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Wapenaar, Kees

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A single-sided representation for the homogeneous Green's function of a unified scalar wave equation

Kees Wapenaar^{a)}

Department of Geoscience and Engineering, Delft University of Technology, Stevinweg 1, 2628 CN Delft, the Netherlands

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A unified scalar wave equation is formulated, which covers three-dimensional (3D) acoustic waves, 2D horizontally-polarised shear waves, 2D transverse-electric EM waves, 2D transverse-magnetic EM waves, 3D quantum-mechanical waves and 2D flexural waves. The homogeneous Green's function of this wave equation is a combination of the causal Green's function and its time-reversal, such that their singularities at the source position cancel each other. A classical representation expresses this homogeneous Green's function as a closed boundary integral. This representation finds applications in holographic imaging, time-reversed wave propagation and Green's function retrieval by cross correlation. The main drawback of the classical representation in those applications is that it requires access to a closed boundary around the medium of interest, whereas in many practical situations the medium can be accessed from one side only. Therefore, a single-sided representation is derived for the homogeneous Green's function of the unified scalar wave equation. Like the classical representation, this single-sided representation fully accounts for multiple scattering. The single-sided representation has the same applications as the classical representation, but unlike the classical representation it is applicable in situations where the medium of interest is accessible from one side only. © 2017 Acoustical Society of America.

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I. INTRODUCTION

The homogeneous Green's function is defined as the combination of the causal Green's function and its time-reversed function. Unlike the standard causal Green's function, which is singular at the position of the source, the homogeneous Green's function is regular throughout space. It can be represented in an exact form by a closed boundary integral.¹ This representation finds its applications in optical, acoustic and seismic holographic imaging methods.^{1–5} Moreover, it plays an important role in the fields of time-reversed wave propagation^{6–8} and Green's function retrieval from controlled-source or ambient-noise data by cross correlation.^{9–12} In many situations the closed boundary integral is for practical reasons replaced by an open boundary integral, for example because the medium to be imaged can be accessed from one side only. This induces approximations in the representation of the homogeneous Green's function, which can be quite severe when there is significant multiple scattering due to inhomogeneities in the medium. In recent work we have derived a single-sided homogeneous Green's function representation, which circumvents the need of omni-directional accessibility of the medium but nevertheless accounts for multiple scattering.¹³ Subsequently, we derived a unified form of this representation for a specific class of vectorial fields in lossless media.¹⁴ Here we derive a unified form of the single-sided homogeneous Green's function representation for a broad class of scalar fields in media with losses.

The setup of this paper is as follows. We start by introducing a unified scalar wave equation¹⁵ and discuss briefly how the coefficients and operators in this wave equation are defined for a variety of scalar wave phenomena. Next, we derive general reciprocity theorems (of the convolution type and of the correlation type) for two independent wave fields obeying the unified wave equation. We use the unified reciprocity theorem of the correlation type to derive a closed-boundary homogeneous Green's function representation and show that the classical representation¹ follows as a special case of this. Next, we modify the reciprocity theorems and derive a unified form of the single-sided homogeneous Green's function representation. We briefly discuss some applications and end with some conclusions.

II. UNIFIED SCALAR WAVE EQUATION

A broad class of wave phenomena obey a scalar wave equation. In particular, acoustic waves, horizontally-polarised shear waves, transverse-electric and transverse-magnetic EM waves, quantum waves and, finally, flexural waves in a thin plate, can all be captured by the following unified scalar wave equation:¹⁵

$$\left[\mathcal{D} - \sum_{n=0}^N a_n \frac{\partial^n}{\partial t^n} \right] u(\mathbf{x}, t) = -\frac{\partial s(\mathbf{x}, t)}{\partial t}. \quad (1)$$

Here $u(\mathbf{x}, t)$ represents the scalar wave field as a function of space $[\mathbf{x} = (x_1, x_2, x_3)]$ and time (t) . Throughout this paper, the positive x_3 -axis is pointing downward. The source

^{a)}Electronic mail: c.p.a.wapenaar@tudelft.nl

distribution, which causes the wave field, is denoted as $s(\mathbf{x}, t)$. The operator on the left-hand side consists of temporal differential operators (with N indicating the highest order), multiplied by space-dependent isotropic coefficients a_n , and an operator $\mathcal{D}$, containing spatial differential operators and space-dependent isotropic coefficients.

The temporal Fourier transform of a space- and time-dependent function $u(\mathbf{x}, t)$ is defined as

$$u(\mathbf{x}, \omega) = \int_{-\infty}^{\infty} \exp(i\omega t) u(\mathbf{x}, t) dt, \quad (2)$$

where ω is the angular frequency and i the imaginary unit (the sign convention in the exponential is chosen for consistency with Schrödinger's quantum wave equation). Note that, for notational convenience, the same symbol (u) is used for time- and frequency-domain functions. Equation (1) transformed to the frequency domain reads

$$\mathcal{W}u(\mathbf{x}, \omega) = i\omega s(\mathbf{x}, \omega), \quad (3)$$

with the wave operator $\mathcal{W}$ defined as

$$\mathcal{W} = \mathcal{D} - \sum_{n=0}^N (-i\omega)^n a_n. \quad (4)$$

In this paper we consider two specific forms of the operator $\mathcal{D}$, named $\mathcal{D}_2$ and $\mathcal{D}_4$, but any other operator obeying the integral property discussed in Sec. III [Eq. (9)] may be chosen as well. For most wave phenomena considered in this paper, operator $\mathcal{D}$ is defined as

$$\mathcal{D}_2 = \partial_i b \partial_i, \quad (5)$$

with ∂_i standing for spatial differentiation in the x_i -direction. Einstein's summation convention applies to repeated subscripts. The subscript 2 in $\mathcal{D}_2$ denotes this is a second order differential operator. The notation in the right-hand side of Eq. (5) should be understood in the sense that differential operators act on everything to the right of it, hence, $\mathcal{D}_2 f$ stands for $\partial_i (b \partial_i f)$.

Table I shows the definitions of u , s , a_n (for $n = 0, 1, 2$), $\mathcal{D}$ and b for the different wave phenomena considered in this paper. The quantities in the first row correspond to the three-dimensional (3D) acoustic wave equation in a fluid, with p the acoustic pressure, q the volume density of volume injection rate, η the viscosity, κ the compressibility and ρ the

volume density of mass.¹⁶ The second row refers to the 2D elastic wave equation for horizontally-polarised shear waves (SH) in a solid, with v_2 the transverse particle velocity, f_2 the volume density of transverse external force, r the coefficient of frictional force, ρ the volume density of mass and μ the shear modulus.¹⁷ In this paper, 2D wave equations are defined in the $\mathbf{x} = (x_1, x_3)$ -plane, hence, for the 2D situations, subscript i in Eq. (5) takes on the values 1 and 3 only. The third and fourth rows refer to 2D electromagnetic wave equations in matter, with TE and TM standing for “transverse electric” and “transverse magnetic,” respectively. Here E_2 and H_2 are the transverse electric and transverse magnetic field strengths, respectively, J_2^e and J_2^m the volume densities of transverse external electric and magnetic current, respectively, σ the conductivity, ϵ the permittivity and μ the permeability.^{17,18} The fifth row corresponds to the 3D quantum wave equation (Schrödinger equation) for a particle with mass m in a potential V , with ψ the quantum mechanical wave function, and $\hbar = h/2\pi$, with h Planck's constant.^{19,20}

For flexural waves in a thin plate in the $\mathbf{x} = (x_1, x_3)$ -plane, operator $\mathcal{D}_4$ in the sixth row is defined as

$$\mathcal{D}_4 = -\partial_i \partial_j d_1 \partial_i \partial_j - \partial_i \partial_i d_2 \partial_j \partial_j, \quad (6)$$

with

$$d_1 = (1 - \nu)d, \quad (7)$$

$$d_2 = \nu d, \quad (8)$$

where ν is Poisson's ratio and d the bending stiffness (Appendix A). The subscript 4 in $\mathcal{D}_4$ denotes this is a fourth order differential operator. Subscripts i and j take on the values 1 and 3 only. The other quantities in the sixth row in Table I are the transverse particle velocity v_2 , the area density of transverse external force f_2 , and the area density of mass ρ . The expression given for coefficient b in this row can for the moment be ignored. It will be discussed later.

To account for general loss mechanisms, we assume that a_n as well as the coefficients in operator $\mathcal{D}$ may be complex-valued and frequency-dependent, i.e., $a_n = a_n(\mathbf{x}, \omega)$, $b = b(\mathbf{x}, \omega)$, $d_1 = d_1(\mathbf{x}, \omega)$ and $d_2 = d_2(\mathbf{x}, \omega)$, with (for positive ω) $\Re\{(-i)^n a_n, b, d_1, d_2\} \geq 0$ and $\Im\{(-i)^n a_n, b, d_1, d_2\} \leq 0$, where $\Re$ and $\Im$ denote the real and imaginary parts, respectively.

III. RECIPROCITY THEOREMS

A. Integral property of operators $\mathcal{D}$ and $\mathcal{W}$

For the derivation of the unified reciprocity theorems in Secs. III B and III C we will make use of an integral property of the operators $\mathcal{D}$ and $\mathcal{W}$. Consider an arbitrary spatial domain $\mathbb{V}$, enclosed by boundary $\mathbb{S}$, with outward pointing normal vector $\mathbf{n}$ (Fig. 1). For the 3D situation, the domain is a 3D volume and its boundary is a 2D surface with normal vector $\mathbf{n} = (n_1, n_2, n_3)$. For the 2D situation, the domain is a 2D area in the (x_1, x_3) -plane and its boundary is a 1D contour with normal vector $\mathbf{n} = (n_1, n_3)$.

