Splitting methods and invariant imbedding for time-independent wave propagation in focusing media and wave guides

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For time-independent wave propagation in focusing media or wave guides, backscattering and coupling between propagation modes are caused by deterministic or random variations of the refractive index in the distinguished (x) direction of propagation. Various splittings of the wave field into forward and backward traveling components, which lead to coupled equations involving abstract operator coefficients, are presented. Choosing a natural explicit representation for these operators immediately yields a coupled mode form of these equations. The splitting procedure also leads naturally to abstract transmission and reflection operators for slabs of finite thickness $(a \leqslant x \leqslant b)$, and abstract invariant imbedding equations satisfied by these. The coupled mode form of these equations, together with such features as reciprocity (associated with an underlying symplectic structure) are also discussed. The example of a square law medium is used to illustrate some of these concepts.

I. INTRODUCTION

Here we consider only time-independent scalar wave propagation described by the $d \geqslant 2$ dimensional Helmholtz equation. We assume that there is a distinguished direction of propagation chosen as the x direction in a Cartesian coordinate system $(x_1, x_2, x_3, \ldots)$ where $x_1 = x$, $(x_2, x_3, \ldots) = \mathbf{x}_\perp$. The Helmholtz equation is thus written naturally as

$$\psi_{xx} + S\psi = 0 \text{ or } \frac{d}{dx}\begin{pmatrix}\psi \\ \psi_x\end{pmatrix} = \begin{pmatrix}0 & 1 \\ -S & 0\end{pmatrix}\begin{pmatrix}\psi \\ \psi_x\end{pmatrix}, \tag{1.1}$$

where $S = \Delta_\perp + k^2(\mathbf{x})$, and suitable boundary conditions are imposed on ψ if the range of $\mathbf{x}_\perp$ is restricted. Here $\Delta_\perp = \partial^2/\partial \mathbf{x}_\perp{}^2$ is the transverse Laplacian, $k(\mathbf{x}) = kn(\mathbf{x})$, where $n(\mathbf{x})$ is the refractive index, and $k > 0$ is arbitrary. We shall regard $\{S \equiv S(x)\}$ (implicitly including any appropriate boundary conditions) as a generally noncommutative family of unbounded self-adjoint operators on $L^2(\mathbf{x}_\perp)$.

Our treatment of the Helmholtz equation (1.1) is based on a splitting of ψ into right (x increasing) ψ^+, and left (x decreasing) ψ^-, traveling components. This decomposition is achieved in terms of a splitting operator P as

$$\begin{pmatrix}\psi^+ \\ \psi^-\end{pmatrix} = P\begin{pmatrix}\psi \\ \psi_x\end{pmatrix}, \text{ with } P = P(x) = \frac{1}{2}\begin{pmatrix}1 & -iT^{-1/2} \\ 1 & +iT^{-1/2}\end{pmatrix}, \tag{1.2}$$

i.e., $\psi^\pm = \frac{1}{2}(\psi \mp iT^{-1/2}\psi_x)$, so $\psi \equiv \psi^- + \psi^+$. Suitable choices of the operators $T \equiv T(x)$, on $L^2(\mathbf{x}_\perp)$ are discussed below (cf. Refs. 1–6). Formal manipulation of (1.1) now yields (cf. Ref. 4)

$$\frac{d}{dx}\begin{pmatrix}\psi^+ \\ \psi^-\end{pmatrix} = \mathsf{A}(x)\begin{pmatrix}\psi^+ \\ \psi^-\end{pmatrix},$$

$$\mathsf{A}(x) = P\begin{pmatrix}0 & 1 \\ -S & 0\end{pmatrix}P^{-1} + \left(\frac{d}{dx}P\right)P^{-1}, \tag{1.3a}$$

or

$$\frac{d}{dx}\psi^\pm = \pm\frac{1}{2}iT^{-1/2}[(S+T)\psi^\pm + (S-T)\psi^\mp] + \frac{1}{2}(T^{-1/2})_x T^{1/2}(\psi^\pm - \psi^\mp). \tag{1.3b}$$

To motivate (1.2) and (1.3), we note that the choice $T \equiv S$ diagonalizes

$$P\begin{pmatrix}0 & 1 \\ -S & 0\end{pmatrix}P^{-1},$$

thus decoupling (1.3) and providing natural definitions for $\psi^\pm$ in regions where $n(\mathbf{x})$ (or S) is independent of x. We call this choice full *local* splitting, noting that it provides, in some sense, the most complete splitting. It is naturally used (and illustrated in this contribution) for media with deterministic $n(\mathbf{x})$ which varies with x. Clearly, as recognized previously,[2,4] there is no unique natural choice in regions where $n(\mathbf{x})$ varies with x. We now mention some other useful splitting choices. *Reference* splitting where $T(x) \equiv S_0$, independent of x, is also suitable for treating deterministic media where variations in $n(\mathbf{x})$ with respect to x are restricted to some localized region. Here we naturally choose $S_0 \equiv \lim_{|x| \to \infty} S(x)$. We have recently implemented reference splitting to treat wave propagation in random media where the (statistical) mean, $\langle n(\mathbf{x})\rangle$ of $n(\mathbf{x})$, is independent of x, and we choose $S_0 \equiv \langle S \rangle$.[7] Of course (1.2) and (1.3) also allow for the possibility of *intermediate* splittings where $T \not\equiv S$, but T still depends on x, e.g., $T(x) = \langle S(x)\rangle$ for random media where $\langle n(\mathbf{x})\rangle$ also varies with x.

