_B p - B p = s, \tag{3.3}$$

where

$$B = \mathcal{H} - \mathcal{L}^{-1} \partial_B \mathcal{L}, \tag{3.4}$$

with

$$\mathcal{H} = \mathcal{L}^{-1} \mathcal{A} \mathcal{L}, \quad \text{or} \quad \mathcal{A} = \mathcal{L} \mathcal{H} \mathcal{L}^{-1}. \tag{3.5}$$
We subdivide \( N \times N \) matrices \( \mathcal{H} \) and \( \mathcal{L} \) into \( N/2 \times N/2 \) submatrices, according to
\[
\mathcal{H} = \begin{pmatrix} i\mathcal{H}_1^T & 0 \\ 0 & -i\mathcal{H}_1^T \end{pmatrix}, \quad \mathcal{L} = \begin{pmatrix} \mathcal{L}_1^+ & \mathcal{L}_1^- \\ \mathcal{L}_2^+ & \mathcal{L}_2^- \end{pmatrix}.
\] (3.6)

Equation (3.3) is the unified one-way wave equation. Here “one-way” refers to the fact that this equation governs “downward” propagation of subvector \( p^+ \) and “upward” propagation of subvector \( p^- \). Note, however, that the one-way wave fields \( p^+ \) and \( p^- \) are coupled via the matrix \( \mathcal{L}^{-1} \partial_3 \mathcal{L} \). Using so-called power-flux normalisation [13,14,18,24,36], the following symmetry relations hold [24]
\[
N\mathcal{L}^i N = \mathcal{L}^{-1}, \quad NB^i N = B.
\] (3.7)

and
\[
J\mathcal{L}^i K = \mathcal{L}^{-1}, \quad JB^i J = -B.
\] (3.8)

For the symmetry properties in the latter equation evanescent waves are ignored. From the symmetry properties of \( B \) and \( J = -KN = NK \) we find the following additional symmetry property
\[
KB^* K = B.
\] (3.9)

Finally, from equations (2.17), (3.2) and (3.8) it follows (for non-evanescent waves) that the power-flux density in the \( x_3 \)-direction (or the probability current density) is given by
\[
J(x, \omega) = \frac{1}{2} p^+ J p = \frac{1}{2} \left( |p^+|^2 - |p^-|^2 \right).
\] (3.10)

(b) One-way reciprocity theorems

Following a similar derivation as for equations (2.18) and (2.19), but this time using the interaction quantities \( \partial_3 \{ p^+ A N p_B \} \) and \( \partial_3 \{ p^+ J p_B \} \), one-way wave equation (3.3) and symmetry relations (3.7) and (3.8) for operator \( B_A \), we obtain the following one-way reciprocity theorems [24,35]
\[
\int_D (s_A^i N p_B + p_A^i N s_B) d^3 x = \int_D (p_A^i A N p_B n_3) d^2 x - \int_D p_A^i A N (B_B - B_A) p_B d^3 x,
\] (3.11)

and
\[
\int_D (s_A^i J p_B + p_A^i J s_B) d^3 x = \int_D (p_A^i J p_B n_3) d^2 x - \int_D p_A^i J (B_B - B_A) p_B d^3 x.
\] (3.12)

In equation (3.12) evanescent waves are neglected. Note that when there are no sources in \( D \) and the medium parameters in \( D \) are equal in both states, then only the boundary integrals remain. These are then so-called one-way propagation invariants, which have been used in the derivation of relations between reflection and transmission responses, including those used in seismic interferometry [8] and Marchenko imaging [37,38].

(c) One-way homogeneous Green’s function

We introduce the one-way Green’s function \( \Gamma(x, x_B, \omega) \) as a \( N \times N \) matrix obeying wave equation (3.3), with the source vector replaced by a diagonal point-source matrix, according to
\[
\partial_3 \Gamma - B \Gamma = I \delta(x - x_B).
\] (3.13)

As boundary condition we impose the physical radiation condition of outgoing waves at infinity, which corresponds to causality in the time domain, i.e., \( \Gamma(x, x_B, t) = 0 \) for \( t < 0 \). We subdivide the one-way Green’s matrix into \( N/2 \times N/2 \) submatrices, according to
\[
\Gamma(x, x_B, \omega) = \begin{pmatrix} G^{+,+} & G^{+,-} \\ G^{-,+} & G^{-,-} \end{pmatrix}(x, x_B, \omega).
\] (3.14)

The first superscript refers to the type of one-way wave field \( (p^+ \text{ or } p^-) \) observed at \( x \); the second superscript refers to the type of source \( (s^+ \text{ or } s^-) \) at \( x_B \); see Figure 2.
To find a second solution of wave equation (3.13), take the complex conjugate of this equation, and pre- and post-multiply all terms by $K$. Using the property $KK = I$ and equation (3.9), we obtain

$$\partial_3 (K\Gamma^* K) - B(K\Gamma^* K) = I\delta(x - x_B).$$

(3.15)

Hence, $K\Gamma^*(x, x_B, \omega)K$ is a second solution of wave equation (3.13). Subtracting wave equations (3.13) and (3.15), we obtain

$$\partial_3 \Gamma h(x, x_B, \omega) - B\Gamma h(x, x_B, \omega) = 0,$$

(3.16)

with the one-way homogeneous Green’s function $\Gamma h(x, x_B, \omega)$ defined as

$$\Gamma h(x, x_B, \omega) = \Gamma(x, x_B, \omega) - K\Gamma^*(x, x_B, \omega)K.$$

(3.17)