Using the theorem of Gauss, it can be shown that

TABLE I. Definition of the wave fields, sources, operators and coefficients in the wave equation [Eq. (3)] for the wave phenomena considered in this paper.

	u	s	a_0	a_1	a_2	$\mathcal{D}$	b
Acoustic waves (3D)	p	q	0	$\frac{1}{\eta}$	κ	$\mathcal{D}_2$	$\frac{1}{\rho}$
SH-waves (2D)	v_2	f_2	0	r	ρ	$\mathcal{D}_2$	μ
TE-waves (2D)	E_2	$-J_2^e$	0	σ	ϵ	$\mathcal{D}_2$	$\frac{1}{\mu}$
TM-waves (2D)	H_2	$-J_2^m$	0	0	μ	$\mathcal{D}_2$	$\frac{1}{\epsilon - \frac{\sigma}{i\omega}}$
Quantum waves (3D)	ψ		V	$-i\hbar$	0	$\mathcal{D}_2$	$\frac{\hbar^2}{2m}$
Flexural waves (2D)	v_2	f_2	0	0	ρ	$\mathcal{D}_4$	$2\omega\sqrt{\rho d}$

FIG. 1. Domain $\mathbb{V}$, enclosed by boundary $\mathbb{S}$, with outward pointing normal vector $\mathbf{n}$. Outside a sphere with finite radius, the medium is homogeneous and lossless.

$$\int_{\mathbb{V}} [f(\mathcal{D}g) - (\mathcal{D}f)g] d\mathbf{x} = \oint_{\mathbb{S}} \mathcal{J}(f, g) d\mathbf{x}, \quad (9)$$

where, for $\mathcal{D} = \mathcal{D}_2$, the interaction quantity $\mathcal{J}$ is defined as

$$\mathcal{J}_2(f, g) = [f(b\partial_i g) - (b\partial_i f)g]n_i, \quad (10)$$

and, for $\mathcal{D} = \mathcal{D}_4$,

$$\begin{aligned} \mathcal{J}_4(f, g) = & [(\partial_i f)(d_1 \partial_i \partial_j g) - (d_1 \partial_i \partial_j f)(\partial_j g) \\ & + (\partial_j d_1 \partial_i \partial_j f)g - f(\partial_j d_1 \partial_i \partial_j g) \\ & + (\partial_i f)(d_2 \partial_j \partial_j g) - (d_2 \partial_j \partial_j f)(\partial_i g) \\ & + (\partial_i d_2 \partial_j \partial_j f)g - f(\partial_i d_2 \partial_j \partial_j g)]n_i. \end{aligned} \quad (11)$$

Here $f=f(\mathbf{x})$ and $g=g(\mathbf{x})$ are arbitrary space-dependent functions [not necessarily solutions of Eq. (3)]. The left-hand side of Eq. (9) is unaltered when we add an arbitrary function to $\mathcal{D}$. In particular, we may replace $\mathcal{D}$ by $\mathcal{W}$, as defined in Eq. (4), hence

$$\int_{\mathbb{V}} [f(\mathcal{W}g) - (\mathcal{W}f)g] d\mathbf{x} = \oint_{\mathbb{S}} \mathcal{J}(f, g) d\mathbf{x}. \quad (12)$$

B. Reciprocity theorem of the convolution type

We consider two independent wave states A and B for which we derive a reciprocity theorem. The source distributions and wave fields in these states are distinguished by subscripts A and B . Outside a sphere (or, in 2D, a circle) with finite radius, the medium (or, for quantum mechanics, the potential) is homogeneous and lossless in both states (Fig. 1).

For the derivation of the first reciprocity theorem, the coefficients a_n , b , etc. inside $\mathbb{V}$ are chosen the same in both states (outside $\mathbb{V}$ the coefficients in the two states may be different). Hence, in the frequency domain the wave fields $u_A(\mathbf{x}, \omega)$ and $u_B(\mathbf{x}, \omega)$ obey in $\mathbb{V}$ the following two equations:

$$\mathcal{W}u_A(\mathbf{x}, \omega) = i\omega s_A(\mathbf{x}, \omega), \quad (13)$$

$$\mathcal{W}u_B(\mathbf{x}, \omega) = i\omega s_B(\mathbf{x}, \omega). \quad (14)$$

We obtain a reciprocity theorem by substituting $f=u_A$ and $g=u_B$ into Eq. (12), using Eqs. (13) and (14). We thus obtain

$$i\omega \int_{\mathbb{V}} [u_A s_B - s_A u_B] d\mathbf{x} = \oint_{\mathbb{S}} \mathcal{J}(u_A, u_B) d\mathbf{x}. \quad (15)$$

We call this the reciprocity theorem of the convolution type,^{17,21} because products like $u_A s_B$ in the frequency domain correspond to convolutions in the time domain.

C. Reciprocity theorem of the correlation type

We consider again two independent wave states A and B for which we derive a second reciprocity theorem. The wave field in state B obeys in $\mathbb{V}$ again Eq. (14). For state A we define an adjoint medium (or, for quantum mechanics, an adjoint potential), with coefficients $\bar{a}_n = (-1)^n a_n^*$, $\bar{b} = b^*$, $\bar{d}_1 = d_1^*$ and $\bar{d}_2 = d_2^*$. Here the bar denotes the adjoint medium and the asterisk denotes complex conjugation. When the original medium is dissipative, the adjoint medium is effectual^{22–24} (a wave propagating through an effectual medium gains energy; effectual media are usually associated with a computational state). The wave operator for the adjoint medium is defined as

$$\bar{\mathcal{W}} = \bar{\mathcal{D}} - \sum_{n=0}^N (-i\omega)^n \bar{a}_n. \quad (16)$$

Note that

$$\bar{\mathcal{W}} = \mathcal{W}^*. \quad (17)$$

We define $\bar{u}_A$ as the solution of the wave equation for the adjoint medium, hence

$$\bar{\mathcal{W}}\bar{u}_A(\mathbf{x}, \omega) = i\omega s_A(\mathbf{x}, \omega). \quad (18)$$

Taking the complex conjugate of both sides of this equation, using Eq. (17), gives

$$\mathcal{W}\bar{u}_A^*(\mathbf{x}, \omega) = -i\omega s_A^*(\mathbf{x}, \omega). \quad (19)$$

We obtain our second reciprocity theorem by substituting $f=\bar{u}_A^*$ and $g=u_B$ into Eq. (12), using Eqs. (19) and (14). We thus obtain

$$i\omega \int_{\mathbb{V}} [\bar{u}_A^* s_B + s_A^* u_B] d\mathbf{x} = \oint_{\mathbb{S}} \mathcal{J}(\bar{u}_A^*, u_B) d\mathbf{x}. \quad (20)$$

We call this the reciprocity theorem of the correlation type,^{21,25} because products like $\bar{u}_A^* s_B$ in the frequency domain correspond to correlations in the time domain.

A special case is obtained when we consider a lossless medium (which implies we may omit the bars) and take states A and B identical (implying we may also omit the subscripts A and B). Equation (20) yields for this situation

$$\frac{1}{4} \int_{\mathbb{V}} [u^* s + s^* u] d\mathbf{x} = \frac{1}{4i\omega} \oint_{\mathbb{S}} \mathcal{J}(u^*, u) d\mathbf{x}. \quad (21)$$

This expression formulates power conservation, except for the Schrödinger equation, in which case Eq. (21), multiplied by $4\omega/\hbar$, stands for conservation of probability.

IV. CLOSED-BOUNDARY GREEN'S FUNCTION REPRESENTATION

A. Reciprocity of the Green's function

We apply the reciprocity theorem of the convolution type [Eq. (15)] to Green's functions. For state A we define the Green's function $G(\mathbf{x}, \mathbf{x}_A, \omega)$ as the solution of wave Eq. (13), with the source replaced by a unit point source, $\delta(\mathbf{x} - \mathbf{x}_A)$, with $\mathbf{x}_A$ inside $\mathbb{V}$. Hence

$$\mathcal{W}G(\mathbf{x}, \mathbf{x}_A, \omega) = i\omega\delta(\mathbf{x} - \mathbf{x}_A). \quad (22)$$

In a similar way, for state B we define $G(\mathbf{x}, \mathbf{x}_B, \omega)$ as the response to a unit point source at $\mathbf{x}_B$ inside $\mathbb{V}$, hence

$$\mathcal{W}G(\mathbf{x}, \mathbf{x}_B, \omega) = i\omega\delta(\mathbf{x} - \mathbf{x}_B). \quad (23)$$

The coefficients of $\mathcal{W}$ are the same in both states, inside as well as outside $\mathbb{V}$. As boundary condition we impose the physical radiation condition of outgoing waves at infinity, which corresponds to causality in the time domain, i.e., $G(\mathbf{x}, \mathbf{x}_A, t) = G(\mathbf{x}, \mathbf{x}_B, t) = 0$ for $t < 0$. In other words, $G(\mathbf{x}, \mathbf{x}_A, \omega)$ and $G(\mathbf{x}, \mathbf{x}_B, \omega)$ are forward propagating Green's functions. We make the following substitutions in the reciprocity theorem of the convolution type [Eq. (15)]:

$$s_A = \delta(\mathbf{x} - \mathbf{x}_A), \quad (24)$$

$$u_A = G(\mathbf{x}, \mathbf{x}_A, \omega), \quad (25)$$

$$s_B = \delta(\mathbf{x} - \mathbf{x}_B), \quad (26)$$

$$u_B = G(\mathbf{x}, \mathbf{x}_B, \omega). \quad (27)$$

The boundary integral on the right-hand side is independent of the choice for $\mathbb{S}$ (as long as it encloses $\mathbf{x}_A$ and $\mathbf{x}_B$). Hence, it vanishes on account of the Sommerfeld radiation condition for outgoing waves at infinity. As a result, Eq. (15) yields for this situation

$$G(\mathbf{x}_B, \mathbf{x}_A, \omega) = G(\mathbf{x}_A, \mathbf{x}_B, \omega). \quad (28)$$

This expression formulates source-receiver reciprocity.