Neglecting $\pm$ coupling in (1.3) produces a "unidirectional propagation approximation" which will be of the WKB (parabolic) type for local (reference) splitting. Such an approximation constitutes the lead term in an iterative Bremmer-type series expansion[1] of the exact solution of (1.3). For either an exact or approximate treatment, it is clearly necessary to develop an operational calculus for the splitting operator $T(x)$. This is trivial if one simply makes a scalar choice for $T(x)$ [e.g., $T(\mathbf{x}) \equiv k^2(x, \mathbf{x}_\perp = 0)$ (or the $|x| \to \infty$ limit, should it exist) which produces an Arnaud[3] (Leontovich–Fock[8]) approximation], but instead we con-

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sider only "more complete" abstract operator choices in an attempt to avoid "kinematic" contributions to backscattering [i.e., those not associated with variations of $k(\mathbf{x})$ with respect to x]. The spectral theory for $T(x)$ is only trivial for stratified media where T is multiplicative in the transverse Fourier transform variables. More generally, Weyl pseudodifferential operator calculus can be used,[9] but here we utilize conventional self-adjoint operator spectral theory, which, for focusing media or wave guides, corresponds to a wave field decomposition into a complete set of guided and radiation modes.

Mode-coupled equations, obtained by evaluating the abstract operator splitting equations (1.3) in a natural explicit representation, are displayed in Sec. II. A "more conventional" derivation of these equations is also provided. The explicit example of a square law medium with one lateral dimension is treated in Sec. III, and a diagrammatic representation of the Bremmer-type series solutions is provided. Invariant imbedding equations for transmission and reflection operators for slabs of finite thickness are presented in Sec. IV, and the symplectic structure of the underlying splitting equations is shown to generate important reciprocity conditions.

II. LOCAL SPLITTING APPLIED TO DETERMINISTIC FOCUSING MEDIA AND WAVEGUIDES

The infinite focusing media (or open waveguides) considered here have the following properties: (i) $n(\mathbf{x})$ attains its maximum near $\mathbf{x}_\perp = 0$; (ii) $n(\mathbf{x}) \to n_\infty(x)$, as $|\mathbf{x}_\perp| \to \infty$, for each x; and (iii) $n(\mathbf{x})$ is independent of x outside of the interval $(0<)\ a<x<b$. Thus any guided wave propagation is along the x axis, and scattering is restricted to $a<x<b$. The self-adjoint operator $T(x) \equiv S(x)$ here in general has several discrete eigenvalues satisfying $\lambda \in (k^2 n_\infty^2(x), k^2 \max n^2(\mathbf{x}))$. The corresponding $L^2(\mathbf{x}_\perp)$-normalized eigenfunctions describe the guided modes.[10,11] We note that if $d=3$ and $\delta n(\mathbf{x}) \equiv n(\mathbf{x}) - n_\infty(x) \in C_0^\infty(R^2)$ is non-negative, then there exists at least one such guided mode,[12] no matter how small k! (This is also a property of symmetric, but not asymmetric, slab waveguides[10].) In addition, each $\lambda \in [-\infty, k^2 n_\infty^2(x)]$ is in the continuous spectrum. Specifically, $\lambda_{\mathbf{k}_\perp} = k^2 n_\infty^2(x) - |\mathbf{k}_\perp|^2$ is associated with "weak" radiation mode eigenfunctions $\sim e^{i\mathbf{k}_\perp \cdot \mathbf{x}_\perp}$ as $|\mathbf{x}_\perp| \to \infty$. Modes with $\lambda > 0$ (<0) are described as propagating (evanescent) for reasons which will become obvious. A schematic of the spectrum of $T = S$ is shown in Fig. 1. Radiation modes can plan an important role in wave propagation, but one encounters fundamental problems associated with singularities in associated coupling terms[11] (see below). A guided mode can also disappear into the continuum of radiation modes as x varies, as a result of changes in the shape of $n(\mathbf{x})$. Such a *cutoff* highlights a fundamental problem with an "adiabatic" treatment neglecting mode coupling.[11] This problem will not be addressed here.

For a closed waveguide, $\mathbf{x}_\perp$ is restricted to a finite region for each x. Its boundary (where conditions are imposed on the wavefield) is assumed to vary smoothly with x for $a<x<b$, and to be fixed elsewhere. Here the spectrum of

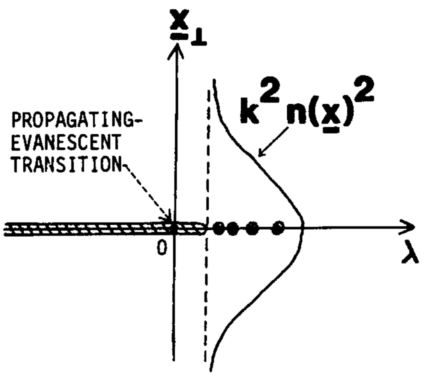

FIG. 1. A schematic of the continuum spectrum (cross-hatched line) and point spectrum (circles) of $T \equiv S$.

$T \equiv S$ is purely discrete, each eigenvalue λ corresponding to one or more guided modes. A mode which is propagating $(\lambda > 0)$, for large x, could become evanescent for part of $a<x<b$ (the quantum mechanical analog of which is "barrier tunneling"[13]). In this case one sees singularities in the splitting procedure (certain $\lambda^{-1/2} \to \infty$) generating a strong coupling between forward and back propagating modes (cf. the connection formulas for barrier tunneling[13]). We shall not discuss this further here.

