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A NOTE ON SCATTERING OPERATOR SYMBOLS FOR ELLIPTIC WAVE PROPAGATION

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ABSTRACT. The ill-posed elliptic wave propagation problems can be transformed into well-posed initial value problems of the reflection and transmission operators characterizing the material structure of the given model by the combination of wave field splitting and invariant imbedding methods. In general, the derived scattering operator equations are of first-order in range, nonlinear, nonlocal, and stiff and oscillatory with a subtle fixed and movable singularity structure. The phase space and path integral analysis reveals that construction and reconstruction algorithms depend crucially on a detailed symbol analysis of the scattering operators. Some information about the singularity structure of the scattering operator symbols is presented and analyzed in the transversely homogeneous limit.

1. Introduction

For many realistic three-dimensional wave propagation problems, one-way marching methods are incorporated into the solution algorithm for the inherently elliptic, frequency-domain, scalar Helmholtz formulation, as in Fishman's articles [3] and [4], which has widespread applicability in acoustics, quantum mechanics, etc. In general, marching elliptic methods require not only the back propagation of a backward wave field component but also the knowledge of both the wave field and its normal derivative on an initial plane. The first requirement leads to an ill-posed problem which requires a regularization that effectively filters out the evanescent portion of the spectrum. For strongly backscattering environments, such filtering can result in spurious oscillations in the wave field,

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which suggests the important role played by the high-frequency portion of the spectrum under such conditions. Since both wave field and its normal derivative can not be independently specified on the initial plane, on the other hand, the second requirement provides more troubles. Given the initial wave field, the determination of the corresponding normal derivative requires scattering data from the entire domain. Constructing this scattering information, however, effectively solves the original problem. Therefore, one recognizes that the two-point Helmholtz boundary value problem basically as scattering problems in terms of a transition region and transversely inhomogeneous half-spaces and it is desirable to develop an algorithm for the elliptic propagation problem which can use marching methods as much as possible in a well-posed manner.

Wave field splitting, invariant imbedding, and phase space and infinite functional analysis have been combined to transform the Helmholtz two-point boundary value problem on wave fields into an initial value problem on the scattering operators characterizing inhomogeneity of the transition region. The wave field splitting incorporates the kinematically correct physics and provide an effective representation for the weak range-dependent limit. Invariant imbedding provides the derivation of the scattering operator equations. The combined wave splitting and invariant imbedding methods were initiated by Bremmer [1] and developed by Corones and coworkers [2] and [8]. The phase space (or microscopic) and path integral methods transform the ill-behaved operator equations into equations on well-behaved functions and also provide the one-way propagation algorithms. Refer to [5] for phase space methods and [9] for path integral representations. The system of the resulting equations for the reflection and transmission operators is now well-posed but stiff and oscillatory. The reflected and transmitted wave fields can be computed in a very efficient manner while the wave field in the transition region can be computed by essentially a layer stripping algorithm. In principle, the transition region can be divided into subregions, allowing for parallel computations and subsequent recombination.

Associated with the reflection, transmission, and square root Helmholtz operators, the operator symbol analysis plays an important role for both direct and inverse problems. The operator symbols provide the natural multidimensional extension of the scattering coefficients in the one-dimensional formulation and the framework to quantize classical theories in quantum physics. In general, the resulting equations for the scattering operators are first-order in range, nonlinear, nonlocal, and stiff and oscillatory with a fixed and movable singularity structure.

Motivated by this observation, the analysis and subsequent exploitation of the singularity structure associated with the scattering operator symbols are the essential focus of the direct and inverse developments. The constructions of exact and approximate scattering operator symbols illustrate the general singularity structure and scattering theory, provide numerical benchmarks, and serve as an independent source of scattering data for the inverse problem. As an initial step toward the general case where the equations are nonlocal and of the composition type, the transversely homogeneous case is studied in this paper.

2. One-way evolution equations

The initial model for the problem of present interest is given by the scalar Helmholtz equation

$$(\nabla^2 + \bar{k}^2 K^2(\mathbf{x}))\phi(\mathbf{x}) = 0, \tag{1}$$

where $\bar{k}$ is a reference wave number and $K(\mathbf{x})$ is a refractive index field as a (sufficiently) smooth function of $\mathbf{x}$ in the n-dimensional space R^n. The environment can be characterized by $K(\mathbf{x})$ with a transition region of arbitrary variability superimposed upon a transversely inhomogeneous background profile. The vertical lines define the boundary of the transition region. The adopted model can be thought of as an infinite waveguide.