B. The closed-boundary homogeneous Green's function representation

We apply the reciprocity theorem of the correlation type [Eq. (20)] to Green's functions. For state A we define the Green's function $\bar{G}(\mathbf{x}, \mathbf{x}_A, \omega)$ in the adjoint medium as the solution of

$$\bar{\mathcal{W}}\bar{G}(\mathbf{x}, \mathbf{x}_A, \omega) = i\omega\delta(\mathbf{x} - \mathbf{x}_A), \quad (29)$$

with $\mathbf{x}_A$ in $\mathbb{V}$, and we impose again the condition of outgoing waves at infinity. Taking the complex conjugate of both sides of Eq. (29) gives

$$\mathcal{W}\bar{G}^*(\mathbf{x}, \mathbf{x}_A, \omega) = -i\omega\delta(\mathbf{x} - \mathbf{x}_A). \quad (30)$$

$\bar{G}^*(\mathbf{x}, \mathbf{x}_A, \omega)$ obeys the non-physical radiation condition of incoming waves at infinity, which corresponds to

acausality in the time domain, i.e., $\bar{G}(\mathbf{x}, \mathbf{x}_A, -t) = 0$ for $t > 0$. In other words, $\bar{G}^*(\mathbf{x}, \mathbf{x}_A, \omega)$ is a backward propagating Green's function. For state B we choose again $G(\mathbf{x}, \mathbf{x}_B, \omega)$, obeying Eq. (23), with $\mathbf{x}_B$ in $\mathbb{V}$. We substitute

$$s_A = \delta(\mathbf{x} - \mathbf{x}_A), \quad (31)$$

$$\bar{u}_A = \bar{G}(\mathbf{x}, \mathbf{x}_A, \omega), \quad (32)$$

for state A , and Eqs. (26) and (27) for state B , into the reciprocity theorem of the correlation type (Eq. 20). This gives

$$\begin{aligned} G(\mathbf{x}_A, \mathbf{x}_B, \omega) + \bar{G}^*(\mathbf{x}_B, \mathbf{x}_A, \omega) \\ = \frac{1}{i\omega} \oint_{\mathbb{S}} \mathcal{J}(\bar{G}^*(\mathbf{x}, \mathbf{x}_A, \omega), G(\mathbf{x}, \mathbf{x}_B, \omega)) d\mathbf{x}. \end{aligned} \quad (33)$$

Using Eq. (28) this can be rewritten as

$$G_h(\mathbf{x}_B, \mathbf{x}_A, \omega) = \frac{1}{i\omega} \oint_{\mathbb{S}} \mathcal{J}(\bar{G}^*(\mathbf{x}, \mathbf{x}_A, \omega), G(\mathbf{x}, \mathbf{x}_B, \omega)) d\mathbf{x}, \quad (34)$$

with the homogeneous Green's function $G_h(\mathbf{x}_B, \mathbf{x}_A, \omega)$ defined as

$$G_h(\mathbf{x}_B, \mathbf{x}_A, \omega) = G(\mathbf{x}_B, \mathbf{x}_A, \omega) + \bar{G}^*(\mathbf{x}_B, \mathbf{x}_A, \omega). \quad (35)$$

By combining Eqs. (22) and (30), it follows that $G_h(\mathbf{x}, \mathbf{x}_A, \omega)$ obeys the following wave equation

$$\mathcal{W}G_h(\mathbf{x}, \mathbf{x}_A, \omega) = 0. \quad (36)$$

This is a homogeneous differential equation, hence the name "homogeneous Green's function" for its solution $G_h(\mathbf{x}, \mathbf{x}_A, \omega)$.

Equation (34) is akin to the classical homogeneous Green's function representation.^{1,5} To demonstrate this, we write the integrand in Eq. (34) in explicit form for the wave phenomena in the first five rows of Table I. Using $\mathcal{J}_2$, as defined in Eq. (10), we obtain

$$\begin{aligned} G_h(\mathbf{x}_B, \mathbf{x}_A, \omega) = \frac{1}{i\omega} \oint_{\mathbb{S}} b(\mathbf{x}, \omega) (\bar{G}^*(\mathbf{x}, \mathbf{x}_A, \omega) \partial_i G(\mathbf{x}, \mathbf{x}_B, \omega) \\ - \partial_i \bar{G}^*(\mathbf{x}, \mathbf{x}_A, \omega) G(\mathbf{x}, \mathbf{x}_B, \omega)) n_i d\mathbf{x}. \end{aligned} \quad (37)$$

Next, we take b constant and real-valued, and introduce a modified Green's function $\mathcal{G}(\mathbf{x}, \mathbf{x}_A, \omega)$, obeying the wave equation

$$\frac{1}{b} \mathcal{W}\mathcal{G}(\mathbf{x}, \mathbf{x}_A, \omega) = -\delta(\mathbf{x} - \mathbf{x}_A). \quad (38)$$

Comparing this with Eq. (22), it follows that

$$\mathcal{G}(\mathbf{x}, \mathbf{x}_A, \omega) = -\frac{b}{i\omega} G(\mathbf{x}, \mathbf{x}_A, \omega). \quad (39)$$

Using this relation, Eq. (37) can be rewritten as

$$\begin{aligned} G_h(\mathbf{x}_B, \mathbf{x}_A, \omega) = \oint_{\mathbb{S}} (\bar{G}^*(\mathbf{x}, \mathbf{x}_A, \omega) \partial_i \mathcal{G}(\mathbf{x}, \mathbf{x}_B, \omega) \\ - \partial_i \bar{G}^*(\mathbf{x}, \mathbf{x}_A, \omega) \mathcal{G}(\mathbf{x}, \mathbf{x}_B, \omega)) n_i d\mathbf{x}, \end{aligned} \quad (40)$$

with

$$\mathcal{G}_h(\mathbf{x}_B, \mathbf{x}_A, \omega) = \mathcal{G}(\mathbf{x}_B, \mathbf{x}_A, \omega) - \bar{\mathcal{G}}^*(\mathbf{x}_B, \mathbf{x}_A, \omega). \quad (41)$$

For the lossless situation we may omit the bars, in which case Eq. (40) is the classical homogeneous Green's function representation,^{1,5} with $\mathcal{G}_h(\mathbf{x}_B, \mathbf{x}_A, \omega) = 2i\Im\{\mathcal{G}(\mathbf{x}_B, \mathbf{x}_A, \omega)\}$.

C. Applications of the closed-boundary representation

We briefly discuss a number of applications of the closed-boundary homogeneous Green's function representation [Eq. (34)].

1. Holographic imaging (closed-boundary approach)

We apply source-receiver reciprocity [Eq. (28)] to two of the three Green's functions in Eq. (34), and replace $\mathbf{x}_A$ by the variable $\mathbf{x}'$. This gives

$$G_h(\mathbf{x}', \mathbf{x}_B, \omega) = \frac{1}{i\omega} \oint_{\mathbb{S}} \mathcal{J}(\bar{G}^*(\mathbf{x}', \mathbf{x}, \omega), G(\mathbf{x}, \mathbf{x}_B, \omega)) d\mathbf{x}. \quad (42)$$

The interpretation is as follows, see also Fig. 2(a). The coordinate vector $\mathbf{x}_B$ denotes the position of a source inside $\mathbb{V}$. This source may be either a real source, or it may represent a secondary source caused by a scatterer at $\mathbf{x}_B$. $G(\mathbf{x}, \mathbf{x}_B, \omega)$ represents the response to this source, observed by receivers at $\mathbf{x}$ on the boundary $\mathbb{S}$. The complex-conjugate Green's function $\bar{G}^*(\mathbf{x}', \mathbf{x}, \omega)$ back-propagates this response from the boundary $\mathbb{S}$ to any image point $\mathbf{x}'$ in $\mathbb{V}$. The integral in Eq. (42) is taken along all receivers at $\mathbf{x}$ on $\mathbb{S}$. The homogeneous Green's function $G_h(\mathbf{x}', \mathbf{x}_B, \omega)$ at the left-hand side quantifies the properties of the image. Its (finite) value for $\mathbf{x}' = \mathbf{x}_B$ represents the image amplitude at the position of the source. The behaviour of $G_h(\mathbf{x}', \mathbf{x}_B, \omega)$ in some region around $\mathbf{x}_B$ [indicated by the dashed circle in Fig. 2(a)] quantifies the spatial resolution function. For a lossless medium [omitting the bars in Eqs. (42) and (35)], this summarises the essence of holographic imaging methods in optics,¹ acoustics,⁵ and seismology.³ For a medium with losses, the bar in $\bar{G}^*(\mathbf{x}', \mathbf{x}, \omega)$ denotes that the back propagation is carried out in the adjoint medium.^{26,27} Because of the exponential growth of this Green's function with distance, care must be taken when the response at $\mathbb{S}$ is contaminated with noise.

2. Time-reversed wave propagation (closed-boundary approach)

Using $\mathcal{J}(f, g) = -\mathcal{J}(g, f)$ [see Eqs. (10) and (11)] and source-receiver reciprocity [Eq. (28)], replacing $\mathbf{x}_B$ by the variable $\mathbf{x}'$, and assuming the medium is lossless, we obtain from Eq. (34)

$$-i\omega G_h(\mathbf{x}', \mathbf{x}_A, \omega) = \oint_{\mathbb{S}} \mathcal{J}(G(\mathbf{x}', \mathbf{x}, \omega), G^*(\mathbf{x}, \mathbf{x}_A, \omega)) d\mathbf{x}, \quad (43)$$

or, in the time domain,

$$\frac{\partial G_h(\mathbf{x}', \mathbf{x}_A, t)}{\partial t} = \oint_{\mathbb{S}} \mathcal{J}_t(G(\mathbf{x}', \mathbf{x}, t), G(\mathbf{x}, \mathbf{x}_A, -t)) d\mathbf{x}. \quad (44)$$