It is convenient to introduce generic mode labels κ and to denote all $(T \equiv S)$-mode eigenfunctions by $\psi_\kappa(\mathbf{x}_\perp | x) \equiv \langle \mathbf{x}_\perp | \kappa, x\rangle$ (using Dirac notation), and corresponding eigenvalues by $\lambda_\kappa(x)$. Thus if Σ_κ represents a sum/integral over all modes, then one has that

$$f(T(x)) = \sum_\kappa f(\lambda_\kappa(x)) |\kappa,x\rangle \langle \kappa,x| .$$

The modal coefficients $\phi_\kappa(x) = \langle \kappa,x|\phi\rangle$ of $\phi(\mathbf{x})$ satisfy

$$\phi(\mathbf{x}) \equiv \sum_\kappa \phi_\kappa(x) \langle \mathbf{x}_\perp | \kappa,x\rangle . \tag{2.1}$$

We note here that

$$(\psi_x)_\kappa = \left\langle \kappa,x \left| \frac{d}{dx} \right| \psi \right\rangle = \frac{d}{dx} \langle \kappa,x|\psi\rangle - \left(\frac{d}{dx} \langle \kappa,x| \right) |\psi\rangle$$
$$= \frac{d}{dx} \psi_\kappa + \sum_{\kappa'} \left\langle \kappa,x \left| \frac{d}{dx} \right| \kappa',x \right\rangle \psi_{\kappa'} , \tag{2.2}$$

so, from (1.2), one has

$$\psi_\kappa^\pm = \frac{1}{2} \left(\psi_\kappa \mp i\lambda_\kappa^{-1/2} \frac{d}{dx} \psi_\kappa \right)$$
$$\mp \frac{i}{2} \lambda_\kappa^{-1/2} \sum_{\kappa'} \left\langle \kappa,x \left| \frac{d}{dx} \right| \kappa',x \right\rangle \psi_{\kappa'} . \tag{2.3}$$

We can obtain *directly* from (1.3), with $T(x) \equiv S(x)$, coupled equations for $\psi_\kappa^\pm$, which after some rearrangement become

$$\frac{d}{dx} \psi_\kappa^\pm(x) + \left\{ \mp i\lambda_\kappa(x)^{1/2} + \frac{1}{4} \frac{d}{dx} \ln \lambda_\kappa(x) \right\} \psi_\kappa^\pm(x)$$
$$= \frac{1}{4} \frac{d}{dx} \ln \lambda_\kappa(x) \psi_\kappa^\mp(x)$$
$$+ \frac{1}{2} \sum_{\kappa'} \left\langle \kappa,x \left| \frac{d}{dx} \right| \kappa',x \right\rangle \left\{ \left[\left(\frac{\lambda_{\kappa'}(x)}{\lambda_\kappa(x)} \right)^{1/2} - 1 \right] \psi_{\kappa'}^\mp(x) \right.$$

$$-\left[\left(\frac{\lambda_{\kappa'}(x)}{\lambda_\kappa(x)}\right)^{1/2}+1\right]\psi_{\kappa'}^{\pm}(x)\Bigg\}$$

$$\equiv F_\kappa^{\pm}(x), \text{ say.} \tag{2.4}$$

Note that contributions to $(T(x)^{-1/2})_x$ come from the x dependence of both eigenvalues and eigenfunctions (here bras and kets). For evanescent $\lambda_\kappa<0$, we set $\lambda_\kappa^{1/2}=i|\lambda_\kappa|^{1/2}$ guaranteeing that the corresponding components of ψ^+ (ψ^-) are exponentially decreasing as x increases (decreases). The singular behavior of the coupling coefficients, $\langle\kappa,x|d/dx|\kappa',x\rangle$, where κ, κ' are both radiation modes, is discussed in Appendix A for $d=3$.

Clearly (2.4) provides a natural starting point for the analysis of backscattering effects on wave propagation. For boundary conditions corresponding to one or more right-propagating guided modes at $x=0$ [$\psi_\kappa^+(0)\neq 0$, for such κ], and no left-propagating waves at $x=\infty$ [$\psi_\kappa^-(\infty)=0$], (2.4) can be rewritten in integral form as

$$\psi_\kappa^+(x)=\phi_\kappa^+(x)+\int_0^x dx'\,G_\kappa^+(x|x')F_\kappa^+(x'),$$
$$\psi_\kappa^-(x)=-\int_x^\infty dx'\,G_\kappa^-(x|x')F_\kappa^-(x'), \tag{2.5}$$

where

$$\phi_\kappa^+(x)\equiv G_\kappa^+(x|0)\psi_\kappa^+(0)$$

and

$$G_\kappa^{\pm}(x|x')\equiv\left(\frac{\lambda_\kappa(x')}{\lambda_\kappa(x)}\right)^{1/4}\exp\left(\pm i\int_{x'}^x dx''\,\lambda_\kappa^{1/2}(x'')\right).$$

The only contribution to the integrals, associated with inhomogeneity in $n(\mathbf{x})$ with respect to x, comes from the scattering region $x'\in[a,b]$. If coupling between guided modes is weak and coupling to radiation modes can be ignored, then the iterative solution of (2.5) is viable.

It is instructive to consider the relationship of (2.4) to the more conventional mode-coupled equations for ψ_κ, $(\psi_x)_\kappa$. We show, in Appendix B, how the latter can be used to generate a standard second-order equation for the ψ_κ [as could have been obtained from an explicit propagation mode representation of (1.1)]. By introducing an appropriate infinite matrix splitting operator, we can also recover (2.4).