The basic idea of the first step of analysis for the problem is to apply wave field splitting and invariant imbedding methods to transform the boundary value problems into initial value problems. As defined in the book [11], the following equation is taken to define the wave splitting employed in the general inhomogeneous medium.

$$\phi^{\pm}(\mathbf{x}) = (1/2)(\phi(\mathbf{x}) \mp (i/\bar{k})\mathbf{B}^{-1}\partial_x \phi(\mathbf{x})) \tag{2}$$

$$\mathbf{B} \equiv (K^2(\mathbf{x}) + (1/\bar{k}^2)\nabla_t^2)^{1/2}, \tag{3}$$

where $x \in R$ and $\mathbf{x}_t \in R^{n-1}$ are designated as the principal global propagation direction and the transverse direction, respectively. For the general inhomogeneous transition region, $\phi^+(\mathbf{x})$ and $\phi^-(\mathbf{x})$ do not have a physical meaning whereas they represent physically identificable forward and backward wave field components of the total wave field $\phi(\mathbf{x})$, respectively, in the transversely inhomogeneous environments. The latter case corresponds to the diagonal system of the following complete system for $\phi^+(\mathbf{x})$ and $\phi^-(\mathbf{x})$ holding in all three regions:

(4) $\partial_x \phi^+(\mathbf{x}) = ((-i/2)\partial_x \mathbf{B}_1^{-1} + 1)i\mathbf{B}_1\phi^+(\mathbf{x}) + ((i/2)\partial_x \mathbf{B}_2^{-1})i\mathbf{B}_2\phi^-(\mathbf{x}),$

(5) $\partial_x \phi^-(\mathbf{x}) = ((i/2)\partial_x \mathbf{B}_1^{-1})i\mathbf{B}_1\phi^+(\mathbf{x}) + ((-i/2)\partial_x \mathbf{B}_2^{-1} + 1)i\mathbf{B}_2\phi^-(\mathbf{x}),$

where $\mathbf{B}_1$, $\mathbf{B}_2$ are $-\bar{k}\mathbf{B}$, $\bar{k}\mathbf{B}$, respectively; $\mathbf{B}_1$ was chosen to correspond to the forward wave radiation condition and $\mathbf{B}_2$ to correspond to the backward wave radiation condition. In the transversely inhomogeneous environments, the forward and backward evolution equations are

(6) $(i/\bar{k})\partial_x \phi^\pm(x, \mathbf{x}_t) \pm (K^2(\mathbf{x}_t) + (1/\bar{k}^2)\nabla_t^2)^{1/2}\phi^\pm(x, \mathbf{x}_t) = 0.$

These uncoupled equations are the formally exact wave equations supplemented with appropriate outgoing wave radiation and initial value conditions.

For wave propagation problems in the presence of two transversely inhomogeneous half-spaces separated by a planar transition region of arbitrary length and inhomogeneity, system (4)–(5) represents a type of two-point boundary value problem for the reflected, transmitted, and internal wave fields. This first-order system is ill-posed for marching in the sense that both $\phi^+(x, \mathbf{x}_t)$ and $\phi^-(x, \mathbf{x}_t)$ cannot be marched in the same direction in a well-posed manner although their one-way equations are well-posed only in the $+x$ and $-x$ directions, respectively. Even if (4)–(5) was well-posed for marching, it would still be necessary to determine either $\phi^-(x, \mathbf{x}_t)$ or $\phi^+(x, \mathbf{x}_t)$ in the left or right half-space, respectively. This can be accomplished by explicitly using the scattering nature of the propagating problem. Let the left and right boundaries of the transition region be located at $x = a$ and $x = b$, respectively, and a source at one point in each half-space. Then the incident wave fields are related to the scattered wave fields through scattering operators as follows.