Here the time-domain homogeneous Green's function is defined as

$$G_h(\mathbf{x}', \mathbf{x}_A, t) = G(\mathbf{x}', \mathbf{x}_A, t) + G(\mathbf{x}', \mathbf{x}_A, -t) \quad (45)$$

and $\mathcal{J}_t(f, g)$ denotes the time-domain equivalent of $\mathcal{J}(f, g)$, meaning that products of functions in Eqs. (10) and (11) are replaced by convolutions. The interpretation of Eq. (44) is as follows, see also Fig. 2(b). $G(\mathbf{x}, \mathbf{x}_A, t)$ represents the impulse response to a source at $\mathbf{x}_A$, observed by receivers at $\mathbf{x}$ on the boundary $\mathbb{S}$. In a time-reversal experiment, the time-reversed response $G(\mathbf{x}, \mathbf{x}_A, -t)$ is fed to sources at $\mathbf{x}$ on the boundary $\mathbb{S}$, which physically emit a wave field into the medium. The propagation of this wave field through the medium to any location $\mathbf{x}'$ is described by $G(\mathbf{x}', \mathbf{x}, t)$. The integral in Eq. (44) is taken along all sources at $\mathbf{x}$ on $\mathbb{S}$. The left-hand side of Eq. (44), with the homogeneous Green's function defined by Eq. (45), quantifies the fact that, for $t < 0$, a back propagating field $\partial G(\mathbf{x}', \mathbf{x}_A, -t)/\partial t$ converges to the focal point $\mathbf{x}_A$ and, for $t > 0$, a forward propagating field $\partial G(\mathbf{x}', \mathbf{x}_A, t)/\partial t$ propagates from a virtual source at $\mathbf{x}_A$ to any observation point $\mathbf{x}'$. This summarises the mathematical justification^{28,29} of the principle of time-reversed wave propagation.^{7,30–32}

3. Green's function retrieval (closed-boundary approach)

Using $\mathcal{J}(f, g) = -\mathcal{J}(g, f)$ and source-receiver reciprocity, and assuming the medium is lossless, we obtain from Eq. (34)

$$\frac{\partial G_h(\mathbf{x}_B, \mathbf{x}_A, t)}{\partial t} = \oint_{\mathbb{S}} \mathcal{J}_t(G(\mathbf{x}_B, \mathbf{x}, t), G(\mathbf{x}_A, \mathbf{x}, -t)) d\mathbf{x}. \quad (46)$$

The interpretation is as follows, see also Fig. 2(c). $G(\mathbf{x}_A, \mathbf{x}, t)$ and $G(\mathbf{x}_B, \mathbf{x}, t)$ represent the response to a source at $\mathbf{x}$ on $\mathbb{S}$, observed by two receivers at $\mathbf{x}_A$ and $\mathbf{x}_B$, respectively. According to Eqs. (10) and (11), the integrand describes a specific combination of convolutions of $G(\mathbf{x}_A, \mathbf{x}, -t)$ and $G(\mathbf{x}_B, \mathbf{x}, t)$, which is equivalent to cross correlations of $G(\mathbf{x}_A, \mathbf{x}, t)$ and $G(\mathbf{x}_B, \mathbf{x}, t)$. The integration in Eq. (46) takes place along the sources at $\mathbf{x}$ on $\mathbb{S}$. According to the left-hand side, this results in the retrieval of the (time-derivative of) the Green's function and its time-reversal between the receivers at $\mathbf{x}_A$ and $\mathbf{x}_B$. In other words, the receiver at $\mathbf{x}_A$ is turned into a virtual source, of which the response is observed by a receiver at $\mathbf{x}_B$. This summarises the mathematical justification^{11,33,34} of the principle of Green's function retrieval by cross correlation in open systems.^{10,12,35–37}

V. SINGLE-SIDED GREEN'S FUNCTION REPRESENTATION

A. Modified reciprocity theorems

The applications discussed in Sec. IV C all rely on the assumption that the medium (or potential) can be accessed

FIG. 2. Applications of the closed-boundary homogeneous Green's function representation [Eq. (34)]. (a) Holographic imaging. (b) Time-reversed wave propagation. (c) Green's function retrieval. For simplicity the Green's functions in these figures are represented by simple straight rays, however, they fully account for propagation and (primary and multiple) scattering in an arbitrary inhomogeneous medium (or potential).

from a closed boundary $\mathbb{S}$. In many practical situations the medium can be accessed from one side only. To account for this, we modify the reciprocity theorems of Eqs. (15) and (20). We replace the closed boundary configuration of Fig. 1 by that of Fig. 3, where $\mathbb{S}$ consists of $\mathbb{S}_0$, $\mathbb{S}_A$, and $\mathbb{S}_{\text{cyl}}$. Here $\mathbb{S}_0$ is the accessible boundary, i.e., the boundary at which measurements can be carried out. This boundary may be horizontal (defined as $x_3 = x_{3,0}$), or curved. $\mathbb{S}_A$ is a horizontal boundary below $\mathbb{S}_0$, containing $\mathbf{x}_A$. Hence, it is defined as $x_3 = x_{3,A}$. Finally, $\mathbb{S}_{\text{cyl}}$ is, for the 3D situation, a cylindrical boundary with a vertical axis through $\mathbf{x}_A$ and infinite radius

FIG. 3. Modified domain $\mathbb{V}_A$, enclosed by boundary $\mathbb{S}_0 \cup \mathbb{S}_A \cup \mathbb{S}_{\text{cyl}}$.

($r \rightarrow \infty$). This cylindrical boundary exists between $\mathbb{S}_0$ and $\mathbb{S}_A$ and closes the boundary $\mathbb{S}$. For the 2D situation, $\mathbb{S}_{\text{cyl}}$ consists of two vertical lines between $\mathbb{S}_0$ and $\mathbb{S}_A$, one at $x_1 \rightarrow -\infty$ and one at $x_1 \rightarrow +\infty$. The domain enclosed by $\mathbb{S}$ is named $\mathbb{V}_A$ (the subscript A denoting that this domain depends on the depth of $\mathbf{x}_A$). Outside a sphere (or, in 2D, a circle) with finite radius the medium is again homogeneous and lossless in both states.

The contributions of the boundary integrals over $\mathbb{S}_{\text{cyl}}$ in Eqs. (15) and (20) vanish, but [specifically for Eq. (20)] for another reason than Sommerfeld's radiation condition. The reasoning is as follows.³⁸ The integrands contain products of functions which each decay with $1/r$ (in 3D), or $1/\sqrt{r}$ (in 2D), for $r \rightarrow \infty$. Hence, the integrands decay with $1/r^2$ (in 3D), or $1/r$ (in 2D), for $r \rightarrow \infty$. The surface area of $\mathbb{S}_{\text{cyl}}$ is proportional to r (in 3D) or 1 (in 2D), hence, the integrals decay with $1/r$ (in 3D and in 2D), and thus vanish for $r \rightarrow \infty$. This implies that we can restrict the integration in the right-hand sides of Eqs. (15) and (20) to the boundaries $\mathbb{S}_0$ and $\mathbb{S}_A$.

For the interaction quantity at the horizontal boundary $\mathbb{S}_A$ (at which $n_3 = +1$), we take

$$\mathcal{J}(f, g) = b[f(\partial_3 g) - (\partial_3 f)g]. \quad (47)$$

This strictly holds for the wave phenomena represented by the first five rows in Table I [see Eq. (10)], and it holds under the assumption of slowly varying medium parameters for the flexural wave equation, represented by the sixth row in Table I [see Eqs. (A18) and (A19) in Appendix A, where b in the sixth row in Table I is defined]. For the boundary integrals along $\mathbb{S}_A$ we derive in Appendix B

$$\int_{\mathbb{S}_A} \mathcal{J}(u_A, u_B) d\mathbf{x} = -i\omega \int_{\mathbb{S}_A} (u_A^+ u_B^- - u_A^- u_B^+) d\mathbf{x}, \quad (48)$$

$$\int_{\mathbb{S}_A} \mathcal{J}(\bar{u}_A^*, u_B) d\mathbf{x} = i\omega \int_{\mathbb{S}_A} ((\bar{u}_A^+)^* u_B^+ - (\bar{u}_A^-)^* u_B^-) d\mathbf{x}. \quad (49)$$

Here u^+ and u^- represent the flux-normalised downgoing (+) and upgoing (−) constituents of the wave field u at $\mathbb{S}_A$. According to Eq. (B24), they are related via

$$u = \mathcal{L}_1\{u^+ + u^-\}, \quad (50)$$

with composition operator $\mathcal{L}_1$ defined in Eq. (B19). Similarly, the fields in the adjoint medium are at $\mathbb{S}_A$ related via

$$\bar{u} = \bar{\mathcal{L}}_1\{\bar{u}^+ + \bar{u}^-\}. \quad (51)$$

Using Eqs. (48) and (49) in Eqs. (15) and (20), respectively, yields for the configuration of Fig. 3 the following two modified reciprocity theorems

$$\begin{aligned} i\omega \int_{\mathbb{V}_A} [u_A s_B - s_A u_B] d\mathbf{x} \\ = \int_{\mathbb{S}_0} \mathcal{J}(u_A, u_B) d\mathbf{x} - i\omega \int_{\mathbb{S}_A} (u_A^+ u_B^- - u_A^- u_B^+) d\mathbf{x} \end{aligned} \quad (52)$$

and

$$\begin{aligned} i\omega \int_{\mathbb{V}_A} [\bar{u}_A^* s_B + s_A^* u_B] d\mathbf{x} \\ = \int_{\mathbb{S}_0} \mathcal{J}(\bar{u}_A^*, u_B) d\mathbf{x} + i\omega \int_{\mathbb{S}_A} ((\bar{u}_A^+)^* u_B^+ - (\bar{u}_A^-)^* u_B^-) d\mathbf{x}. \end{aligned} \quad (53)$$

B. The single-sided homogeneous Green's function representation

We use Eqs. (52) and (53) to derive a single-sided representation for the homogeneous Green's function.

For state A we introduce a focusing function $f_1(\mathbf{x}, \mathbf{x}_A, \omega)$ in a truncated version of the actual medium, i.e., in a medium which is identical to the actual medium in $\mathbb{V}_A$, but homogeneous and lossless above $\mathbb{S}_0$ and below $\mathbb{S}_A$ (Fig. 4). In $\mathbb{V}_A$ it obeys the source-free wave equation

$$\mathcal{W}f_1(\mathbf{x}, \mathbf{x}_A, \omega) = 0. \quad (54)$$

FIG. 4. Illustration of the focusing function $f_1(\mathbf{x}, \mathbf{x}_A, \omega)$, defined in a truncated version of the actual medium.