III. WAVE PROPAGATION IN SQUARE LAW MEDIA (WITH VARIABLE FOCUSING)

When the guided mode wave propagation in focusing media is effectively confined laterally to a region near the maximum of $n(\mathbf{x})$, one might expect a quadratic approximation for $n(\mathbf{x})$ to be reasonable. This motivates the analysis of "square-law" media where

$$n(\mathbf{x})^2=1-B^2(x)|\mathbf{x}_\perp|^2, \tag{3.1}$$

which, of course, is unphysical for $|\mathbf{x}_\perp|>B^{-1}$. Relation (3.1) provides a useful description for certain optical fibers. Although replacing the physical $n(\mathbf{x})$ by (3.1) may have minimal effect on the highest (guided mode) eigenvalues and eigenfunctions of $T(x)\equiv S(x)$ and the corresponding eigenfunctions, it affects those of lower eigenvalues more dramatically, and replaces the continuous radiation mode spectrum with a "spurious" point spectrum.

For simplicity we confine our attention to $d=2$ here (a single lateral dimension). Here the eigenfunctions and eigenvalues of

$$T(x)\equiv S(x)=\frac{\partial^2}{\partial x_\perp^{\,2}}+k^2(1-B^2(x)x_\perp^{\,2})$$

are given by

$$\psi_m(x_\perp|x)=(2^{-m}/m!)^{1/2}(kB(x)/\pi)^{1/4}$$
$$\times H_m(k^{1/2}B(x)^{1/2}x_\perp)e^{-kB(x)x_\perp^2/2}, \tag{3.2}$$
$$\lambda_m(x)=k^2-2kB(x)(m+\tfrac{1}{2}),\quad \text{for } m\geqslant 0,$$

where H_m is the mth-order Hermite polynomial. Using standard relationships for the H_m, one can show that

$$\frac{d}{dx}|m,x\rangle=\frac{B'(x)}{4B(x)}[m^{1/2}(m-1)^{1/2}|m-2,x\rangle$$
$$-(m+2)^{1/2}(m+1)^{1/2}|m+2,x\rangle], \tag{3.3a}$$

so

$$\left\langle m,x\left|\frac{d}{dx}\right|n,x\right\rangle=\frac{B'(x)}{4B(x)}[(m+2)^{1/2}(m+1)^{1/2}\delta_{m+2,n}$$
$$-m^{1/2}(m-1)^{1/2}\delta_{m-2,n}]. \tag{3.3b}$$

It is elucidating to consider the high wavenumber (k) regime here where $d/dx\ln\lambda_m$ and $(\lambda_{m\pm2}/\lambda_m)^{1/2}-1=O(1/k)$, which indicates the small coupling between forward and backward propagating modes. In this regime (2.4) becomes

$$\frac{d}{dx}\psi_m^{\pm}\mp i\left[k-B\left(m+\frac{1}{2}\right)\right]\psi_m^{\pm}$$
$$=\frac{B'(x)}{4B(x)}[m^{1/2}(m-1)^{1/2}\psi_{m-2}^{\pm}$$
$$-(m+2)^{1/2}(m+1)^{1/2}\psi_{m+2}^{\pm}]+O\left(\frac{1}{k}\right). \tag{3.4}$$

Let us now utilize the integral form (2.5) of the mode coupled equations (2.4) for a scattering problem with boundary conditions $\psi_m^+(0)\propto\delta_{m,0}$, $\psi_m^-(\infty)=0$ for all $m\geqslant 0$. Clearly, from (3.3) and (2.4), one has that $\psi_m^{\pm}(x)\equiv 0$, for m odd. Expressions for $\psi_m^{\pm}$, with m even, can be obtained from the iterative solution of (2.5) [assuming that no $\lambda_m(x)$ changes sign or becomes zero, as x varies]. It is natural to represent contributions to these solutions diagrammatically in terms of paths on a lattice of points labeled by the modes $(m,\pm)$. The zero length path $(0,+)$ and segments connecting different points have the interpretation shown in Fig. 2. Then $\psi_m^{\pm}$ is represented as a sum over all paths connecting $(0,+)$ to $(m,\pm)$ (see Fig. 3). One can straightforwardly extend these considerations to higher dimensional ($d\geqslant 3$) square law media.

IV. INVARIANT IMBEDDING, SYMPLECTIC STRUCTURE AND RECIPROCITY, AND OTHER SYMMETRIES

We have shown that the basic differential equation associated with any splitting has the form

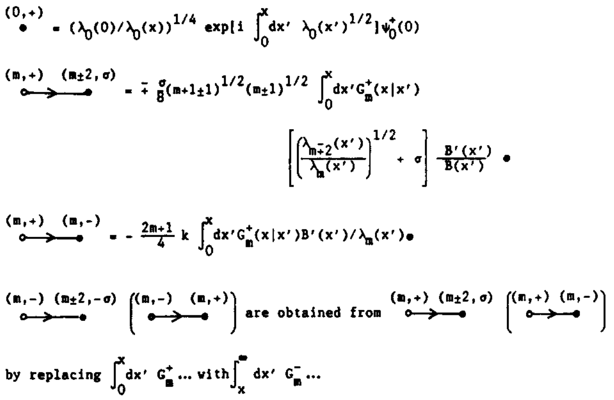

FIG. 2. Operator theoretic interpretation of path segments appearing in the diagrammatic representation of solutions of the coupled wave equations. Here $\sigma = +1$ or -1.