(7) $$\phi^+(b, \mathbf{x}_t) = \mathbf{T}^+(a, b)\phi^+(a, \mathbf{x}_t) + \mathbf{R}^-(a, b)\phi^-(b, \mathbf{x}_t),$$

(8) $$\phi^-(a, \mathbf{x}_t) = \mathbf{R}^+(a, b)\phi^+(a, \mathbf{x}_t) + \mathbf{T}^-(a, b)\phi^-(b, \mathbf{x}_t),$$

where the scattering operators $\mathbf{R}^\pm(a, b)$ and $\mathbf{T}^\pm(a, b)$ denote the forward and backward reflection and transmission operators, respectively, associated with the transition region $a \le x \le b$. From (7)–(8), the construction of the scattering operators leads to the determination of $\phi^-(a, \mathbf{x}_t)$ and $\phi^+(b, \mathbf{x}_t)$, which provides the initial data for the computation of the reflected and transmitted wave fields by one-way marching algorithms. Finally, the transition region wave field is computed in a layer-stripping way.

The construction of the operator-valued scattering matrix can be achieved by invariant imbedding methods. Invariant imbedding intuitively views the scattering matrix for a finite region as being composed of scattering matrices of a large number of contiguous subregions and thus computes the effect of adjoining a very thin slab to the one side of the transition region. These ideas are well known techniques not only for deterministic problem but also for stochastic problems (for example, [7]) of linear wave equations in both the time and frequency domains. The first step for obtaining the scattering matrix is to start from a finite number of transversely inhomogeneous layers and the corresponding combinatorial equations of the forward and backward reflection and transmission operators. The next step is to represent the operators in terms of the square root operator $\mathbf{B}$ and its inverse. Then writing the equations to an order of Δx has to be accomplished. Finally, taking the limit of equations as Δx goes to zero leads to the continuum limit for the smoothly imbedded transition region. If one follows the prescribed steps, then with brief notation

$$\mathbf{R}_1^{\pm} = \mathbf{R}^{\pm}(a,x), \qquad \mathbf{T}_1^{\pm} = \mathbf{T}^{\pm}(a,x), \tag{9}$$

$$\mathbf{R}_2^{\pm} = \mathbf{R}^{\pm}(x,b), \qquad \mathbf{T}_2^{\pm} = \mathbf{T}^{\pm}(x,b), \tag{10}$$

the resultant imbedding equations are given by the following Riccati equations for reflection and transmission operators. For $\mathbf{R}^{\pm}(a,x)$ and $\mathbf{T}^{\pm}(a,x)$,

$$(i/\bar{k})\partial_x \mathbf{R}_1^{+} = \mathbf{T}_1^{-}\boldsymbol{\beta}\mathbf{T}_1^{+}, \tag{11}$$

$$(i/\bar{k})\partial_x \mathbf{T}_1^{+} = \alpha\mathbf{T}_1^{+} + \mathbf{R}_1^{-}\boldsymbol{\beta}\mathbf{T}_1^{+}, \tag{12}$$

$$(i/\bar{k})\partial_x \mathbf{R}_1^{-} = -\boldsymbol{\beta} + \boldsymbol{\alpha}\mathbf{R}_1^{-} - \mathbf{R}_1^{-}\boldsymbol{\delta} + \mathbf{R}_1^{-}\boldsymbol{\beta}\mathbf{R}_1^{-}, \tag{13}$$

$$(i/\bar{k})\partial_x \mathbf{T}_1^{-} = -\mathbf{T}_1^{-}\boldsymbol{\delta} + \mathbf{T}_1^{-}\boldsymbol{\beta}\mathbf{R}_1^{-}, \tag{14}$$

which are well-posed for one-way marching in the $+x$ direction, and for $\mathbf{R}^{\pm}(x,b)$ and $\mathbf{T}^{\pm}(x,b)$

$$(i/\bar{k})\partial_x \mathbf{R}_2^{+} = -\boldsymbol{\beta} + \boldsymbol{\delta}\mathbf{R}_2^{+} - \mathbf{R}_2^{+}\boldsymbol{\alpha} + \mathbf{R}_2^{+}\boldsymbol{\beta}\mathbf{R}_2^{+}, \tag{15}$$

$$(i/\bar{k})\partial_x \mathbf{T}_2^{+} = -\mathbf{T}_2^{+}\boldsymbol{\alpha} + \mathbf{T}_2^{+}\boldsymbol{\beta}\mathbf{R}_2^{+}, \tag{16}$$

$$(i/\bar{k})\partial_x \mathbf{R}_2^{-} = \mathbf{T}_2^{+}\boldsymbol{\beta}\mathbf{T}_2^{-}, \tag{17}$$