Using equation (3.14) and the definition of $K$ in equation (2.13), equation (3.17) can be written as

$$\Gamma h(x, x_B, \omega) = \left\{ \begin{array}{l} G^{+,+} - (G^{-,-})^* \\ G^{-,+} - (G^{+,+})^* \\ G^{+,+} - (G^{+,+})^* \\ G^{-,+} - (G^{+,+})^* \end{array} \right\} (x, x_B, \omega).$$

(3.18)

Following a similar derivation as for equation (2.30), this time starting with the one-way convolution-type reciprocity theorem (equation 3.11), we find the following reciprocity relation for the one-way Green’s function

$$N\Gamma^t(x_B, x_A, \omega)N = \Gamma(x_A, x_B, \omega).$$

(3.19)

Using $KN = -NK$ it follows that the same relation holds for the one-way homogeneous Green’s function defined in equation (3.17), i.e.,

$$N\Gamma^t h(x_B, x_A, \omega)N = \Gamma h(x_A, x_B, \omega).$$

(3.20)

(d) Double-sided one-way homogeneous Green’s function representation

Following a similar derivation as for equation (2.33), starting with the one-way correlation-type reciprocity theorem (equation 3.12), we find the following double-sided one-way homogeneous Green’s function representation

$$\Gamma h(x_A, x_B, \omega) = \int_{\partial D_1 \cup \partial D_2} J\Gamma^t(x, x_A, \omega)J\Gamma(x, x_B, \omega)n_3 d^2 x.$$

(3.21)

Like the double-sided two-way homogeneous Green’s function representation in equation (2.33), this representation can only be used when the medium is accessible from two sides, see Figure 3.
4. Unified single-sided one-way representation

We derive a single-sided one-way representation of the homogeneous Green’s function from the one-way reciprocity theorems. In section (a) we briefly discuss the two states that will be used in the reciprocity theorems (a one-way Green’s function and a one-way focusing function). In section (b) we discuss the one-way focusing function in more detail, and in section (c) we use this focusing function and the Green’s function in the one-way reciprocity theorems to derive the single-sided one-way representation of the homogeneous Green’s function.

(a) Introduction of the two states

For the derivation of the single-sided representation we consider another configuration than for the double-sided representations. Instead of the domain $\mathbb{D}$ enclosed by $\partial \mathbb{D}_0$ and $\partial \mathbb{D}_1$ (Figures 1 and 3), we define a domain $\mathbb{D}_A$, enclosed by two infinite horizontal boundaries $\partial \mathbb{D}_0$ and $\partial \mathbb{D}_A$ (with $\partial \mathbb{D}_A$ below $\partial \mathbb{D}_0$), together denoted by $\partial \mathbb{D}$, see Figure 4. Here $\partial \mathbb{D}_0$ represents the accessible upper boundary of the medium (defined by $x_3 = x_3^A$) and $\partial \mathbb{D}_A$ is chosen at the depth of $x_A$, hence, it is defined by $x_3 = x_3^A$. The boundary $\partial \mathbb{D}_1$, which is indicated by dotted lines in Figures 4(a) and (b), is obsolete in the following derivations. In section (c) we will apply the one-way reciprocity theorems to domain $\mathbb{D}_A$, enclosed by $\partial \mathbb{D} = \partial \mathbb{D}_0 \cup \partial \mathbb{D}_A$. For state $B$ we take again the one-way Green’s function $\Gamma(x, x_B, \omega)$ that we also used in the previous section. This Green’s function is illustrated (for the acoustic case) in Figure 4(b), with more detail than in Figure 3. The orange lines in Figure 4(b) indicate some interfaces between layers with different medium parameters, and the green rays between $x_B$ (inside the medium) and $x$ (at the upper boundary $\partial \mathbb{D}_0$) represent some of the primary and multiply reflected waves in the Green’s function $\Gamma(x, x_B, \omega)$. The green rays between $x_B$ and $x_A$ represent the Green’s function $\Gamma(x_A, x_B, \omega)$. Note that $x_B$ may lie above or below $x_A$, hence inside or outside domain $\mathbb{D}_A$ (in this example it lies outside $\mathbb{D}_A$). Note that the solid black lines, indicating the integration boundaries $\partial \mathbb{D}_0$ and $\partial \mathbb{D}_A$, do not represent interfaces.

For state $A$ we introduce a one-way focusing function $F(x, x_A, \omega)$. Whereas a Green’s function propagates from a source at $x_A$ to $x$, a focusing function propagates from $x$ to $x_A$, where it focuses. In the double-sided representations, discussed in sections 2 and 3, the backpropagating Green’s functions $KG^\dagger(x, x_A, \omega)K$ and $JF^\dagger(x, x_A, \omega)J$ played this role. This “backpropagation approach” breaks down when the medium is accessible from one side only (here $\partial \mathbb{D}_0$), which is why we need a focusing function instead. In section (b) this focusing function will be formally defined. Here we introduce it intuitively at the hand of the ray diagram of Figure 4(a). This figure

Figure 3. Visualisation of the double-sided one-way homogeneous Green’s function representation (equation 3.21).
shows a reference medium, which is identical to the actual medium of Figure 4(b) in the domain \( \Omega_A \), whereas it is reflection-free in the half-spaces above \( \partial D_0 \) and below \( \partial D_A \). A downgoing focusing function \( F^+ (x, x_A, \omega) \) is incident from above (we consider the acoustic case, so the focusing function is a scalar field in this example). The outer red rays indicate the direct arrival of the downward propagating focusing function, converging to the focal point at \( x_A \) (these are only two of many direct rays converging to \( x_A \)). Before arriving at the focal point, these rays are reflected upward, indicated by the blue rays and denoted as \( F^- (x, x_A, \omega) \). If no further measures were taken, these rays would reflect downward again, giving rise to additional rays reaching the depth level \( \partial D_A \) but at other positions than the focal point. However, as can be seen in Figure 4(a), additional red rays are launched from the upper half-space into the medium, which reach the interfaces at the same positions as the upgoing blue rays, in such a way that they annihilate the aforementioned downward reflected rays. As a consequence, only the direct arrival of the downward propagating focusing function reaches \( \partial D_A \) and converges at the focal point. Interestingly, assuming the direct arrival of the focusing function \( F^+ (x, x_A, \omega) \) is known, the remainder of this function and the entire function \( F^- (x, x_A, \omega) \) (both for \( x \) at \( \partial D_0 \)) can be retrieved from reflection measurements at the accessible boundary \( \partial D_0 \), using a 3D version of the Marchenko method [38,41].