Analogous to Eq. (50), for $\mathbf{x}$ on $\mathbb{S}_A$ we express the focusing function as a superposition of flux-normalised downgoing and upgoing constituents, according to

$$f_1(\mathbf{x}, \mathbf{x}_A, \omega) = \mathcal{L}_1(\mathbf{x})\{f_1^+(\mathbf{x}, \mathbf{x}_A, \omega) + f_1^-(\mathbf{x}, \mathbf{x}_A, \omega)\}. \quad (55)$$

The focusing function is incident to the inhomogeneous medium from the homogeneous lossless half-space above $\mathbb{S}_0$, propagates and scatters in the truncated actual medium in $\mathbb{V}_A$, focuses at $\mathbf{x}_A$ on $\mathbb{S}_A$, and continues as a downgoing wave field in the homogeneous lossless half-space below $\mathbb{S}_A$. The focusing conditions read^{39–41}

$$[f_1^+(\mathbf{x}, \mathbf{x}_A, \omega)]_{x_3=x_{3,A}} = \delta(\mathbf{x}_H - \mathbf{x}_{H,A}) \quad (56)$$

and

$$[f_1^-(\mathbf{x}, \mathbf{x}_A, \omega)]_{x_3=x_{3,A}} = 0. \quad (57)$$

Here $\mathbf{x}_H$ denotes the horizontal components of the coordinate vector $\mathbf{x}$, hence, $\mathbf{x}_H = (x_1, x_2)$ in the 3D case, and $\mathbf{x}_H = x_1$ in the 2D case. Similarly, $\mathbf{x}_{H,A}$ denotes the horizontal components of the coordinate vector $\mathbf{x}_A$. In practice $f_1(\mathbf{x}, \mathbf{x}_A, \omega)$ must be filtered to avoid unstable behaviour for the evanescent wave components. This implies that the delta function in the focusing condition (Eq. 56) is spatially band-limited.

For state B we choose again $G(\mathbf{x}, \mathbf{x}_B, \omega)$, obeying Eq. (23) in the actual medium throughout space. Because $\mathbb{S}_A$ (i.e., the lower boundary of $\mathbb{V}_A$) is determined by the depth of $\mathbf{x}_A$, it follows that $\mathbf{x}_B$ may lie inside or outside $\mathbb{V}_A$, depending on its position relative to $\mathbf{x}_A$. To account for this, we define the characteristic function χ_A as

$$\chi_A(\mathbf{x}_B) = \begin{cases} 1, & \text{for } \mathbf{x}_B \text{ inside } \mathbb{V}_A, \\ \frac{1}{2}, & \text{for } \mathbf{x}_B \text{ on } \mathbb{S}, \\ 0, & \text{for } \mathbf{x}_B \text{ outside } \mathbb{V}_A. \end{cases} \quad (58)$$

Analogous to Eq. (50), for $\mathbf{x}$ on $\mathbb{S}_A$ we express the Green's function $G(\mathbf{x}, \mathbf{x}_B, \omega)$ as a superposition of flux-normalised downgoing and upgoing constituents, according to

$$G(\mathbf{x}, \mathbf{x}_B, \omega) = \mathcal{L}_1(\mathbf{x})\{G^+(\mathbf{x}, \mathbf{x}_B, \omega) + G^-(\mathbf{x}, \mathbf{x}_B, \omega)\}. \quad (59)$$

We make the following substitutions in the modified reciprocity theorem of the convolution type [Eq. (52)]

$$s_A = 0, \quad (60)$$

$$u_A = f_1(\mathbf{x}, \mathbf{x}_A, \omega), \quad (61)$$

$$u_A^\pm = f_1^\pm(\mathbf{x}, \mathbf{x}_A, \omega), \quad (62)$$

$$s_B = \delta(\mathbf{x} - \mathbf{x}_B), \quad (63)$$

$$u_B = G(\mathbf{x}, \mathbf{x}_B, \omega), \quad (64)$$

$$u_B^\pm = G^\pm(\mathbf{x}, \mathbf{x}_B, \omega). \quad (65)$$

Using focusing conditions (56) and (57), this gives

$$\begin{aligned} & \chi_A(\mathbf{x}_B) i\omega f_1(\mathbf{x}_B, \mathbf{x}_A, \omega) + i\omega G^-(\mathbf{x}_A, \mathbf{x}_B, \omega) \\ &= \int_{\mathbb{S}_0} \mathcal{J}(f_1(\mathbf{x}, \mathbf{x}_A, \omega), G(\mathbf{x}, \mathbf{x}_B, \omega)) d\mathbf{x}. \end{aligned} \quad (66)$$

Next, for state A we define a focusing function $\bar{f}_1(\mathbf{x}, \mathbf{x}_A, \omega)$ in the adjoint of the truncated medium.⁴² In $\mathbb{V}_A$ it obeys the source-free wave equation

$$\mathcal{W}\bar{f}_1^*(\mathbf{x}, \mathbf{x}_A, \omega) = 0. \quad (67)$$

For $\mathbf{x}$ on $\mathbb{S}_A$, $\bar{f}_1(\mathbf{x}, \mathbf{x}_A, \omega)$ consists of downgoing and upgoing constituents, according to

$$\bar{f}_1(\mathbf{x}, \mathbf{x}_A, \omega) = \bar{\mathcal{L}}_1(\mathbf{x})\{\bar{f}_1^+(\mathbf{x}, \mathbf{x}_A, \omega) + \bar{f}_1^-(\mathbf{x}, \mathbf{x}_A, \omega)\}, \quad (68)$$

with $\bar{\mathcal{L}}_1 = \mathcal{L}_1^*$. The focusing conditions for $\bar{f}_1(\mathbf{x}, \mathbf{x}_A, \omega)$ are the same as those for $f_1(\mathbf{x}, \mathbf{x}_A, \omega)$, described by Eqs. (56) and (57). We substitute

$$s_A = 0, \quad (69)$$

$$\bar{u}_A = \bar{f}_1(\mathbf{x}, \mathbf{x}_A, \omega), \quad (70)$$

$$\bar{u}_A^\pm = \bar{f}_1^\pm(\mathbf{x}, \mathbf{x}_A, \omega), \quad (71)$$

for state A, and Eqs. (63)–(65) for state B, into the modified reciprocity theorem of the correlation type [Eq. (53)]. We thus obtain

$$\begin{aligned} & \chi_A(\mathbf{x}_B) i\omega \bar{f}_1^*(\mathbf{x}_B, \mathbf{x}_A, \omega) - i\omega G^+(\mathbf{x}_A, \mathbf{x}_B, \omega) \\ &= \int_{\mathbb{S}_0} \mathcal{J}(\bar{f}_1^*(\mathbf{x}, \mathbf{x}_A, \omega), G(\mathbf{x}, \mathbf{x}_B, \omega)) d\mathbf{x}. \end{aligned} \quad (72)$$

We obtain two more relations by replacing the medium parameters in both states in Eqs. (66) and (72) by their adjoints, followed by complex conjugating both sides of the resulting equations. We thus obtain

$$\begin{aligned} & -\chi_A(\mathbf{x}_B) i\omega \bar{f}_1^*(\mathbf{x}_B, \mathbf{x}_A, \omega) - i\omega \{\bar{G}^-(\mathbf{x}_A, \mathbf{x}_B, \omega)\}^* \\ &= \int_{\mathbb{S}_0} \mathcal{J}(\bar{f}_1^*(\mathbf{x}, \mathbf{x}_A, \omega), \bar{G}^*(\mathbf{x}, \mathbf{x}_B, \omega)) d\mathbf{x} \end{aligned} \quad (73)$$

and

$$\begin{aligned} & -\chi_A(\mathbf{x}_B) i\omega f_1(\mathbf{x}_B, \mathbf{x}_A, \omega) + i\omega \{\bar{G}^+(\mathbf{x}_A, \mathbf{x}_B, \omega)\}^* \\ &= \int_{\mathbb{S}_0} \mathcal{J}(f_1(\mathbf{x}, \mathbf{x}_A, \omega), \bar{G}^*(\mathbf{x}, \mathbf{x}_B, \omega)) d\mathbf{x}. \end{aligned} \quad (74)$$

Applying $\mathcal{L}_1(\mathbf{x}_A)$ to both sides of Eqs. (66) and (72) and combining the results, using Eqs. (28) and (59), gives

$$\begin{aligned} & \chi_A(\mathbf{x}_B) i\omega F(\mathbf{x}_B, \mathbf{x}_A, \omega) + i\omega G(\mathbf{x}_B, \mathbf{x}_A, \omega) \\ &= \int_{\mathbb{S}_0} \mathcal{J}(F(\mathbf{x}, \mathbf{x}_A, \omega), G(\mathbf{x}, \mathbf{x}_B, \omega)) d\mathbf{x}, \end{aligned} \quad (75)$$

with

$$F(\mathbf{x}, \mathbf{x}_A, \omega) = \mathcal{L}_1(\mathbf{x}_A)\{f_1(\mathbf{x}, \mathbf{x}_A, \omega) - \bar{f}_1^*(\mathbf{x}, \mathbf{x}_A, \omega)\}. \quad (76)$$

Note that on the right-hand side of Eq. (75) we interchanged the order of the application of operator $\mathcal{L}_1(\mathbf{x}_A)$ and the integration, which is allowed because the operator acts on the coordinate $\mathbf{x}_A$ at $\mathbb{S}_A$, whereas the integration takes place along the coordinate $\mathbf{x}$ at $\mathbb{S}_0$. Similarly, applying $\mathcal{L}_1(\mathbf{x}_A)$ to both sides of Eqs. (73) and (74) and combining the results, using $\bar{\mathcal{L}}_1^* = \mathcal{L}_1$ and Eqs. (28), (59), and (76), gives

$$\begin{aligned} & -\chi_A(\mathbf{x}_B) i\omega F(\mathbf{x}_B, \mathbf{x}_A, \omega) + i\omega \bar{G}^*(\mathbf{x}_B, \mathbf{x}_A, \omega) \\ &= \int_{\mathbb{S}_0} \mathcal{J}(F(\mathbf{x}, \mathbf{x}_A, \omega), \bar{G}^*(\mathbf{x}, \mathbf{x}_B, \omega)) d\mathbf{x}. \end{aligned} \quad (77)$$

By combining Eqs. (75) and (77), the focusing functions $F(\mathbf{x}_B, \mathbf{x}_A, \omega)$ on the left-hand sides cancel, hence

$$G_h(\mathbf{x}_B, \mathbf{x}_A, \omega) = \frac{1}{i\omega} \int_{\mathbb{S}_0} \mathcal{J}(F(\mathbf{x}, \mathbf{x}_A, \omega), G_h(\mathbf{x}, \mathbf{x}_B, \omega)) d\mathbf{x}, \quad (78)$$

where $G_h(\mathbf{x}_B, \mathbf{x}_A, \omega)$ is the homogeneous Green's function, defined in Eq. (35). Equation (78) is the main result of this paper. It is a representation of the unified homogeneous Green's function $G_h(\mathbf{x}_B, \mathbf{x}_A, \omega)$ between any two points $\mathbf{x}_A$ and $\mathbf{x}_B$ in an inhomogeneous medium (or potential), expressed in terms of an integral over a single accessible boundary $\mathbb{S}_0$. In contrast, the closed-boundary representation for the same unified homogeneous Green's function [Eq. (34)] is expressed in terms of an integral over a boundary $\mathbb{S}$ which encloses the two points $\mathbf{x}_A$ and $\mathbf{x}_B$.