$$(i/\bar{k})\partial_x \mathbf{T}_2^{-} = \boldsymbol{\delta}\mathbf{T}_2^{-} + \mathbf{R}_2^{+}\boldsymbol{\beta}\mathbf{T}_2^{-}, \tag{18}$$

which are well-posed for one-way marching in the $-x$ direction, where the operators $\boldsymbol{\alpha}(x)$, $\boldsymbol{\beta}(x)$ and $\boldsymbol{\delta}(x)$ are given by $\boldsymbol{\alpha} = ((i/2\bar{k})\partial_x\mathbf{B}^{-1} - 1)\mathbf{B}$, $\boldsymbol{\beta} = ((i/2\bar{k})\partial_x\mathbf{B}^{-1})\mathbf{B}$, $\boldsymbol{\delta} = ((i/2\bar{k})\partial_x\mathbf{B}^{-1} + 1)\mathbf{B}$. These first-order, coupled (except for $\mathbf{R}_1^{-}$ and $\mathbf{R}_2^{+}$), non-linear system of operator equations have the initial conditions

$$\mathbf{R}_1^{\pm}(x=a)=0, \quad \mathbf{T}_1^{\pm}(x=a)=1, \tag{19}$$

$$\mathbf{R}_2^{\pm}(x=b)=0, \quad \mathbf{T}_2^{\pm}(x=b)=1. \tag{20}$$

Therefore, a well-posed, one-way, initial value problem has been obtained from the ill-posed, two-point, Helmholtz boundary value problem; the two wave field components are ill-posed for simultaneous marching, whereas the wave field $\phi^+(x,\mathbf{x}_t)$ (or $\phi^-(x,\mathbf{x}_t)$) and the scattering operators $\mathbf{R}_2^{\pm}$ and $\mathbf{T}_2^{\pm}$ (or $\mathbf{R}_1^{\pm}$ and $\mathbf{T}_1^{\pm}$) can be marched in opposite directions to solve the (two-way) elliptic problem.

3. Phase space analysis and path integral representation

Considering the transition region modeled by a (large) finite number of transversely inhomogeneous layers, it is assumed that $\mathbf{B}$ depends upon x parametrically. Then it suffices to look at equation (6). This formal one-way wave equation is a singular integrodifferential equation. The square root of two noncommuting operators must be constructed. While functions of a finite set of commuting self-adjoint operators can be constructed through spectral theory, nontrivial functions of noncommuting operators have to be represented by pseudodifferential operators. The pseudodifferential operator theory can extend homogeneous Fourier analysis to inhomogeneous environments. See [10] for general reference. Now, using the results from [6], the formal one-way wave equation (6) can be written explicitly as a Weyl pseudodifferential equation in the form

$$\begin{aligned}(21)\ (i/\bar{k})\partial_x\phi^+(x,\mathbf{x}_t) + (\bar{k}/2\pi)^{n-1}\int_{R^{2(n-1)}} d\mathbf{x}_t^{'}\, d\mathbf{p}_t\, \Omega_{\mathbf{B}}(\mathbf{p}_t,(\mathbf{x}_t+\mathbf{x}_t^{'})/2)\cdot \\ \cdot\exp(i\bar{k}\mathbf{p}_t\cdot(\mathbf{x}_t-\mathbf{x}_t^{'}))\phi^+(x,\mathbf{x}_t^{'})=0,\end{aligned}$$

where $\Omega_{\mathbf{B}}(\mathbf{p},\mathbf{q})$ is the operator symbol associated with the square root Helmholtz operator $\mathbf{B}\equiv(K^2(\mathbf{q})+(1/\bar{k}^2)\nabla_{\mathbf{q}}^2)^{1/2}$. The singular operator (kernel) calculus is now replaced by a calculus for a smooth, well-behaved functions, i.e., operator symbols, which contain the complete spectral information in just the appropriate manner to lead to the infinitesimal propagator.