(b) One-way focusing function

Here we discuss the one-way focusing function in a more formal way. We introduce \( F(x, x_A, \omega) \) as a \( N \times N/2 \) matrix obeying wave equation (3.3) without a source function on the right-hand side and with an operator matrix \( B \) defined in a reference medium, hence

\[
\partial_3 F - BF = 0. \tag{4.1}
\]

The reference medium is equal to the actual medium between \( \partial D_0 \) and \( \partial D_A \) and reflection-free above \( \partial D_0 \) and below \( \partial D_A \). Hence, in \( \Omega_A \) we have \( B = B \), with \( B = \mathcal{H} - L^{-1} \partial_3 L \), see equation (3.4). Outside \( \Omega_A \), where the reference medium is reflection-free, the coupling matrix \( L^{-1} \partial_3 L \) is zero, hence \( B = \mathcal{H} \) outside \( \Omega_A \). We subdivide the one-way focusing function into \( N/2 \times N/2 \) submatrices, according to

\[
F(x, x_A, \omega) = \begin{pmatrix}
F^+(x, x_A, \omega) \\
F^-(x, x_A, \omega)
\end{pmatrix}, \tag{4.2}
\]

where the superscripts denote downward (+) and upward (−) propagation at \( x \). The downgoing focusing function \( F^+ (x, x_A, \omega) \) (variable \( x \), fixed \( x_A \)) is incident to the medium from the reflection-free upper half-space (above \( \partial D_0 \)). It propagates through the domain \( \Omega_A \), where it...
interacts with \( F^+(x, x_A, \omega) \) and vice versa due to the inhomogeneities of the medium, after which it focuses at \( x_A \). The focusing condition is denoted as

\[
F^+(x, x_A, \omega)|_{x_3=x_{3,A}} = I\delta(x_H - x_{H,A}), \tag{4.3}
\]

where \( x_H = (x_1, x_2) \) and \( x_{H,A} = (x_1, x_2, x_A) \) denote the horizontal coordinates of \( x \) and \( x_A \), respectively. The field at \( x_3 = x_{3,A} \) can also be written as

\[
F^+(x, x_A, \omega)|_{x_3=x_{3,A}} = \int_{\partial\Omega_0} T^+(x, x', \omega)F^+(x', x_A, \omega)d^2x', \tag{4.4}
\]

where \( T^+(x, x', \omega) \) is the transmission response of the medium between \( \partial\Omega_0 \) and \( \partial\Omega_A \). Replacing the left-hand side of equation (4.4) by the right-hand side of equation (4.3), it follows that \( T^+(x', x_A, \omega) \) for \( x' \) at \( \partial\Omega_0 \), i.e., the focusing function emitted from the upper boundary, is the inverse of the transmission response \( T^+(x, x', \omega) \) of the medium between \( \partial\Omega_0 \) and \( \partial\Omega_A \). This implies that the focusing function not only compensates for the geometrical spreading of the transmission response, but also for its multiple scattering (as illustrated in Figure 4(a)) and, in the elastodynamic situation, for wave conversion. Because there is no sink at \( x_A \), the focused downgoing field at \( x_A \) acts as a virtual source for downgoing waves in the half-space below \( \partial\Omega_A \). Because in the reference medium this half-space is reflection free, there is no upgoing field at and below \( \partial\Omega_A \). Hence, the focusing condition of equation (4.3) can be extended to

\[
F(x, x_A, \omega)|_{x_3=x_{3,A}} = \left( \begin{array}{c} I\delta(x_H - x_{H,A}) \\ O \end{array} \right) = I_1 \delta(x_H - x_{H,A}), \quad \text{with} \quad I_1 = \left( \begin{array}{c} I \\ 0 \end{array} \right). \tag{4.5}
\]

To avoid unstable behaviour of the focusing function, evanescent waves are excluded. This means that the delta function in equations (4.3) and (4.5) should be interpreted as a spatially band-limited delta function. Note that the sifting property of the delta function, \( h(x_{H,A}) = \int \delta(x_{H,A} - x_{H,A})h(x_{H,A})dx_{H,A} \), remains valid for a spatially band-limited delta function, assuming \( h(x_{H}) \) is also spatially band-limited (which is the case when evanescent waves are excluded).