C. Applications of the single-sided representation

We discuss the same applications as in Sec. IV C, but this time using as starting point the single-sided homogeneous Green's function representation [Eq. (78)]. Since each of these applications makes use of the focusing function $F(\mathbf{x}, \mathbf{x}_A, \omega)$, or, in the time domain, $F(\mathbf{x}, \mathbf{x}_A, t)$, we first briefly indicate how to obtain this function in practice. For this, we distinguish between model-driven and data-driven approaches. When the medium between $\mathbb{S}_0$ and $\mathbb{S}_A$ is

accurately known (including all scatterers), the transmission response between these boundaries can be numerically modeled (including multiple scattering) and subsequently inverted.⁴¹ This forms the basis for obtaining $F(\mathbf{x}, \mathbf{x}_A, \omega)$ in a model-driven way. Alternatively, to avoid inversion of the transmission response, the focusing function can be modeled directly, following a recursive Kirchhoff-Helmholtz wavefield extrapolation approach,^{43,44} starting with the focused field at $\mathbb{S}_A$ and recursively moving upward. These model-driven approaches hold for media with or without losses. When only a smooth background medium is known, the focusing function (including multiple scattering) can be retrieved from reflection measurements at the boundary $\mathbb{S}_0$, using a 2D or 3D version of the single-sided Marchenko method.³⁹ This data-driven approach holds for media without losses. It can be extended to media with losses,⁴² but this requires measurements at $\mathbb{S}_0$ and $\mathbb{S}_A$.

1. Holographic imaging (single-sided approach)

We apply source-receiver reciprocity to the Green's function at the left-hand side of Eq. (78), and replace $\mathbf{x}_A$ by the variable $\mathbf{x}'$. This gives

$$G_h(\mathbf{x}', \mathbf{x}_B, \omega) = \frac{1}{i\omega} \int_{\mathbb{S}_0} \mathcal{J}(F(\mathbf{x}, \mathbf{x}', \omega), G_h(\mathbf{x}, \mathbf{x}_B, \omega)) d\mathbf{x}, \quad (79)$$

see Fig. 5(a). The main difference with the holographic imaging method, described by Eq. (42) (Sec. IVC 1), is that the closed integration boundary $\mathbb{S}$ has been replaced by the single (open) boundary $\mathbb{S}_0$ and that the back-propagating Green's function $\bar{G}^*(\mathbf{x}', \mathbf{x}, \omega)$ has been replaced by the focusing function $F(\mathbf{x}, \mathbf{x}', \omega)$. Moreover, the response to which the focusing function is applied is the homogeneous Green's function $G_h(\mathbf{x}, \mathbf{x}_B, \omega)$, instead of $G(\mathbf{x}, \mathbf{x}_B, \omega)$ in Eq. (42). The integral in Eq. (79) is taken along all receivers at $\mathbf{x}$ on $\mathbb{S}_0$. The homogeneous Green's function on the left-hand side is the same as that in Eq. (42), hence, it quantifies the spatial resolution function in some region around $\mathbf{x}_B$ [indicated by the dashed circle in Fig. 5(a)].

2. "Time-reversed" wave propagation (single-sided approach)

In the time-reversal approach discussed in Sec. IVC 2, a time-reversed field is physically emitted into the medium. For the single-sided version we cannot make use of Eq. (78), because the homogeneous Green's function $G_h(\mathbf{x}, \mathbf{x}_B, \omega)$ in the integrand is not physical. Therefore, we return to Eq. (75), in which the integrand contains the physical (i.e., causal) Green's function $G(\mathbf{x}, \mathbf{x}_B, \omega)$. Using $\mathcal{J}(f, g) = -\mathcal{J}(g, f)$ and source-receiver reciprocity, replacing $\mathbf{x}_B$ by the variable $\mathbf{x}'$, and assuming the medium is lossless, we obtain from Eq. (75)

$$\begin{aligned} & \frac{\partial G(\mathbf{x}', \mathbf{x}_A, t)}{\partial t} + \chi_A(\mathbf{x}') \frac{\partial F(\mathbf{x}', \mathbf{x}_A, t)}{\partial t} \\ &= \int_{\mathbb{S}_0} \mathcal{J}_t(G(\mathbf{x}', \mathbf{x}, t), F(\mathbf{x}, \mathbf{x}_A, t)) d\mathbf{x}, \end{aligned} \quad (80)$$

FIG. 5. Applications of the single-sided homogeneous Green's function representation [Eq. (78)]. (a) Holographic imaging. (b) "Time-reversed" wave propagation. (c) Green's function retrieval. For simplicity the focusing functions and Green's functions in these figures are represented by simple straight rays, however, they fully account for propagation and (primary and multiple) scattering in an arbitrary inhomogeneous medium (or potential).

see Fig. 5(b). In comparison with the time-reversal method, described by Eq. (44), the focusing function $F(\mathbf{x}, \mathbf{x}_A, t)$ instead of $G(\mathbf{x}, \mathbf{x}_A, -t)$ is fed to the sources at $\mathbf{x}$ on $\mathbb{S}_0$ (instead of $\mathbb{S}$) and physically emitted into the medium. The integral in Eq. (80) is taken along all sources at $\mathbf{x}$ on $\mathbb{S}_0$. The left-hand side shows that, for $\mathbf{x}'$ below $\mathbf{x}_A$ [where $\chi_A(\mathbf{x}') = 0$], the field $\partial G(\mathbf{x}', \mathbf{x}_A, t)/\partial t$ propagates from a virtual source at $\mathbf{x}_A$ to any observation point $\mathbf{x}'$. For $\mathbf{x}'$ above $\mathbf{x}_A$ the virtual-source field is contaminated by the focusing function $\partial F(\mathbf{x}', \mathbf{x}_A, t)/\partial t$. Note, however, that only the direct arrival of the Green's function overlaps with the focusing function.⁴¹ Beyond the direct arrival time the focusing function is zero and hence does not contaminate the virtual-source field $\partial G(\mathbf{x}', \mathbf{x}_A, t)/\partial t$.

3. Green's function retrieval (single-sided approach)

Using $\mathcal{J}(f, g) = -\mathcal{J}(g, f)$ and source-receiver reciprocity, and assuming the medium is lossless, we obtain from Eq. (78)

$$\frac{\partial G_h(\mathbf{x}_B, \mathbf{x}_A, t)}{\partial t} = \int_{\mathbb{S}_0} \mathcal{J}_t(G_h(\mathbf{x}_B, \mathbf{x}, t), F(\mathbf{x}, \mathbf{x}_A, t)) d\mathbf{x}, \quad (81)$$

see Fig. 5(c). Instead of cross correlating the Green's functions $G(\mathbf{x}_A, \mathbf{x}, t)$ and $G(\mathbf{x}_B, \mathbf{x}, t)$, as in Eq. (46) (Sec. IV C 3), here the homogeneous Green's function $G_h(\mathbf{x}_B, \mathbf{x}, t)$, observed by a receiver at $\mathbf{x}_B$, is convolved with the focusing function $F(\mathbf{x}, \mathbf{x}_A, t)$, focused at a receiver at $\mathbf{x}_A$. The integration takes place along the sources at $\mathbf{x}$ on $\mathbb{S}_0$ (instead of $\mathbb{S}$). The left-hand side is the same as in Eq. (46), i.e., the response to a virtual source at $\mathbf{x}_A$, observed by a receiver at $\mathbf{x}_B$, and its time reversal. Note that, since the focusing function $F(\mathbf{x}, \mathbf{x}_A, t)$ is related to the inverse of the transmission response between $\mathbb{S}_0$ and $\mathbb{S}_A$, Green's function retrieval using Eq. (81) is akin to a method called "Green's function retrieval by multidimensional deconvolution,"^{45,46} in which the Green's function $G(\mathbf{x}_A, \mathbf{x}, t)$ is inverted rather than reversed in time.

VI. CONCLUSIONS

We have derived a representation for the homogeneous Green's function of a unified scalar wave equation. Unlike the classical representation, which involves an integral along a closed boundary, this representation is expressed as an integral over a single boundary only. It accounts for multiple scattering and holds in media with losses. This representation is particularly useful when the medium of interest is accessible from one side only. Applications are found in holographic imaging methods, time-reversed wave propagation and Green's function retrieval.