Therefore, operator symbols must be constructed. The square root of an operator is constructed in terms of its square. For the Weyl pseudodifferential operator calculus, it implies that the operator symbol $\Omega_{\mathbf{B}}(\mathbf{p},\mathbf{q})$

is defined through the Weyl composition equation

$$
\begin{aligned}
\Omega_{\mathbf{B}^2}(\mathbf{p},\mathbf{q}) &= K^2(\mathbf{q}) - \mathbf{p}^2 \\
&= (\bar{k}/\pi)^{2(n-1)} \int_{R^{4(n-1)}} d\mathbf{t}\, d\mathbf{x}\, d\mathbf{y}\, d\mathbf{z}\, \Omega_{\mathbf{B}}(\mathbf{t}+\mathbf{p},\mathbf{x}+\mathbf{q}) \\
&\quad \cdot \Omega_{\mathbf{B}}(\mathbf{y}+\mathbf{p},\mathbf{z}+\mathbf{q}) \exp(2i\bar{k}(\mathbf{x}\cdot\mathbf{y} - \mathbf{t}\cdot\mathbf{z})),
\end{aligned} \tag{22}
$$

where $\Omega_{\mathbf{B}^2}(\mathbf{p},\mathbf{q})$ is the operator symbol associated with the square of $\mathbf{B}$. For a given $K^2(\mathbf{q})$, the Weyl composition equation must be solved with the outgoing wave radiation condition.

Solution representation for the pseudodifferential equation (21) can be directly expressed in terms of Feynman's path integrals following from the semigroup property of the propagator. The path integral representation for the propagator takes the form

$$
\begin{aligned}
&G^{+}(x,\mathbf{x}_t|0,\mathbf{x}_t') \\
(23)= \;& \lim_{N\to\infty} \int_{R^{(n-1)(2N-1)}} \prod_{j=1}^{N-1} d\mathbf{x}_{jt} \prod_{j=1}^{N} (\bar{k}/2\pi)^{n-1} d\mathbf{p}_{jt} \\
&\cdot \exp\left(i\bar{k} \sum_{j=1}^{N} (\mathbf{p}_{jt}\cdot(\mathbf{x}_{jt} - \mathbf{x}_{j-1t}) + (x/N) H(\mathbf{p}_{jt},\mathbf{x}_{jt},\mathbf{x}_{j-1t})) \right),
\end{aligned}
$$

where

$$
\begin{aligned}
(24)\; H(\mathbf{p},\mathbf{q}'',\mathbf{q}') = \;& (\bar{k}/2\pi)^{n-1} \int_{R^{2(n-1)}} d\mathbf{s}\, d\mathbf{t} \\
& F(\mathbf{q}' - \mathbf{q}'', \mathbf{s}) h_{\mathbf{B}}(\mathbf{p}, (\mathbf{q}'' + \mathbf{q}')/2 - \mathbf{t}) \exp(i\bar{k}\mathbf{s}\cdot\mathbf{t}).
\end{aligned}
$$

Here, $F(\mathbf{u},\mathbf{v})$ and $h_{\mathbf{B}}$ (the standard pseudodifferential operator symbol) are related to the operator symbol $\Omega_{\mathbf{B}}(\mathbf{p},\mathbf{q})$ through $\hat{\Omega}_{\mathbf{B}}(\mathbf{u},\mathbf{v}) = F(\mathbf{u},\mathbf{v})\hat{h}_{\mathbf{B}}(\mathbf{u},\mathbf{v})$, where $\hat{\Omega}_{\mathbf{B}}$ and $\hat{h}_{\mathbf{B}}(\mathbf{p},\mathbf{q})$ denote the corresponding Fourier transforms. The path in phase space in equation (23) is defined by the prescription $\mathbf{x}_{0t} = \mathbf{x}_t'$, $\mathbf{x}_{jt} = \mathbf{x}_t(j/N)$, $\mathbf{x}_{Nt} = \mathbf{x}_t$, $\mathbf{p}_{jt} = \mathbf{p}_t((j-1/2)/N)$ placing $\mathbf{p}_{jt}$ halfway between $\mathbf{x}_{jt}$ and $\mathbf{x}_{j-1t}$. Note the analogy between present wave propagation problem and the quantum mechanical problem. In quantum mechanics, $h_B(\mathbf{p},\mathbf{q})$ is the classical Hamiltonian and $F(\mathbf{u},\mathbf{v})$ is a function determining the ordering of the two noncommuting operators $\mathbf{Q} = \mathbf{q}$ and $\mathbf{P} = (-i/\bar{k})\partial_{\mathbf{q}}$.