(c) Single-sided one-way homogeneous Green’s function representation

We use the convolution-type and correlation-type one-way reciprocity theorems (equations 3.11 and 3.12), with \( \partial\Omega = \partial\Omega_0 \cup \partial\Omega_A \), to derive a single-sided representation for the one-way homogeneous Green’s function \( \Gamma_1(x_A, x_B, \omega) \). For state \( A \) we substitute the one-way focusing function defined in the reference medium, hence, we replace wave vector \( p_A(x, \omega) \) by matrix \( F(x, x_A, \omega) \), source vector \( s_A(x, \omega) \) by zero, and operator \( B_A \) by \( B \), which in \( \Omega_A \) is equal to \( B \). For state \( B \) we substitute the one-way Green’s function defined in the actual medium, hence, we replace wave vector \( p_B(x, \omega) \) by matrix \( \Gamma(x, x_B, \omega) \), source vector \( s_B(x, \omega) \) by \( I\delta(x - x_B) \) (with \( x_B \) below \( \partial\Omega_0 \)), and operator \( B_B \) by \( B \). Making these substitutions in the one-way reciprocity theorems, using the focusing condition defined in equation (4.5), yields

\[
I_1^1 \left( N\Gamma(x_A, x_B, \omega) - H(x_{3,A} - x_{3,B})F(x_B, x_A, \omega) \right)N = \int_{\partial\Omega_0} F(x, x_A, \omega)N\Gamma(x, x_B, \omega)d^2x \tag{4.6}
\]

and

\[
I_1^1 \left( J\Gamma^*(x_A, x_B, \omega) - H(x_{3,A} - x_{3,B})F(x_B, x_A, \omega) \right)J = \int_{\partial\Omega_0} F(x, x_A, \omega)J\Gamma^*(x, x_B, \omega)d^2x, \tag{4.7}
\]

where we used \( n_3 = -1 \) at \( \partial\Omega_0 \). \( H(x_B) \) is the Heaviside step function, hence, the second term on the left-hand sides of equations (4.6) and (4.7) only contributes when \( x_B \) lies above \( x_A \). Post-multiplying all terms in equation (4.7) by \( K \), using \( J = NK \) and \( JK = N \), and subtracting the
resulting equation from equation (4.6), gives

\[ I_1^2 \mathbf{N} \mathbf{\Gamma}_h(x_A, x_B, \omega) = \int_{\partial D_0} \mathbf{F}^t(x, x_A, \omega) \mathbf{N} \mathbf{\Gamma}_h(x, x_B, \omega) d^2 x, \]  

with the one-way homogeneous Green’s function \( \mathbf{\Gamma}_h(x, x_B, \omega) \) defined in equation (3.17). Note that the matrix \( I_1 \mathbf{N} \) on the left-hand side selects the lower two submatrices of \( \mathbf{\Gamma}_h \). We can recover the complete matrix \( \mathbf{\Gamma}_h \) as follows. First we define a matrix \( \mathbf{\Gamma}_2 \) by pre-multiplying the left-hand side of equation (4.8) by \( I_2 \) (defined below). Using equation (3.18) this gives

\[ \mathbf{\Gamma}_2 = I_2 \mathbf{N} \mathbf{\Gamma}_h = \begin{bmatrix} \mathbf{G}^- & \mathbf{O} \\ \mathbf{G}^+ & \mathbf{O} \end{bmatrix} = \begin{bmatrix} \mathbf{G}^- & \mathbf{0} \\ \mathbf{G}^+ & \mathbf{0} \end{bmatrix}, \quad \text{with} \quad I_2 = \begin{bmatrix} \mathbf{0} & \mathbf{I} \end{bmatrix}. \]  

Matrix \( \mathbf{\Gamma}_h(x_A, x_B, \omega) \), as defined in equation (3.18), is thus recovered via

\[ \mathbf{\Gamma}_h(x_A, x_B, \omega) = \mathbf{\Gamma}_2(x_A, x_B, \omega) = \mathbf{\Gamma}_2^t(x_A, x_B, \omega) \mathbf{K}, \]  

where, according to equations (4.8) and (4.9), \( \mathbf{\Gamma}_2(x_A, x_B, \omega) \) is given by

\[ \mathbf{\Gamma}_2(x_A, x_B, \omega) = \int_{\partial D_0} I_2 \mathbf{F}^t(x, x_A, \omega) \mathbf{N} \mathbf{\Gamma}_h(x, x_B, \omega) d^2 x. \]  

Equations (4.10) and (4.11) together form the single-sided one-way homogeneous Green’s function representation, which is illustrated in Figure 5(a). This representation states that the one-way homogeneous Green’s function \( \mathbf{\Gamma}_h(x_A, x_B, \omega) \), with \( x_A \) and \( x_B \) both below \( \partial D_0 \), can be obtained when the medium is accessible from the upper boundary \( \partial D_0 \) only.

It is interesting to note that \( \mathbf{\Gamma}_h(x, x_B, \omega) \) in the right-hand side of equation (4.11) can be represented in a similar way. To this end, in equation (4.8) we replace \( x \) by \( x' \) at \( \partial D_0' \), which we define just above \( \partial D_0 \). Furthermore, we replace \( x_B \) by \( x \) at \( \partial D_0 \) and \( x_A \) by \( x_B \). This gives

\[ I_1^t \mathbf{N} \mathbf{\Gamma}_h(x_B, x, \omega) = \int_{\partial D_0'} \mathbf{F}^t(x', x_B, \omega) \mathbf{N} \mathbf{\Gamma}_h(x', x, \omega) d^2 x', \]  

or, post-multiplying all terms by \( \mathbf{N} \) and transposing the result (using equation (3.20)),

\[ \mathbf{\Gamma}_h(x, x_B, \omega) I_1 = \int_{\partial D_0'} \mathbf{\Gamma}_h(x, x', \omega) \mathbf{F}^t(x', x_B, \omega) d^2 x'. \]  

Note that the matrix \( I_1 \) on the left-hand side selects the left two submatrices of \( \mathbf{\Gamma}_h \). Post-multiplying both sides of this equation by \( I_1^t \), we find in a similar way as above that the complete
matrix $\Gamma_h(x, x_B, \omega)$ is recovered as follows

$$
\Gamma_h(x, x_B, \omega) = \Gamma_1(x, x_B, \omega) - K \Gamma_1^*(x, x_B, \omega) K,
$$

(4.14)

with

$$
\Gamma_1(x, x_B, \omega) = \int_{\partial \Omega_0} \Gamma_h(x, x', \omega) F(x', x_B, \omega) \mathcal{L}^1 d^2 x',
$$

(4.15)

see Figure 5(b). Here $\Gamma_h(x, x', \omega)$ is a one-way homogeneous Green’s function with its source at $x'$ and receiver at $x$, both at the upper boundary.