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APPENDIX A: FLEXURAL WAVES

Consider a 2D inhomogeneous isotropic thin plate in the (x_1, x_3) -plane. The equation of motion reads^{47,48}

$$\partial_i Q_i - \rho \frac{\partial^2 u_2}{\partial t^2} = -f_2, \quad (A1)$$

where

$$Q_i = \partial_j M_{ij}, \quad (A2)$$

with $u_2(\mathbf{x}, t)$ the transverse particle displacement, $f_2(\mathbf{x}, t)$ the area density of transverse external force, $Q_i(\mathbf{x}, t)$ the shear stress, $M_{ij}(\mathbf{x}, t)$ the moment and $\rho(\mathbf{x})$ the area density of mass. The subscripts i and j take on the values 1 and 3 only. Einstein's summation convention applies to repeated subscripts. For an isotropic plate, the moments are defined as^{47,48}

$$M_{11} = -[d\partial_1\partial_1 + \nu d\partial_3\partial_3]u_2, \quad (A3)$$

$$M_{33} = -[\nu d\partial_1\partial_1 + d\partial_3\partial_3]u_2, \quad (A4)$$

$$M_{13} = M_{31} = -(1 - \nu)d\partial_1\partial_3u_2, \quad (A5)$$

with $d(\mathbf{x})$ the bending stiffness and $\nu(\mathbf{x})$ the Poisson ratio. These equations can be captured by the single equation

$$M_{ij} = -[(1 - \nu)d\partial_i\partial_j + \delta_{ij}\nu d\partial_k\partial_k]u_2, \quad (A6)$$

where δ_{ij} is the Kronecker delta function. Substitution of Eqs. (A2) and (A6) into Eq. (A1) gives the flexural wave equation for the transverse particle velocity $v_2(\mathbf{x}, t) = \partial u_2(\mathbf{x}, t)/\partial t$, hence,

$$-[\partial_i\partial_j d_1\partial_i\partial_j + \partial_i\partial_i d_2\partial_j\partial_j]v_2 - \rho \frac{\partial^2 v_2}{\partial t^2} = -\frac{\partial f_2}{\partial t}, \quad (A7)$$

with

$$d_1 = (1 - \nu)d, \quad (A8)$$

$$d_2 = \nu d. \quad (A9)$$

Equation (A7), transformed to the frequency domain, reads

$$-[\partial_i\partial_j d_1\partial_i\partial_j + \partial_i\partial_i d_2\partial_j\partial_j]v_2 + \rho\omega^2 v_2 = i\omega f_2, \quad (A10)$$

with $v_2(\mathbf{x}, \omega)$ and $f_2(\mathbf{x}, \omega)$ being the Fourier transforms of $v_2(\mathbf{x}, t)$ and $f_2(\mathbf{x}, t)$ in Eq. (A7). Equation (A10) is covered by the unified wave equation in the frequency domain [Eqs. (3) and (4)], with the quantities u , s , and a_2 given in the sixth row of Table I and the differential operator $\mathcal{D}_4$ defined in Eq. (6). To account for general loss mechanisms, we assume that $\rho(\mathbf{x}, \omega)$, $d_1(\mathbf{x}, \omega)$ and $d_2(\mathbf{x}, \omega)$ may be complex-valued and frequency-dependent. This exact wave equation underlies the closed-boundary representation of the homogeneous Green's function, Eq. (34), for the situation of flexural waves.

For the derivation of the single-sided representation we assume that the plate is only weakly inhomogeneous, so that the spatial derivatives of the coefficients $\rho(\mathbf{x}, \omega)$, $d_1(\mathbf{x}, \omega)$, and $d_2(\mathbf{x}, \omega)$ are small in comparison with those of the wave field $v_2(\mathbf{x}, \omega)$. With this assumption, Eq. (A10) simplifies to

$$-d\partial_i\partial_i\partial_j\partial_j v_2 + \rho\omega^2 v_2 = i\omega f_2. \quad (A11)$$

We now define operator $\mathcal{D}_4$ as

$$\mathcal{D}_4 = -d\partial_i\partial_i\partial_j\partial_j. \quad (A12)$$

For $\mathcal{J}_4(f, g)$, obeying Eq. (9), we thus obtain

$$\begin{aligned} \mathcal{J}_4(f, g) = & d[(\partial_i\partial_j\partial_i\partial_j)g - f(\partial_i\partial_j\partial_j\partial_i) \\ & + (\partial_i f)(\partial_j\partial_j\partial_i) - (\partial_j\partial_j f)(\partial_i g)]n_i. \end{aligned} \quad (A13)$$

This expression can be further simplified. To this end we first rewrite Eq. (A11) as follows

$$(\partial_i\partial_i - k_F^2)(\partial_j\partial_j + k_F^2)v_2 = -i\omega f_2/d, \quad (A14)$$

with the flexural wave number k_F defined as

$$k_F^2 = \omega \sqrt{\frac{\rho}{d}}. \quad (\text{A15})$$

In any source-free region, Eq. (A14) decouples into the following two equations

$$(\partial_i \partial_i - k_F^2) v_2 = 0, \quad (\text{A16})$$

$$(\partial_j \partial_j + k_F^2) v_2 = 0. \quad (\text{A17})$$

Equation (A16) accounts for damped solutions of Eq. (A14), whereas Eq. (A17) accounts for waves. Assuming that $\mathbb{S}$ [where $\mathcal{J}_4(f, g)$ is defined] is source-free and that f and g both obey wave Eq. (A17), Eq. (A13) simplifies to

$$\mathcal{J}_4(f, g) = 2k_F^2 d [f(\partial_i g) - (\partial_i f)g] n_i. \quad (\text{A18})$$

Note that this expression is the same as that for $\mathcal{J}_2(f, g)$, given in Eq. (10), if we define

$$b = 2k_F^2 d = 2\omega \sqrt{\rho d}. \quad (\text{A19})$$

APPENDIX B: DECOMPOSITION

Our aim is to derive decomposed versions of the boundary integrals in reciprocity theorems (15) and (20) for the part $\mathbb{S}_A$ of the closed boundary $\mathbb{S}$. Hence, we seek decomposed versions of

$$\int_{\mathbb{S}_A} \mathcal{J}(u_A, u_B) d\mathbf{x} \quad \text{and} \quad \int_{\mathbb{S}_A} \mathcal{J}(\bar{u}_A^*, u_B) d\mathbf{x}. \quad (\text{B1})$$

Since $\mathbb{S}_A$ is a horizontal boundary, its normal vector is defined as $\mathbf{n} = (n_1, n_2, n_3) = (0, 0, 1)$ for 3D situations, and $\mathbf{n} = (n_1, n_3) = (0, 1)$ for 2D situations. In the following, we define the interaction quantity at $\mathbb{S}_A$ as

$$\mathcal{J}(f, g) = b[f(\partial_3 g) - (\partial_3 f)g], \quad (\text{B2})$$

which strictly holds for the wave phenomena represented by the first five rows in Table I [see Eq. (10)], and which holds under the assumption of slowly varying medium parameters for the flexural wave equation, represented by the sixth row in Table I [see Eqs. (A18) and (A19)].

According to Eq. (B2), we need expressions for the first order derivative ∂_3 , which we derive from expressions for second order derivatives. For the wave phenomena represented by the first five rows in Table I, we find from Eqs. (3), (4), and (5), assuming the medium is source-free at $\mathbb{S}_A$,

$$\partial_3(b\partial_3 u) = -\mathcal{K}_2 u, \quad (\text{B3})$$

with

$$\mathcal{K}_2 = -\sum_{n=0}^N (-i\omega)^n \alpha_n + \partial_\nu b \partial_\nu, \quad (\text{B4})$$

with $\alpha_n = a_n$. For the 3D situation, Greek subscripts take on the values 1 and 2, and the summation convention holds for repeated subscripts. For the 2D situation, Greek subscripts

take on the value 1 only. Subscript 2 in operator $\mathcal{K}_2$ denotes that this operator accounts for second order differentiation in the x_3 -direction.

For flexural waves, represented by the sixth row in Table I, we assume that the plate is weakly inhomogeneous, so that the spatial derivatives of the coefficients are small in comparison with those of the wave field. Under these assumptions (and the assumption that $\mathbb{S}_A$ is source-free), Eqs. (A15), (A17), and (A19) yield again Eqs. (B3) and (B4), but this time with $\alpha_0 = \alpha_1 = 0$ and $\alpha_2 = 2a_2 = 2\rho$. We define an operator $\mathcal{H}_2$ as

$$\mathcal{H}_2 = b^{-1/2} \mathcal{K}_2 b^{-1/2} = -\sum_{n=0}^N \alpha'_n (-i\omega)^n + \partial_\nu b \partial_\nu, \quad (\text{B5})$$

with^{38,49}

$$\alpha'_0 = \alpha_0/b - \frac{(\partial_\nu b)(\partial_\nu b)}{4b^2} + \frac{\partial_\nu b \partial_\nu b}{2b}, \quad (\text{B6})$$

$$\alpha'_n = \alpha_n/b \quad \text{for } n > 0. \quad (\text{B7})$$

Note that $\partial_\nu b \partial_\nu$ in operator $\mathcal{K}_2$ [Eq. (B4)] has been simplified into $\partial_\nu b \partial_\nu$ in operator $\mathcal{H}_2$ [Eq. (B5)]. Using this definition of $\mathcal{H}_2$, we rewrite Eq. (B3) as

$$\partial_3(b\partial_3 u) = -b^{1/2} \mathcal{H}_2(b^{1/2} u). \quad (\text{B8})$$

We define an operator $\mathcal{H}_1$ as the square root of $\mathcal{H}_2$, according to^{50–52}

$$\mathcal{H}_1 \mathcal{H}_1 = \mathcal{H}_2 \quad \text{or} \quad \mathcal{H}_1 = \mathcal{H}_2^{1/2}. \quad (\text{B9})$$

Note that $\mathcal{H}_1$ is a pseudo-differential operator.^{24,53–56} The square root of an operator is not uniquely defined. We take the square root such that the imaginary part of the eigenvalue spectrum of $\mathcal{H}_1$ has the same sign as that of $\mathcal{H}_2$, i.e., positive for a dissipative medium and negative for an effectual medium (for details see Ref. 24, keeping in mind that the imaginary unit j in that paper has been replaced by $-i$ in the present paper, to be consistent with the use of i in Schrödinger's equation).