$$\frac{d}{dx}\begin{pmatrix}\psi^+\\ \psi^-\end{pmatrix} = \mathsf{A}(x)\begin{pmatrix}\psi^+\\ \psi^-\end{pmatrix} \equiv \mathsf{j}\mathsf{H}(x)\begin{pmatrix}\psi^+\\ \psi^-\end{pmatrix},$$

$$\text{where } \mathsf{j} = \begin{pmatrix}0 & I\\ -I & 0\end{pmatrix}, \tag{4.1}$$

defining $\mathsf{H}(x) \equiv -\mathsf{j}\mathsf{A}(x)$ and noting that $-\mathsf{j}^2 = \mathsf{I}$ (the identity). Since (4.1) is linear, one naturally defines the abstract transmission $T^\pm$ and reflection $R^\pm$ operators for slabs $[x,y]$ of finite thickness, by

$$\begin{pmatrix}\psi^-(x)\\ \psi^+(y)\end{pmatrix} = \begin{pmatrix}R^+(x,y) & T^-(x,y)\\ T^+(x,y) & R^-(x,y)\end{pmatrix}\begin{pmatrix}\psi^+(x)\\ \psi^-(y)\end{pmatrix}$$

$$\equiv \mathsf{S}(x,y)\begin{pmatrix}\psi^+(x)\\ \psi^-(y)\end{pmatrix}, \tag{4.2}$$

where S is called the scattering operator and clearly $T^\pm(x,x) = I$, $R^\pm(x,x) = 0$. The operator S satisfies the differential equation (cf. Refs. 4, 5, and 14)

$$\frac{\partial}{\partial y}\mathsf{S} = \begin{pmatrix}T^- & 0\\ R^- & I\end{pmatrix}\mathsf{H}(y)\begin{pmatrix}T^+ & R^-\\ 0 & I\end{pmatrix}. \tag{4.3}$$

Taking the four components of (4.3) provides the familiar Ambarzumian form of the invariant imbedding equations.[14] An equivalent set may be obtained from these by making the replacements $\partial/\partial y \to \partial/\partial x$, $T^- \leftrightarrow T^+$, $R^- \leftrightarrow R^+$, $H_{\pm\pm}(y) \to H_{\mp\mp}(x)$, $H_{\pm\mp}(y) \to H_{\mp\pm}(x)$.

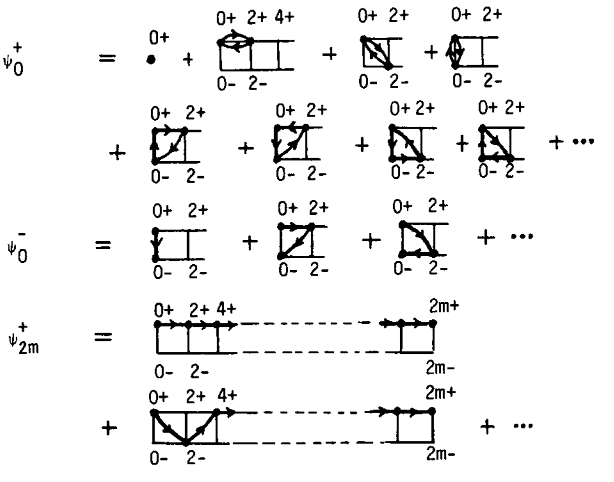

FIG. 3. Diagrammatic expansions for various forward and backward traveling modal components of the wave field.

Since these equations have a structure generic to many problems in wave propagation and transport theory, we anticipate that there exist basic relationships between the reflection and transmission operators. To fully elucidate this structure, it is appropriate to introduce several new quantities. Let $\mathsf{C}(x,y)$ be the operator which propagates the wavefields $\psi^\pm$ from x to y, i.e.,

$$\begin{pmatrix}\psi^+(y)\\ \psi^-(y)\end{pmatrix} = \mathsf{C}(x,y)\begin{pmatrix}\psi^+(x)\\ \psi^-(x)\end{pmatrix}, \tag{4.4}$$

where, from (4.2),

$$C_{++} = T^+ - R^-[T^-]^{-1}R^+, \quad C_{+-} = R^-[T^-]^{-1},$$
$$C_{-+} = -[T^-]^{-1}R^+, \quad C_{--} = [T^-]^{-1}. \tag{4.5}$$

Though C is less physical than S, we shall see that in certain cases it can be regarded as a (linear) canonical transformation. Note that from (4.1) and (4.4), one clearly has

$$\mathsf{C}(x,x+\Delta x) = \mathsf{I} + \mathsf{A}(x)\Delta x + O(\Delta x^2), \tag{4.6}$$

where I is the identity. Finally, it is convenient to define

$$\boldsymbol{\theta}^1(x) = \begin{pmatrix}0 & \theta(x)\\ -\tilde{\theta}(x) & 0\end{pmatrix}, \quad \boldsymbol{\theta}(x,y) = \begin{pmatrix}\theta(x) & 0\\ 0 & \tilde{\theta}(y)\end{pmatrix}, \tag{4.7}$$

where the operator $\theta(x)$ will be specified later, and $\tilde{}$ denotes a *real* involution operation (so $\tilde{\tilde{A}} = A$, $\tilde{i} = i$). Now using (4.1)–(4.7) as defining relations, one has the following.