5. Applications of the single-sided representation

We briefly discuss applications of the single-sided homogeneous Green’s function representation in holographic imaging and inverse scattering, time-reversed wave field propagation, and interferometric Green’s function retrieval. The discussions are not meant to be exhaustive but only indicate some applications and possible new research directions.

(a) Holographic imaging and inverse scattering

The central process in acoustic, electromagnetic and elastodynamic imaging and inverse scattering methods is the retrieval of the wave field inside the medium from measurements carried out at the boundary of that medium. The process to obtain the wave field inside the medium is in essence a form of holography. Here we discuss the steps that are needed to obtain the homogeneous Green’s function $G_h(x_A, x_B, t)$, with $x_A$ and $x_B$ inside the medium, from $G(x, x', t)$, with $x$ and $x'$ at the upper boundary of the medium. First, the one-way Green’s function $\Gamma(x, x', t)$ is obtained from the Fourier transform of $G(x, x', t)$, according to

$$
\Gamma(x, x', t) = \mathcal{L}^{-1}(x, \omega) G(x, x', \omega) \mathcal{N} \{ \mathcal{L}^{-1}(x', \omega) \} \mathcal{N},
$$

(5.1)

(see Appendix A, equation (A 7)); a left-arrow underneath an operator denotes that this operator is acting on the quantity left of it). This process is called decomposition. Examples for acoustic and elastodynamic wave fields can be found in reference [12].

Next, equations (4.14) and (4.15) are used to retrieve $\Gamma_h(x, x_B, \omega)$. The one-way homogeneous Green’s function $\Gamma_h(x, x', \omega)$ in equation (4.15) is obtained from $\Gamma(x, x', t)$ via equation (3.17), with $x_B$ replaced by $x'$. The time-domain version of the focusing function, $F(x', x_B, t)$, can be derived from $\Gamma(x, x', t)$ with the Marchenko method. For the 1D acoustic situation this does not require any additional information [37,39]. For the 2D and 3D acoustic situation, apart from $\Gamma(x, x', t)$, an estimate of the direct arrival between $x_B$ and $x'$ is needed to obtain $F(x', x_B, t)$, but no other information about the medium is required [38,40]. For the elastodynamic situation, also the forward scattered response between $x_B$ and $x'$ is needed [41], although in moderately inhomogeneous media a reasonable estimate of $F(x', x_B, t)$ can be obtained when only the direct arrival is known [42]. Once $F(x', x_B, t)$ has been retrieved, its Fourier transform is, according to equations (4.14) and (4.15), applied to $\Gamma_h(x, x', \omega)$ to obtain the one-way homogeneous Green’s function $\Gamma_h(x, x_B, \omega)$ (Figure 5(b)). Next, according to equations (4.10) and (4.11), the Fourier transform of $F(x, x_A, t)$ is applied to $\Gamma_h(x, x_B, \omega)$ to obtain $\Gamma_h(x_A, x_B, \omega)$ (Figure 5(a)). The combination of these two steps, i.e.

$$
\Gamma_h(x, x', \omega) \xrightarrow{F(x', x_B, \omega)} \Gamma_h(x, x_B, \omega) \xrightarrow{F(x, x_A, \omega)} \Gamma_h(x_A, x_B, \omega),
$$

(5.2)

is visualised in Figure 6. Note that in the first step the sources at all $x'$ at the boundary are focused to $x_B$, whereas in the second step the receivers at all $x$ at the boundary are focused to $x_A$. The resulting one-way homogeneous Green’s function $\Gamma_h(x_A, x_B, \omega)$ can be seen as the response to a virtual source at $x_B$, observed by a virtual receiver at $x_A$ (note that $x_A$ and $x_B$ can be chosen anywhere inside the medium). This two-step procedure resembles a method called “source-receiver redatuming” in exploration seismology [43,44], except that in that method only
multiple scattering and wave conversion. Primary waves are accounted for, whereas equation (5.2) accounts for primaries and all orders of scattering \[45–47\]. Note, however, that $G$ used for imaging the internal structures or finding the local medium parameters via inverse scattering occurring at interfaces between layers with different material parameters. Except for this example shows the evolution of $G_h(x_A, x_B, t)$ for variable $x_A, x_B$ and $t$ contains a wealth of additional information about the interior of the medium, of which the advantages need to be further explored.

An example of obtaining $G_h(x_A, x_B, t)$ from $G(x, x', t)$ for the acoustic situation can be found in [9]. This example shows the evolution of $G_h(x_A, x_B, t)$ through space and time, with multiple scattering occurring at interfaces between layers with different material parameters. Except for imaging and inverse scattering, the elastodynamic version could be very useful to predict the propagation of microseismic signals through an unknown complex subsurface.