4. One-way marching algorithm

Now, the wave field splitting, invariant imbedding, and phase space and path integral analysis can be combined to yield an explicit one-way marching algorithm. The algorithmic application of the solution method proceeds in the following way. The basic idea is to compute the reflection and transmission operator symbols and then, in the manner prescribed by the Weyl symbol calculus, apply them to the appropriate incoming fields to produce the appropriate initial data for well-posed, one-way marching.

For a detailed illustration, it is assumed that there is a wave source only in the left half-space. The embedding equations for reflection and transmission operators are changed into equations for operator symbols. These symbols can be simultaneously solved in an efficient manner due to their own one-way nature; the equations are marched from $x = b$ in incremental step to $x = a$ and then recovers the physical medium. Each incremental strip is transversely inhomogeneous. If only scattering fields are desired, the storage requirements are minimal since only the operator symbols for the physical medium are required. If the wave field in the transition region is also desired, then the incremental reflection operator symbols corresponding to the successive imbedding problems must be stored. Starting from the physical problem at $x = a$, $\phi^-(a^-, \mathbf{x}_t)$ is determined from the given $\phi^+(a^-, \mathbf{x}_t)$, the determined reflection operator symbol $\Omega_{\mathbf{R}_2^+}(a, b)$, and the Weyl symbol calculus. The continuous wave fields $\phi(a, \mathbf{x}_t)$ and $\partial_x \phi(a, \mathbf{x}_t)$ at $x = a$ then follow from the wave splitting equations

$$\phi(x, \mathbf{x}_t) = \phi^+(x, \mathbf{x}_t) + \phi^-(x, \mathbf{x}_t), \tag{25}$$

$$\partial_x \phi(x, \mathbf{x}_t) = i\mathbf{B}_1 \phi^+(x, \mathbf{x}_t) + i\mathbf{B}_2 \phi^-(x, \mathbf{x}_t), \tag{26}$$

and $\phi^+(a^+, \mathbf{x}_t)$ is now determined by (2). The Weyl symbol calculus and the approximate constructions of the square root operator symbols are used in the applications of (2) and (25)–(26). In the transversely inhomogeneous strip, $\phi^+(a^+, \mathbf{x}_t)$ is now marched to $x = (a + \Delta x)^-$, producing $\phi^+((a + \Delta x)^-, \mathbf{x}_t)$. Then one now has the problem of an incoming wave field incident upon a new slab $a + \Delta x \leq x \leq b$ with a known reflection operator symbol previously calculated and stored in the invariant imbedding procedure. The above outlined procedure is then repeated in a layer-stripping manner to $x = b$. The traveling wave fields are always propagated in their well-posed directions. The two-way nature of the elliptic problem in the transition region is accounted for by first marching the reflection operator symbol equation from $x = b$ to $x = a$, and then successively calculating the wave field by marching back from $x = a$ to $x = b$.

5. Symbol analysis in the transversely homogeneous limit

Wave field splitting, invariant imbedding, and phase space and path integral methods have been put together to transform the ill-posed Helmholtz two-point boundary value problem of wave fields into well-posed initial value problems of the scattering operators characterizing the transition region. This is a natural way to incorporate well-posed marching methods into the inherently two-way problem. For the computational one-way algorithm, the operator symbols associated with reflection, transmission, and square root Helmholtz operators play a pivotal role. In general, the resulting equations for the reflection and transmission operator symbols are first-order in range, nonlinear, nonlocal, and stiff and oscillatory with a subtle fixed and movable singularity structure. Essentially the analysis and subsequent exploitation of the singularity structure with the scattering operator symbols are the focus of the direct and inverse developments. Toward the exact and approximate constructions of the operator symbols in the general inhomogeneous medium, the transversely homogeneous case is considered from now on. This problem is mathematically simpler but contains both mathematical and computational complications including the singularity structure of the multidimensional general case.

The profile in the transversely homogeneous limit is defined by

$$K^2(x, \mathbf{x}_t) = \begin{cases} K_1^2, & x \le a \\ K^2(x), & x \in [a, b] \\ K_2^2, & x \ge b \end{cases} \tag{27}$$

where K_1 and K_2 are constants and $K(x)$, $a \le x \le b$, is assumed to be smoothly continuous with the constants.