Theorem: The following conditions are equivalent for any differentiable $\theta(x)$:

$$\text{(i) } \boldsymbol{\theta}(x,y)\mathsf{S}(x,y) = \tilde{\mathsf{S}}(x,y)\tilde{\boldsymbol{\theta}}(x,y), \tag{4.8}$$

i.e.,

$$\theta(x)R^+(x,y) = \tilde{R}^+(x,y)\tilde{\theta}(x),$$
$$\tilde{\theta}(y)R^-(x,y) = \tilde{R}^-(x,y)\theta(y)$$

and

$$\theta(x)T^-(x,y) = \tilde{T}^+(x,y)\theta(y);$$

$$\text{(ii) } \tilde{\mathsf{C}}(x,y)\boldsymbol{\theta}^1(y)\mathsf{C}(x,y) = \boldsymbol{\theta}^1(x), \tag{4.9}$$

i.e., a symplectic condition for C;

$$\text{(iii) } \tilde{\mathsf{A}}(x)\boldsymbol{\theta}^1(x) + \boldsymbol{\theta}^1(x)\mathsf{A}(x) + \boldsymbol{\theta}^1_x(x) = \mathsf{O}, \tag{4.10}$$

or equivalently,

$$\tilde{\mathsf{H}}(x)\tilde{\boldsymbol{\theta}}(x,x) - \boldsymbol{\theta}(x,x)\mathsf{H}(x) + \boldsymbol{\theta}^1_x(x) = 0,$$

i.e.,

$$\tilde{H}_{++}(x)\tilde{\theta}(x) = \theta(x)H_{++}(x),$$
$$\tilde{H}_{--}(x)\theta(x) = \tilde{\theta}(x)H_{--}(x),$$

and

$$\tilde{H}_{-+}(x)\theta(x) - \theta(x)H_{+-}(x) + \theta_x(x) = 0.$$

Proof: (i) $\Rightarrow$ (ii): Calculation of the components of $\tilde{\mathsf{C}}(x,y)\boldsymbol{\theta}^1(y)\mathsf{C}(x,y)$, followed by substitution of identities from (i), shows straightforwardly that this quantity equals $\boldsymbol{\theta}^1(x)$.

(ii) $\Rightarrow$ (iii): Substituting the expansions

$$\tilde{\mathsf{C}}(x,x+\Delta x) = \mathsf{I} + \tilde{\mathsf{A}}\Delta x + O(\Delta x^2),$$
$$\mathsf{C}(x,x+\Delta x)^{-1} = \mathsf{I} - \mathsf{A}\Delta x + O(\Delta x^2), \tag{4.11}$$

and

$$\theta^1(x+\Delta x) = \theta^1(x) + \theta^1_x(x)\Delta x + O(\Delta x^2),$$

into the identity

$$\tilde{C}(x,x+\Delta x)\theta^1(x+\Delta x) = \theta^1(x)C(x,x+\Delta x)^{-1}, \tag{4.12}$$

and equating terms $O(\Delta x)$ yields (iii).

(iii) $\Rightarrow$ (i): Using Eqs. (4.3) and identities from (iii), one obtains

$$\begin{aligned}\frac{\partial}{\partial y}[\theta(x)R^+] &= \theta(x)T^-H_{++}(y)T^+ \\ &= \tilde{T}^+\theta(y)H_{++}(y)T^+ \\ &\quad + [\theta(x)T^- - \tilde{T}\theta(y)]H_{++}(y)T^+,\end{aligned}$$

and

$$\begin{aligned}\frac{\partial}{\partial y}[\tilde{R}^+\tilde{\theta}(x)] &= \tilde{T}^+\tilde{H}_{++}(y)\tilde{T}^-\tilde{\theta}(x) \\ &= \tilde{T}^+\tilde{H}_{++}(y)\tilde{\theta}(y)T^+ + \tilde{T}^+\tilde{H}_{++}(y) \\ &\quad \times[\tilde{T}^-\tilde{\theta}(x) - \tilde{\theta}(y)T^+],\end{aligned} \tag{4.13}$$

so

$$\begin{aligned}&\frac{\partial}{\partial y}[\theta(x)R^+ - \tilde{R}^+\tilde{\theta}(x)] \\ &\quad = [\theta(x)T^- - \tilde{T}^+\theta(y)]H_{++}(y)T^+ - I,\end{aligned} \tag{4.14}$$

where I denotes the involution of the first term. Similarly,

$$\begin{aligned}&\frac{\partial}{\partial y}[\tilde{\theta}(y)R^- - \tilde{R}^-\theta(y)] \\ &\quad = [\tilde{\theta}(y)R^- - \tilde{R}^-\theta(y)] \\ &\quad \times[H_{++}(y)\overline{R} + H_{++}(y)] - I,\end{aligned} \tag{4.15}$$

$$\begin{aligned}&\frac{\partial}{\partial y}[\tilde{\theta}(y)T^+ - \tilde{T}^-\tilde{\theta}(x)] \\ &\quad = [\tilde{\theta}(y)R^- - \tilde{R}^-\theta(y)]H_{++}(y)T^+ \\ &\quad - [\tilde{R}^-\tilde{H}_{++}(y) + \tilde{H}_{++}(y)] \\ &\quad \times[\tilde{T}^-\tilde{\theta}(x) - \tilde{\theta}(y)T^+].\end{aligned} \tag{4.16}$$

Since the identities (i) [i.e., (4.8)] are trivially satisfied when $x=y$, (4.14)–(4.16) show that they are satisfied for all $y \geqslant x$. □

Now we apply these results to the specific choice of splitting of ψ into $\psi^\pm$ defined by (1.2) and thus associated with the operator $T = T(x)$. The corresponding components of H can be determined from (1.3). For this application it is necessary to choose the real involution ˜ to correspond to the real transpose (rather than Hermitian adjoint) and to note that appropriate choices of T satisfy $\tilde{T} = T$, i.e.,

$$\begin{aligned}\int d\mathbf{x}_\perp\, \psi(\mathbf{x}_\perp)(\tilde{T}\phi)(\mathbf{x}_\perp) &\equiv \int d\mathbf{x}_\perp\, \phi(\mathbf{x}_\perp)(T\psi)(\mathbf{x}_\perp) \\ &= \int d\mathbf{x}_\perp\, \psi(\mathbf{x}_\perp)(T\phi)(\mathbf{x}_\perp).\end{aligned} \tag{4.17}$$