(b) Time-reversed wave field propagation

In the field of time-reversal acoustics, the response to a source inside a medium is recorded at the boundary, reversed in time and emitted back from the boundary into the medium \[48\]. The back-propagated field focuses at the position of the source and after that the focal point acts as a virtual source. The generalisation of time-reversal acoustics for other types of waves we call time-reversed wave field propagation. The back-propagated field can be quantified with the homogeneous Green’s function representation, as follows. Transposing both sides of equation (2.33), using symmetry properties (2.30) and (2.31), we obtain

$$G_h(x_B, x_A, \omega) = \int_{D_D \cup D_I} \frac{G(x_B, x, \omega)}{J} G^*(x, x_A, \omega) J \, n_3 d^2 x.$$  
(5.4)

In the time domain this becomes

$$G_h(x_B, x_A, t) = \int_{D_D \cup D_I} \frac{G(x_B, x, t)}{J} * \frac{J G(x, x_A, -t)}{J} \, n_3 d^2 x,$$  
(5.5)

where the inline asterisk denotes temporal convolution. The Green’s function $G(x, x_A, t)$ represents the response to a source at $x_A$ inside the medium, observed at $x$ at the boundary. According to the right-hand side of equation (5.5), this field is reversed in time and used as a source function which is injected from all $x$ at the boundary $\partial D_0 \cup \partial D_1$ into the medium. The

Figure 6. Visualisation of the two-step procedure (equation 5.2). Starting with $\Gamma_h(x, x', \omega)$, the sources at all $x'$ at the boundary are focused to $x_B$, yielding $\Gamma_h(x, x_B, \omega)$. Next, the receivers at all $x$ at the boundary are focused to $x_A$, giving $\Gamma_h(x_A, x_B, \omega)$. 

primary waves are accounted for, whereas equation (5.2) accounts for primaries and all orders of multiple scattering and wave conversion. 

Next, the two-way homogeneous Green’s function $G_h(x_A, x_B, \omega)$ can be obtained from $\Gamma_h(x_A, x_B, \omega)$ via

$$G_h(x_A, x_B, \omega) = \mathcal{L}(x_A, \omega) \Gamma_h(x_A, x_B, \omega) N \mathcal{L}^*(x_B, \omega) N$$  
(5.3)

(see Appendix A, equation (A 10)). This process is called composition. Finally, $G_h(x_A, x_B, t)$ is obtained by an inverse Fourier transformation. This homogeneous Green’s function can be used for imaging the internal structures or finding the local medium parameters via inverse scattering \[45–47\]. Note, however, that $G_h(x_A, x_B, t)$ (for variable $x_A, x_B$ and $t$) contains a wealth of additional information about the interior of the medium, of which the advantages need to be further explored.

In the time domain this becomes

$$G_h(x_B, x_A, t) = \int_{\partial D_0 \cup \partial D_1} \frac{G(x_B, x, t)}{J} * \frac{J G(x, x_A, -t)}{J} \, n_3 d^2 x,$$  
(5.5)

where the inline asterisk denotes temporal convolution. The Green’s function $G(x, x_A, t)$ represents the response to a source at $x_A$ inside the medium, observed at $x$ at the boundary. According to the right-hand side of equation (5.5), this field is reversed in time and used as a source function which is injected from all $x$ at the boundary $\partial D_0 \cup \partial D_1$ into the medium. The
Green’s function \( G(x_B, x, t) \) propagates the field from the boundary to \( x_B \) inside the medium. The homogeneous Green’s function \( G_h(x_B, x_A, t) \) on the left-hand side (fixed \( x_A \), variable \( x_B \) and \( t \)) describes the time-dependent evolution of the injected field through the medium. Note that, according to equation (5.5), standard time-reversed wave field propagation requires that the medium is accessible from two sides. The single-sided homogeneous Green’s function representations developed in this paper provide an alternative. Because time-reversed wave field propagation is a physical process, we cannot use equation (4.11) which contains the non-physical homogeneous Green’s function under the integral on the right-hand side. Therefore we start with equation (4.6). Post-multiplying all terms by \( N \mathcal{L}^t(x_B, \omega) \) and replacing \( N \) in the right-hand side by \( N = -\mathcal{L}^t N \mathcal{L} \) (equation 3.7) gives

\[
I_1^t N \Gamma(x_A, x_B, \omega) N \mathcal{L}^t(x_B, \omega) + H(x_{3A} - x_{3B}) F^t(x_B, x_A, \omega) \mathcal{L}^t(x_B, \omega) = 0,
\]

or, using equation (A 7) and the definition of transposed operators (equation 2.14),

\[
I_1^t N \Gamma(x_A, x_B, \omega) N \mathcal{L}^t(x_B, \omega) + H(x_{3A} - x_{3B}) F^t(x_B, x_A, \omega) \mathcal{L}^t(x_B, \omega) = 0
\]

or, using symmetry relations (2.30) and (3.19) and transposing all terms,

\[
\Gamma^t(x_B, x_A, \omega) I_1 + H(x_{3A} - x_{3B}) F^t(x_B, x_A, \omega) = \int_{\partial D_B} G(x_B, x, \omega) F^t(x, x_A, \omega) d^3x,
\]

where the modified focusing function \( F^t(x, x_A, \omega) \) and the modified Green’s function \( \Gamma^t(x, x_A, \omega) \) are defined as

\[
F^t(x, x_A, \omega) = \mathcal{L}(x, \omega) F(x, x_A, \omega),
\]

\[
\Gamma^t(x, x_A, \omega) = \mathcal{L}(x, \omega) \Gamma(x, x_A, \omega).
\]

The operator \( \mathcal{L}(x, \omega) \) turns a one-way wave field into a two-way wave field, see equation (3.2). Hence, these modified functions consist of two-way fields at \( x \) and one-way fields at \( x_A \). In the time domain equation (5.8) becomes

\[
\Gamma^t(x_B, x_A, t) I_1 + H(x_{3A} - x_{3B}) F^t(x_B, x_A, t) = \int_{\partial D_B} G(x_B, x, t) \overbrace{F(x_B, x_A, t)}^{\text{source}} + \overbrace{F^t(x_B, x_A, t)}^{\text{propagator}} d^3x.
\]

This equation shows that, when the medium is accessible from one side only, the modified focusing function \( F^t(x, x_A, t) \) should be injected into the medium, instead of the time-reversed Green’s function (as in equation 5.5). When reflection measurements are available at the boundary, this focusing function can be obtained in a similar way as described in section (a), except that now the required direct arrival between \( x_A \) and \( x \) can be obtained directly from the measured response to the source at \( x_A \).