We combine Eq. (B8) and the trivial equation $\partial_3 u = \partial_3 u$ in a matrix-vector equation, according to

$$\partial_3 \mathbf{q} = \mathcal{A} \mathbf{q}, \quad (\text{B10})$$

with

$$\mathcal{A} = \begin{pmatrix} 0 & \frac{i\omega}{b} \\ -\frac{1}{i\omega} b^{1/2} \mathcal{H}_2 b^{1/2} & 0 \end{pmatrix}, \quad \mathbf{q} = \begin{pmatrix} b u \\ \frac{b}{i\omega} \partial_3 u \end{pmatrix}. \quad (\text{B11})$$

With this definition of $\mathbf{q}$, the integrals in Eq. (B1) [with $\mathcal{J}$ defined in Eq. (B2)] can be written as

$$\int_{\mathbb{S}_A} \mathcal{J}(u_A, u_B) d\mathbf{x} = i\omega \int_{\mathbb{S}_A} \mathbf{q}_A^T \mathbf{N} \mathbf{q}_B d\mathbf{x}, \quad (\text{B12})$$

$$\int_{\mathbb{S}_A} \mathcal{J}(\bar{u}_A^*, u_B) d\mathbf{x} = i\omega \int_{\mathbb{S}_A} \bar{\mathbf{q}}_A^\dagger \mathbf{K} \mathbf{q}_B d\mathbf{x}, \quad (\text{B13})$$

with

$$\mathbf{N} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \text{and} \quad \mathbf{K} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (\text{B14})$$

In Eq. (B12), $\mathbf{q}_A^t$ denotes the transposed of $\mathbf{q}_A$, whereas $\bar{\mathbf{q}}_A^\dagger$ in Eq. (B13) denotes the adjoint (i.e., the complex conjugate transposed) of $\bar{\mathbf{q}}_A$.

We decompose matrix $\mathcal{A}$ as follows

$$\mathcal{A} = \mathcal{L} \mathcal{H} \mathcal{L}^{-1}, \quad (\text{B15})$$

with

$$\mathcal{L} = \begin{pmatrix} \mathcal{L}_1 & \mathcal{L}_1 \\ \mathcal{L}_2 & -\mathcal{L}_2 \end{pmatrix}, \quad (\text{B16})$$

$$\mathcal{H} = \begin{pmatrix} i\mathcal{H}_1 & 0 \\ 0 & -i\mathcal{H}_1 \end{pmatrix}, \quad (\text{B17})$$

$$\mathcal{L}^{-1} = \frac{1}{2} \begin{pmatrix} \mathcal{L}_1^{-1} & \mathcal{L}_2^{-1} \\ \mathcal{L}_1^{-1} & -\mathcal{L}_2^{-1} \end{pmatrix}. \quad (\text{B18})$$

This decomposition is not unique. We choose

$$\mathcal{L}_1 = (\omega/2)^{1/2} b^{-1/2} \mathcal{H}_1^{-1/2}, \quad (\text{B19})$$

$$\mathcal{L}_2 = (2\omega)^{-1/2} b^{1/2} \mathcal{H}_1^{1/2}, \quad (\text{B20})$$

$$\mathcal{L}_1^{-1} = (\omega/2)^{-1/2} \mathcal{H}_1^{1/2} b^{1/2}, \quad (\text{B21})$$

$$\mathcal{L}_2^{-1} = (2\omega)^{1/2} \mathcal{H}_1^{-1/2} b^{-1/2}. \quad (\text{B22})$$

Here $\mathcal{H}_1^{1/2}$ is the square root of the square root operator $\mathcal{H}_1$ (with the same choices for the sign of the imaginary part of the eigenvalue spectrum).

We introduce a decomposed field vector $\mathbf{p}$ via

$$\mathbf{q} = \mathcal{L} \mathbf{p}, \quad \text{with} \quad \mathbf{p} = \begin{pmatrix} u^+ \\ u^- \end{pmatrix}, \quad (\text{B23})$$

or

$$u = \mathcal{L}_1 \{u^+ + u^-\}, \quad (\text{B24})$$

$$\frac{b}{i\omega} \partial_3 u = \mathcal{L}_2 \{u^+ - u^-\}. \quad (\text{B25})$$

We interpret u^+ and u^- as downgoing (+) and upgoing (−) wave fields.^{24,53–56} With the specific choice for the operators $\mathcal{L}_1$ and $\mathcal{L}_2$, made in Eqs. (B19) and (B20), u^+ and u^- are so-called flux-normalised downgoing and upgoing wave fields. This is explained at the end of this appendix.

Substitution of Eq. (B23) into Eqs. (B12) and (B13) gives

$$\int_{\mathbb{S}_A} \mathcal{J}(u_A, u_B) d\mathbf{x} = i\omega \int_{\mathbb{S}_A} (\mathcal{L} \mathbf{p}_A)^t \mathbf{N} \mathcal{L} \mathbf{p}_B d\mathbf{x}, \quad (\text{B26})$$

$$\int_{\mathbb{S}_A} \mathcal{J}(\bar{u}_A^*, u_B) d\mathbf{x} = i\omega \int_{\mathbb{S}_A} (\bar{\mathcal{L}} \bar{\mathbf{p}}_A)^\dagger \mathbf{K} \mathcal{L} \mathbf{p}_B d\mathbf{x}. \quad (\text{B27})$$

We introduce transposed and adjoint operators via

$$\int_{\mathbb{S}_A} (\mathcal{U} \mathbf{f})^t \mathbf{g} d\mathbf{x} = \int_{\mathbb{S}_A} \mathbf{f}^t (\mathcal{U}' \mathbf{g}) d\mathbf{x}, \quad (\text{B28})$$

$$\int_{\mathbb{S}_A} (\mathcal{U} \mathbf{f})^\dagger \mathbf{g} d\mathbf{x} = \int_{\mathbb{S}_A} \mathbf{f}^\dagger (\mathcal{U}^\dagger \mathbf{g}) d\mathbf{x}. \quad (\text{B29})$$

Here $\mathcal{U}$ is a (pseudo-)differential operator matrix containing the spatial differential operator ∂_ν , whereas $\mathcal{U}'$ and $\mathcal{U}^\dagger$ are the transposed and adjoint (complex conjugate transposed) of $\mathcal{U}$. Furthermore, $\mathbf{f}(\mathbf{x})$ and $\mathbf{g}(\mathbf{x})$ are vector functions with “sufficient decay” at infinity. Using Eqs. (B28) and (B29), we can rewrite Eqs. (B26) and (B27) as follows

$$\int_{\mathbb{S}_A} \mathcal{J}(u_A, u_B) d\mathbf{x} = i\omega \int_{\mathbb{S}_A} \mathbf{p}_A^t \mathcal{L}' \mathbf{N} \mathcal{L} \mathbf{p}_B d\mathbf{x}, \quad (\text{B30})$$

$$\int_{\mathbb{S}_A} \mathcal{J}(\bar{u}_A^*, u_B) d\mathbf{x} = i\omega \int_{\mathbb{S}_A} \bar{\mathbf{p}}_A^\dagger \bar{\mathcal{L}}^\dagger \mathbf{K} \mathcal{L} \mathbf{p}_B d\mathbf{x}. \quad (\text{B31})$$

To simplify this result further, we first consider the transposed and adjoint versions of the scalar operators $\mathcal{H}_1$, $\mathcal{L}_1$, and $\mathcal{L}_2$, which are given by^{24,55}

$$\mathcal{H}_1^t = \bar{\mathcal{H}}_1^\dagger = \mathcal{H}_1, \quad (\text{B32})$$

$$\mathcal{L}_1^t = \bar{\mathcal{L}}_1^\dagger = \frac{1}{2} \mathcal{L}_2^{-1}, \quad (\text{B33})$$

$$\mathcal{L}_2^t = \bar{\mathcal{L}}_2^\dagger = \frac{1}{2} \mathcal{L}_1^{-1}. \quad (\text{B34})$$

Using Eqs. (B14), (B16), (B18), (B32), (B33), and (B34), it follows that

$$\mathcal{L}' \mathbf{N} \mathcal{L} = -\mathbf{N}, \quad (\text{B35})$$

$$\bar{\mathcal{L}}^\dagger \mathbf{K} \mathcal{L} = \mathbf{J}, \quad (\text{B36})$$

with

$$\mathbf{J} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (\text{B37})$$

Using this in Eqs. (B30) and (B31) yields

$$\int_{\mathbb{S}_A} \mathcal{J}(u_A, u_B) d\mathbf{x} = -i\omega \int_{\mathbb{S}_A} \mathbf{p}_A^t \mathbf{N} \mathbf{p}_B d\mathbf{x}, \quad (\text{B38})$$

$$\int_{\mathbb{S}_A} \mathcal{J}(\bar{u}_A^*, u_B) d\mathbf{x} = i\omega \int_{\mathbb{S}_A} \bar{\mathbf{p}}_A^\dagger \mathbf{J} \mathbf{p}_B d\mathbf{x}, \quad (\text{B39})$$

or, using Eqs. (B14), (B23), and (B37),

$$\int_{\mathbb{S}_A} \mathcal{J}(u_A, u_B) d\mathbf{x} = -i\omega \int_{\mathbb{S}_A} (u_A^+ u_B^- - u_A^- u_B^+) d\mathbf{x}, \quad (\text{B40})$$

$$\int_{\mathbb{S}_A} \mathcal{J}(\bar{u}_A^*, u_B) d\mathbf{x} = i\omega \int_{\mathbb{S}_A} ((\bar{u}_A^+)^* u_B^+ - (\bar{u}_A^-)^* u_B^-) d\mathbf{x}. \quad (\text{B41})$$

A special case is obtained when we consider a lossless medium (which implies we may omit the bars) and take states A and B identical (implying we may also omit the subscripts A and B). Equation (B41) yields for this situation

$$\frac{1}{4i\omega} \int_{\mathbb{S}_A} \mathcal{J}(u^*, u) d\mathbf{x} = \frac{1}{4} \int_{\mathbb{S}_A} (|u^+|^2 - |u^-|^2) d\mathbf{x}. \quad (\text{B42})$$

According to Eq. (21), the left-hand side represents the power flux through $\mathbb{S}_A$. Hence, u^+ and u^- on the right-hand side are (power-)flux-normalised downgoing and upgoing wave fields.

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