This is obviously true choosing, e.g., $T = S(x) = \Delta_\perp + k^2(\mathbf{x})$ (local splitting) or $T = S_0 = \Delta_\perp + k^2(x = \pm\infty, \mathbf{x}_\perp)$ (reference splitting) *even if* $k(\mathbf{x}) = kn(\mathbf{x})$ is complex valued corresponding to a dissipative medium. Then condition (iii) is satisfied by the choice

$$\theta = T^{1/2}, \tag{4.18}$$

as may be verified by straightforward calculation.

Another symmetry property for the operator $C(x,y)$ is based on the observation that the (easily verified) relationship

$$\begin{pmatrix}0 & I\\ I & 0\end{pmatrix}\overline{A}(x) = A(x)\begin{pmatrix}0 & I\\ I & 0\end{pmatrix},$$

or

$$A_{++} = \overline{A}_{--},\quad A_{-+} = \overline{A}_{+-}, \tag{4.19}$$

is equivalent to

$$\begin{pmatrix}0 & I\\ I & 0\end{pmatrix}\overline{C}(x,y) = C(x,y)\begin{pmatrix}0 & I\\ I & 0\end{pmatrix},$$

or

$$C_{++}(x,y) = \overline{C}_{--}(x,y),\quad C_{-+}(x,y) = \overline{C}_{+-}(x,y). \tag{4.20}$$

This is representative of a broader class of symmetry relationships.[15] When (4.20) is combined with (4.9) and (4.18), one also obtains

$$\begin{aligned}&\tilde{C}(x,y)\begin{pmatrix}T^{1/2}(y) & 0\\ 0 & -T^{1/2}(y)\end{pmatrix}\overline{C}(x,y) \\ &\quad = \begin{pmatrix}T^{1/2}(x) & 0\\ 0 & -T^{1/2}(x)\end{pmatrix}.\end{aligned} \tag{4.21}$$

Matrix elements of scattering operators are evaluated here using a natural mixed representation with respect to eigenfunctions of (different positioned) splitting operators $T(x)$. For example, $T^+_{\kappa',\kappa}(x,y) = \langle\kappa',y|T^+(x,y)|\kappa,x\rangle$ is the appropriate transmission coefficient connecting right propagating modes κ at x, and κ' at y. Generic Dirac notation is used here for T eigenbras and eigenkets, and corresponding eigenvalues are denoted by $\lambda_\kappa(x)$ (but now these will *not* correspond to S eigenbras and eigenkets and eigenvalues when $S \neq T$). This prescription is automatically compatible with the evaluation of operator products required in (4.3) (or equivalent versions of these equations). Clearly, in (4.3), T bras and kets for all components of $H(y)$ are evaluated at y. The important reciprocity conditions (4.8) [using (4.18)] have the explicit form

$$\begin{aligned}&\lambda_\kappa(x)^{1/2}\langle\kappa,x|R^+(x,y)|\kappa',x\rangle \\ &\quad = \lambda_{\kappa'}(x)^{1/2}\langle\bar{\kappa}',x|R^+(x,y)|\bar{\kappa},x\rangle, \\ &\lambda_\kappa(y)^{1/2}\langle\kappa,y|R^-(x,y)|\kappa',y\rangle \\ &\quad = \lambda_{\kappa'}(y)^{1/2}\langle\bar{\kappa}',y|R^+(x,y)|\bar{\kappa},y\rangle, \\ &\lambda_\kappa(x)^{1/2}\langle\kappa,x|T^-(x,y)|\kappa',y\rangle \\ &\quad = \lambda_{\kappa'}(y)^{1/2}\langle\bar{\kappa}',y|T^+(x,y)|\bar{\kappa},x\rangle,\end{aligned} \tag{4.22}$$

where $\langle\mathbf{x}_\perp|\bar{\kappa},x\rangle = \psi_\kappa(\mathbf{x}_\perp)^*$.

It is a straightforward matter to write down the explicit form of the mode coupled invariant imbedding equations. One could investigate an iterative form of solution which, to the lowest order, gives

$$T^\pm_{\kappa',\kappa} \sim \delta_{\kappa',\kappa}\exp\left(\int_x^y ds\langle\kappa,s|H_{\mp\pm}|\kappa,s\rangle\right) \text{ and } R^\pm_{\kappa',\kappa} \sim 0. \tag{4.23}$$

V. CONCLUSIONS

An abstract splitting operator based formation is shown to provide a powerful and flexible formulation of wave propagation in "imperfect" media. Mode coupled equations connecting forward and backward propagation provide a natural basis for the analysis of backscattering effects. We have, however, noted some difficulties associated with guided mode cutoff, and propagating-evanescent transitions. The formalism also provides a natural basis for derivation of invariant imbedding equations for transmission and reflection operators. The reciprocity relations derived here for these are important from a fundamental and practical perspective.