(c) Interferometric Green’s function retrieval

In the field of interferometric Green’s function retrieval, wave field observations at two points \( x_A \) and \( x_B \) are cross-correlated. Under specific conditions the time-dependent cross-correlation function is proportional to the homogeneous Green’s function between \( x_A \) and \( x_B \) [8,49–51]. For general wave fields, this principle is quantified by the homogeneous Green’s function representation. Using symmetry property (2.30) (which also holds in the time domain), we obtain
from equation (5.5)

\[
G_h(x_B, x_A, t) = -\int_{\partial D_B \cup \partial D_1} G(x_B, x, t) * \{ KG^1(x_A, x, t) K \} n_d d^2 x.
\]  

(5.12)

The integrand on the right-hand side describes a cross-correlation of responses to primary sources at \(x\) on \(\partial D_B \cup \partial D_1\), observed at \(x_A\) and \(x_B\) (actually the inline asterisk denotes a convolution, but because of the time-reversal of the second Green’s function, the integrand can be interpreted as a correlation). The left-hand side represents the response to a virtual source at \(x_A\), observed at \(x_B\).

When the primary sources are present only on a single boundary, the single-sided homogeneous Green’s function representations provide an alternative. Following a similar procedure as in section (b), but this time starting with equation (4.8), using equation (A 10) and symmetry relations (2.31) and (3.20), we obtain

\[
\Gamma_h^c(x_B, x_A, t_1) I_x = \int_{\partial D_B} G_h(x_B, x, t) * F^c(x, x_A, t) d^2 x,
\]

(5.13)

where \(\Gamma_h^c(x_B, x_A, t)\) is the inverse Fourier transform of

\[
\Gamma_h^c(x_B, x_A, \omega) = \mathcal{L}(x_B, \omega) \Gamma_h(x_B, x_A, \omega).
\]  

(5.14)

Equation (5.13) shows that, when sources are present on a single boundary only, instead of cross-correlating two Green’s functions, the homogeneous Green’s function at one observation point should be convolved with the modified focusing function at the other point. A possible way to obtain this focusing function is indicated in sections (a) and (b). Investigating alternative ways to obtain this function from measurements is subject of current research.

Finally, note that instead of \(\Gamma_h^c(x_B, x_A, t_1) I_x\), the homogeneous one-way Green’s function \(\Gamma_1(x_B, x_A, t)\) can be obtained, following a similar procedure as outlined at the end of section 4, according to

\[
\Gamma_h(x_B, x_A, t) = \Gamma_1(x_B, x_A, t) - K \Gamma_1(x_B, x_A, t) K,
\]  

(5.15)

with

\[
\Gamma_1(x_B, x_A, t) = \int_{\partial D_B} \Gamma_h(x_B, x, t) * \Gamma(x, x_A, t) d^2 x.
\]  

(5.16)

From this, the homogeneous two-way Green’s function \(G_h(x_B, x_A, t)\) can be obtained via equation (A 10).

6. Conclusions

We have captured double- and single-sided representations of the homogeneous Green’s function in a unified matrix notation. This notation accounts for acoustic, quantum-mechanical, electromagnetic and elastodynamic wave fields. A double-sided homogeneous Green’s function representation can only be used in situations where the medium of interest is accessible from two sides. Nevertheless, it is often used in an approximate sense in situations where the medium can be accessed from one side only. The inherent approximations are acceptable as long as the effects of multiple scattering (and wave conversion) are negligible. However, in the case of strongly inhomogeneous media (or inhomogeneous potentials in the quantum-mechanical case), the effects of multiple scattering can be quite severe. In this case, approximating a double-sided Green’s function representation by a single-sided representation leads to unacceptable errors. For example, in holographic imaging these errors manifest themselves as artefacts in the image of the interior of the medium. The single-sided homogeneous Green’s function representation, on the other hand, correctly handles multiple scattering (and wave conversion) in situations where the medium can be accessed from one side only. It employs a focusing function instead of a backward propagating Green’s function. Evanescent waves are ignored in the single-sided representation. When reflection measurements are available at the accessible boundary of the medium, the focusing function can be retrieved from these measurements and an estimate of the direct arrival between the boundary and the focal point. By employing the single-sided
homogeneous Green’s function representation in a two-step procedure, sources and receivers at the boundary are focused to virtual sources and virtual receivers inside the medium. The response between these virtual sources and receivers, i.e. the homogeneous Green’s function, includes multiple scattering and wave conversion. We foresee many interesting applications of the unified single-sided homogeneous Green’s function representation in holographic imaging and inverse scattering, time-reversed wave field propagation, and interferometric Green’s function retrieval.

A. Relation between two-way and one-way Green’s functions

Two-way and one-way wave vectors obey the simple relation

\[ \mathbf{q} = \mathbf{Lp} \]  (equation 3.2).