For the limiting case of the transversely homogeneous environment, the embedding equations such as (15)–(16) can be equivalently written as the operator symbol equations in the following local form. The reflection and transmission operator symbol equations are

$$\begin{aligned} (i/\bar{k})\partial_x \Omega_{\mathbf{R}^+}(x, b; p) &= 2(K^2(x) - p^2)^{1/2}\Omega_{\mathbf{R}^+}(x, b; p) \\ &\quad + (i/2\bar{k})(K(x)K'(x)/(K^2(x) - p^2)) \\ &\quad \times \left(1 - \Omega^2_{\mathbf{R}^+}(x, b; p)\right), \quad \Omega_{\mathbf{R}^+}(b, b; p) = 0, \end{aligned} \tag{28}$$

$$
\begin{aligned}
(i/\bar{k})\partial_x \Omega_{\mathbf{T}^+}(x,b;p) &= \Big((i/2\bar{k})K(x)K'(x)/(K^2(x)-p^2) \\
&\qquad +(K^2(x)-p^2)^{1/2}\Big)\Omega_{\mathbf{T}^+}(x,b;p) \\
&\qquad -(i/2\bar{k})(K(x)K'(x)/(K^2(x)-p^2)) \\
&\qquad \times \Omega_{\mathbf{R}^+}(x,b;p)\,\Omega_{\mathbf{T}^+}(x,b;p), \quad \Omega_{\mathbf{T}^+}(b,b;p)=1
\end{aligned} \tag{29}
$$

where an appropriate outgoing wave radiation condition is understood. The above symbol equations are well-posed, stiff, oscillatory Riccati systems with a fixed and movable singularity structure. The stiffness is seen to arise from the local reflections and transmissions.

Since the analysis and subsequent exploitation of the singularity structure associated with the scattering operator symbols are the essential focus of the both direct and inverse algorithm developments, the singularity structures of the operator symbols in the transversely homogeneous limit are presented here in detail. In the limiting case of a transversely homogeneous transition region, the reflection and transmission operator symbols can be written exactly in terms of the solutions of the corresponding one-dimensional, reduced Helmholtz equation and subsequently the singularity structures of the operator symbols are well identified and classified for each fixed variable x or p. To obtain these representations of the scattering operator symbols, let $u_c(x,b;p)$ and $u_s(x,b;p)$ be the solutions of the one-dimensional reduced Helmholtz equations

$$
\begin{aligned}
&\partial^2_{xx} u_{\substack{c\\s}}(x,b;p) + \bar{k}^2(K^2(x)-p^2)u_{\substack{c\\s}}(x,b;p) = 0, \\
&u_c(b,b;p)=1, \quad \partial_x u_c(b,b;p)=0, \\
&u_s(b,b;p)=0, \quad \partial_x u_s(b,b;p)=1,
\end{aligned} \tag{30}
$$

and $\psi(x,b;p)$ denotes a linear combination of these solutions defined by $\psi(x,b;p) = u_c(x,b;p) + i\bar{k}(K^2(b)-p^2)^{1/2}u_s(x,b;p)$. Then, using that in the transversely homogeneous limit $\Omega_{\mathbf{B}^{-1}}(x,b;p) = (K^2(x)-p^2)^{-1/2}$ and combining the symbolic forms of splitting equations (2)–(3) and definitions of the reflection and transmission operators result in

$$
\Omega_{\mathbf{R}^+}(x,b;p) = \frac{-\partial_x\psi(x,b;p) + i\bar{k}(K^2(x)-p^2)^{1/2}\psi(x,b;p)}{\partial_x\psi(x,b;p) + i\bar{k}(K^2(x)-p^2)^{1/2}\psi(x,b;p)}, \tag{31}
$$

$$
\Omega_{\mathbf{T}^+}(x,b;p) = \frac{2i\bar{k}(K^2(x)-p^2)^{1/2}}{\partial_x\psi(x,b;p) + i\bar{k}(K^2(x)-p^2)^{1/2}\psi(x,b;p)}. \tag{32}
$$

From the above representations (31)–(32), one can identify the singularity structure, i.e., fixed singularities (turning points, focal points, cusps, and kinks) and movable singularities (poles), of the scattering operator symbols. For fixed p, the singularities of $\Omega_{\mathbf{R}^+}(x,b;p)$ and $\Omega_{\mathbf{T}^+}(x,b;p)$ are fixed singularities and movable poles. In the case of fixed x, the singularities of $\Omega_{\mathbf{R}^+}(x,b;p)$ and $\Omega_{\mathbf{T}^+}(x,b;p)$ are weak singularities (cusps and kinks) and poles. Using the detailed singularity structure of the scattering operator symbols, one can obtain the following equivalent statements for locating the poles of the scattering operator symbols.