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APPENDIX A: RADIATION MODE EIGENFUNCTIONS AND MATRIX ELEMENTS FOR $d=3$

Here the eigenvalue equation for the radiation mode eigenfunctions, $\psi_{\mathbf{k}_\perp} \sim (1/2\pi)e^{i\mathbf{k}_\perp\cdot\mathbf{x}_\perp}$, as $|\mathbf{x}_\perp| \to \infty$, can be converted to the integral form

$$\psi_{\mathbf{k}_\perp}(\mathbf{x}_\perp|x) = \frac{1}{2\pi} e^{i\mathbf{k}_\perp\cdot\mathbf{x}_\perp} + \frac{ik^2}{4}\int d\mathbf{x}'_\perp \times H_0^1(k_\perp|\mathbf{x}_\perp - \mathbf{x}'_\perp|)\delta n(x,\mathbf{x}'_\perp)\psi_{\mathbf{k}_\perp}(\mathbf{x}'_\perp|x), \tag{A1}$$

where $k_\perp = |\mathbf{k}_\perp|$, and we have used the Hankel function H_0^1 to provide an explicit representation of the two-dimensional free Green's function $(\Delta_\perp + k_\perp^2)^{-1}$ (see Ref. 16a). Let us analyze radiation to radiation mode coupling coefficients, $\langle \mathbf{k}_\perp,x|d/dx|\mathbf{k}'_\perp,x\rangle$, of (2.4). First, one must consider $d/dx\, \psi_{\mathbf{k}'_\perp}$, which can be obtained from (A1) by differentiating under the integral sign. Thus its large $x_\perp = |\mathbf{x}_\perp|$ asymptotic behavior is obtained directly from that of

$$H_0^1(k'_\perp x_\perp) \sim (\pi k'_\perp x_\perp/2)^{-1/2}\exp(ik'_\perp x_\perp - i\pi/4).$$

Second, it is convenient to reexpress the plane wave part of $\psi_{\mathbf{k}_\perp}$ as a linear combination of cylindrical wave eigenfunctions of $\Delta_\perp$, proportional to

$$J_\nu(k_\perp x_\perp) \sim \left(\frac{\pi k_\perp x_\perp}{2}\right)^{-1/2}\cos\left(k_\perp x_\perp - \frac{1}{2\nu\pi} - \frac{1}{4\pi}\right),$$

as $x_\perp \to \infty$.[16b] After writing

$$\int d\mathbf{x}_\perp = \int d\phi \int dx_\perp\, x_\perp \cdot,$$

it is clear that these coupling coefficients involve singular integrals of the form

$$\int_0^\infty dk\, e^{ikx} = \frac{1}{2}\delta(k) + i\mathbb{P}/k, \tag{A2}$$

where $\mathbb{P}$ represents a Cauchy principal value integral.

APPENDIX B: SPLITTING OF CONVENTIONAL MODE-COUPLED EQUATIONS

Let Ψ, Ψ_x denote infinite dimensional vectors with components ψ_κ, $(\psi_x)_\kappa$, respectively. Then, from (1.1), one can readily obtain the following infinite matrix form of the conventional mode-coupled equations[11]:

$$\frac{d}{dx}\begin{pmatrix}\Psi\\ \Psi_x\end{pmatrix} = \left(\begin{array}{c|c} -\mathsf{D} & \mathsf{I} \\ \hline -\lambda & -\mathsf{D}\end{array}\right)\begin{pmatrix}\Psi\\ \Psi_x\end{pmatrix}, \tag{B1}$$

where $(\mathsf{I})_{\kappa,\kappa'} = \delta_{\kappa,\kappa'}$ is the identity, $(\lambda)_{\kappa,\kappa'} = \delta_{\kappa,\kappa'}\lambda_\kappa$ (where the λ_κ are the eigenvalues of $T\equiv S$), and $(\mathsf{D})_{\kappa,\kappa'} = \langle\kappa,x|d/dx|\kappa',x\rangle$. Elimination of Ψ_x from (B1) yields the standard second-order equation for Ψ[11]:

$$\frac{d^2}{dx^2}\Psi + 2\mathsf{D}\frac{d}{dx}\Psi + \left(\mathsf{D}^2 + \frac{d}{dx}\mathsf{D} + \lambda\right)\Psi = 0. \tag{B2}$$

Instead we introduce right, Ψ^+, and left, Ψ^-, traveling vectors in terms of a splitting operator P by

$$\begin{pmatrix}\Psi^+\\ \Psi^-\end{pmatrix} = \mathsf{P}\begin{pmatrix}\Psi\\ \Psi_x\end{pmatrix}, \quad \text{where } \mathsf{P} = \frac{1}{2}\left(\begin{array}{c|c} \mathsf{I} & -i\lambda^{1/2} \\ \hline \mathsf{I} & +i\lambda^{1/2}\end{array}\right), \tag{B3}$$

so the components of $\Psi^\pm$ are just $\psi_\kappa^\pm$ (for local splitting where $T\equiv S$). Deriving equations for $\Psi^\pm$ from (B1) in the obvious way [cf. (1.3)] yields

$$\begin{aligned}\frac{d}{dx}\Psi^\pm = {}& \pm i\lambda^{1/2}\Psi^\pm + \frac{1}{2}(\lambda^{-1/2})_x\lambda^{1/2}(\Psi^\pm - \Psi^\mp), \\ & -\tfrac{1}{2}\lambda^{-1/2}\mathsf{D}\lambda^{1/2}(\Psi^\pm - \Psi^\mp) \\ & -\tfrac{1}{2}\mathsf{D}(\Psi^+ + \Psi^-),\end{aligned} \tag{B4}$$

recovering (2.4).

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(i) $\Phi(y)\overline{\mathsf{C}}(x,y) = \mathsf{C}(x,y)\Phi(x)$,

(ii) $\Phi(x)\overline{\mathsf{A}}(x) - \mathsf{A}(x)\Phi(x) + \Phi_x(x) = 0$.

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