The relation between two-way and one-way Green’s functions is more complex, because it also involves an operator at the source position. We derive this relation from representations for \( \mathbf{q} \) and \( \mathbf{p} \). Consider again the two-way convolution-type reciprocity theorem (equation 2.18). For state \( A \) we replace the wave vector \( \mathbf{q}_A(x, \omega) \) by matrix \( \mathbf{G}(x, x_A, \omega) \) and the source vector \( \mathbf{d}_A(x, \omega) \) by \( \text{I}(x - x_A) \), with \( x_A \) in \( \mathbb{D} \). Here \( \mathbb{D} \) is again enclosed by two horizontal boundaries, together denoted by \( \partial \mathbb{D} \). However, these two horizontal boundaries can be different from \( \partial \mathbb{D}_0 \) and \( \partial \mathbb{D}_1 \) used in the main text. The only condition is that \( x_A \) lies between these boundaries. For state \( B \) we replace \( \mathbf{q}_B(x, \omega) \) by \( \mathbf{q}(x, \omega) \) and assume that this wave field obeys a source-free wave equation. We take the medium parameters the same for both states, hence, the last integral in equation (2.18) vanishes. Making the mentioned substitutions in the remaining integrals and using symmetry relation (2.30), we obtain

\[ \mathbf{q}(x_A, \omega) = -\int_{\partial \mathbb{D}} \mathbf{G}(x_A, x, \omega) \mathbf{q}(x, \omega) n_A d^2 x. \]  (A 1)

In a similar way, we obtain from the one-way convolution-type reciprocity theorem (equation 3.11) and symmetry relation (3.19)

\[ \mathbf{p}(x_A, \omega) = -\int_{\partial \mathbb{D}} \mathbf{\Gamma}(x_A, x, \omega) \mathbf{p}(x, \omega) n_A d^2 x. \]  (A 2)

Using equation (3.2) this becomes

\[ \mathbf{q}(x_A, \omega) = -\mathbf{L}(x_A, \omega) \int_{\partial \mathbb{D}} \mathbf{\Gamma}(x_A, x, \omega) \mathbf{L}^{-1}(x, \omega) \mathbf{q}(x, \omega) n_A d^2 x, \]  (A 3)

or, with the definition of transposed operators (equation 2.14),

\[ \mathbf{q}(x_A, \omega) = -\mathbf{L}(x_A, \omega) \int_{\partial \mathbb{D}} (\mathbf{L}^{-1}(x, \omega))^t \mathbf{\Gamma}^t(x_A, x, \omega) \mathbf{q}(x, \omega) n_A d^2 x, \]  (A 4)

or, using equation (3.7),

\[ \mathbf{q}(x_A, \omega) = -\mathbf{L}(x_A, \omega) \int_{\partial \mathbb{D}} \{ \mathbf{N} \mathbf{L}(x, \omega) \mathbf{N} \mathbf{\Gamma}^t(x_A, x, \omega) \}^t \mathbf{q}(x, \omega) n_A d^2 x. \]  (A 5)

Comparing this with equation (A 1), taking into account that both equations hold for any source-free wave field \( \mathbf{q}(x, \omega) \) and any integration boundary \( \partial \mathbb{D} \) encompassing \( x_A \), we find

\[ \mathbf{G}(x_A, x_B, \omega) = \mathbf{L}(x_A, \omega) \{ \mathbf{N} \mathbf{L}(x_B, \omega) \mathbf{N} \mathbf{\Gamma}^t(x_A, x_B, \omega) \}^t. \]  (A 6)

In the following we denote this as

\[ \mathbf{G}(x_A, x_B, \omega) = \mathbf{L}(x_A, \omega) \mathbf{\Gamma}(x_A, x_B, \omega) \mathbf{N} \mathbf{L}^t(x_B, \omega) \mathbf{N}, \]  (A 7)

where \( \mathbf{L}^t \) is the transposed matrix, containing (non-transposed) operators acting on the quantities left of it. To derive a similar relation between the two-way and one-way homogeneous
Green’s functions, we first consider the second term in equation (2.27), for which we obtain

\[ J G^*(x_A, x_B, \omega) J = J G^*(x_A, \omega) \Gamma^*(x_A, x_B, \omega) N \xi \xi^\dagger(x_B, \omega) N J. \]  

(A 8)

From equations (3.7) and (3.8) we obtain \( \xi \xi^\dagger = J K J \). Using this in equation (A 8) yields

\[ J G^*(x_A, x_B, \omega) J = \xi \xi^\dagger(x_B, \omega) \Gamma(x_A, x_B, \omega) N \xi \xi^\dagger N J J N J, \]

\[ = \xi \xi^\dagger(x_B, \omega) \{ J K^*(x_A, x_B, \omega) K \} N \xi \xi^\dagger(x_B, \omega) N. \]  

(A 9)

Subtracting equations (A 7) and (A 9), using the definitions of the two-way and one-way homogeneous Green’s functions (equations 2.27 and 3.17), we finally obtain

\[ G_h(x_A, x_B, \omega) = \xi \xi^\dagger(x_A, \omega) \Gamma_b(x_A, x_B, \omega) N \xi \xi^\dagger N J J N J. \]  

(A 10)

Ethics. There are no ethical issues.

Data Accessibility. No data were used.

Authors’ Contributions. All authors contributed to the development of the theory and methodology presented in this paper. KW wrote the manuscript. All authors critically read the manuscript, provided revisions, approve the final version and agree to be accountable for all aspects of the work.

Competing Interests. We have no competing interests.

Funding. This research is supported by the Dutch Technology Foundation STW (the applied science division of NWO and the Dutch Technology Program of the Ministry of Economic Affairs; grants 13939 and 13078).

Acknowledgements. We thank the reviewers and editor for their constructive remarks, which helped us to improve the clarity of the paper.

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