- For some fixed $p \geq 0$, $\Omega_{\mathbf{R}^+}(x,b;p)$ (or $\Omega_{\mathbf{T}^+}(x,b;p)$) has a pole at $x = x_0 \in [a,b]$.

- $K^2(b) \leq p^2$, $K^2(x_0) < p^2 \leq K^2_{max}$, and $\partial_x\psi(x_0,b;p) + i\bar{k}(K^2(x_0) - p^2)^{1/2}\psi(x_0,b;p) = 0$.

- **(BVP)** $K^2(b) \leq p^2$, $K^2(x_0) < p^2 \leq K^2_{max}$, and equation
$$\partial^2_{xx}u(x,b;p) + \bar{k}^2(K^2(x) - p^2)u(x,b;p) = 0, \qquad x_0 < x < b,$$
has a solution satisfying the boundary condition $\partial_x u(x_0,b;p) - \bar{k}(p^2 - K^2(x_0))^{1/2}u(x_0,b;p) = 0$ and $\partial_x u(b,b;p) + \bar{k}(p^2 - K^2(b))^{1/2}$ $u(b,b;p) = 0$.
- **(EVP)** $K^2(b) \leq p^2$, $K^2(x_0) < p^2 \leq K^2_{max}$, and equation
$$\partial^2_{xx}v(x,b;p) + \bar{k}^2(\tilde{K}^2(x) - p^2)v(x,b;p) = 0, \qquad -\infty < x < \infty,$$
has a solution satisfying $v(x,b;p) \to 0$ as $x \to -\infty$ and $v(x,b;p) \to 0$ or $u(b,b;p)$ (depending on whether $K_b^2 < p^2$ or $K^2(b) = p^2$) as $x \to \infty$, where $\tilde{K}$ is a smooth extension of K with constants on the intervals $-\infty < x < x_0$ and $b < x < \infty$.

From the Riccati equations of the reflection and transmission operator symbols, the residues of the operator symbols $\Omega_{\mathbf{R}^+}(x,b;p)$ and $\Omega_{\mathbf{T}^+}(x,b;p)$ are given by

$$\begin{aligned}\Omega_{\mathbf{R}^+}(x,b;p) = 2\frac{K^2(x_0) - p^2}{K(x_0)K'(x_0)}\Big\{\frac{1}{x - x_0} - \Big(i\bar{k}\sqrt{K^2(x) - p^2} \\ + \frac{1}{2}\Big(\frac{KK'}{K^2 - p^2}\Big)'\frac{K^2(x) - p^2}{K(x)K'(x)}\Big)_{x=x_0} + \cdots\Big\},\end{aligned} \tag{33}$$

$$\begin{aligned}&\Omega_{\mathbf{T}^+}(x,b;p) \\ &= \tau_0\Big\{\frac{1}{x - x_0} + \Big(\frac{3}{2}\frac{K(x)K'(x)}{K^2(x) - p^2} - \frac{1}{2}\frac{(KK')'}{K(x)K'(x)}\Big) + \cdots\Big\},\end{aligned} \tag{34}$$

where $\partial_x\psi(x_0,b;p)+i\bar{k}(K^2(x)-p^2)^{1/2}\psi(x_0,b;p)=0$ and $\tau_0=2(K^2(x_0)-p^2)/K(x_0)K'(x_0)\psi(x_0,b;p)$.

In conjunction with the singularity structure, as a final remark, it would be interesting to study the deeper mathematical connections between the scattering operator symbols and asymptotics, spectral theory, Sturm-Liouville theory, etc. For example, Sturm-Liouville theory can relate to the number of poles of the scattering operator symbols; this theory, indicating that $\psi(x,b;p)$ has zeros only a finite number of times, implies that if there are an infinite number of poles of the reflection/transmission operator symbols, then the limit point should be either a turning point or a point where $(d/dx)K^2(x)=0$ under the assumption that there are only finite number of zeros of $(d/dx)K^2(x)$ and finite number of turning points.

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