ONE-WAY WAVE EQUATION MODELING IN TWO-WAY WAVE PROPAGATION PROBLEMS

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The exact, well-posed, one-way reformulation of Helmholtz-type wave equations and the generalized Bremmer coupling series are applied to the two-way, scalar, multidimensional Helmholtz equation of mathematical physics. These two constructions provide complementary ways of incorporating one-way wave equation modeling into two-way wave propagation problems. The mathematical framework, for the explicit representation of the appropriate wave propagation operators, one-way wave equations, propagators (fundamental wave field solutions), and computational algorithms, follows upon exploiting the correspondences between the classical wave propagation problem, quantum mechanics, and microlocal analysis. Subsequent detailed, exact and uniform asymptotic constructions, which require going beyond the available results in both the quantum mechanical and microlocal analysis literatures, ultimately provide theoretical insight and computational viability to this approach.

1 Introduction

One-way wave equation modeling plays a prominent role in seismo-acoustic wave propagation and inversion, for example. In this modeling, characterized by complex, layered environments, extending over many wavelengths, it is particularly appropriate to consider a basic scattering picture and subsequent factorization (or wave field decomposition) of the governing, fixed-frequency, two-way wave equation. This is the starting point for both (1) the construction and application of the generalized Bremmer coupling series and (2) the exact, well-posed, one-way reformulation of two-way, Helmholtz-type, wave propagation problems. At the simplest level, the well-known, square-root Helmholtz operator (in the space-frequency domain) is the central object in the generalized Bremmer coupling series. It provides for the construction of the right- and left-traveling wave field components, and, in exponentiated form, represents the formal, fundamental, one-way wave field solution, or propagator, in the tracking of the multiple scattering in the generalized Bremmer coupling series. Clearly, this operator provides for the exact, one-way wave equation in transversely-inhomogeneous (range-independent) environments, and, further, serves as the basis for approximate, one-way wave equations in weakly range-dependent environments. The exact, well-posed, one-way reformulation is accomplished in terms of appropriate Dirichlet-to-Neumann (DtN) operators that provide the desired extension, of the square-root Helmholtz operator, in the range-dependent case. The original, two-way Helmholtz equation, which is ill-posed for the simultaneous marching of the total wave field and its normal derivative in the range direction, is transformed into one-way equations, on the DtN operators and the total wave field, which are successively marched, in a well-posed manner, in opposite directions, to solve the two-way problem. While the generalized Bremmer coupling series accounts for the internal reflections and transmissions through a “multiple sweep” algorithm, the DtN formulation requires only a “single sweep” of the total wave field in the range direction. The complete internal scattering information is contained in the DtN operators.

The initial, formal operator approaches, of both the generalized Bremmer coupling series and the DtN operator reformulation, are made explicit through the application of phase space and path integral methods, which are recognized to provide an appropriate framework to generalize Fourier methods to extended inhomogeneous environments. Underlying these constructions are the correspondences and interplay between the classical wave propagation problem, quantum mechanics, and microlocal analysis. This synthesis of ideas produces explicit representations and defining equations for the appropriate wave propagation operators, one-way wave equations, fundamental wave field solutions (propagators), and marching computational algorithms, in the natural phase space setting. The path integral representations express the fundamental wave field solutions as infinite-dimensional integrals. Historically, similar constructions were previously employed by Wiener, in his study of Brownian motion, and by Feynman, in his reformulation of quantum mechanics. The focus of the analysis is now the relevant operator symbols, which are appropriate transforms of the corresponding operator kernels. Exact and uniform asymptotic constructions of the square-root Helmholtz and DtN operator symbols provide for a theoretically effective and computationally relevant approach to one-way wave equation modeling. These constructions require going beyond the corresponding results in the quantum mechanical and microlocal analysis literatures. Finally, in a complementary manner, coordinate space path integral representations for the general, two-way Helmholtz equation can be considered.

2 One-way wave equation modeling

Seismo-acoustic environments are typically multidimensional, complex, layered environments, distinguished by an inhomogeneous background. This is not an obstacle imbedded in a homogeneous background! The problems of interest are generally large scale, involving strong scattering over many wavelengths, often characterized by both focusing and defocusing regimes. Even the well-known, two-dimensional, variable velocity, constant density, Marmousi model, in seismic wave propagation and inversion, is still, despite the numerous modeling simplifications, a challenging problem, with its fine layering, range of velocities (1,500 – 4,500 m/s), reservoir, etc.

Such environments can be modeled in the context of a basic scattering picture. Consistent with the modeling level of the Marmousi model, the governing wave equation is taken to be the *d*-dimensional, scalar, fixed-frequency Helmholtz equation. The wave propagation problem is modeled as a general radiation formulation, with the Euclidean space partitioned into three contiguous regions with respect to the global propagation, or range, coordinate: left and right transversely-inhomogeneous half spaces connected by a generally-variable transition region. With the source located in the transition region, energy radiates outward from the transition region, propagating one-way in each of the transversely-inhomogeneous half spaces. This model is detailed in (FISHMAN, 1993; FISHMAN *et al.,* 1997; FISHMAN, 2002).

A scattering block decomposition can now be conceptually applied to the general radiation formulation. The three-region model is naturally decomposed into two, individual scattering block problems, to the right and left of the source plane, respectively, the solutions of which must, ultimately, be "glued" together correctly to account for the multiple scattering between the two blocks (FISHMAN *et al.,* 1997; FISHMAN, 2002). This essentially reduces the Helmholtz radiation problem to the fundamental scattering problem of a wave field reflecting and transmitting from a generally-variable block imbedded in a transversely-inhomogeneous background environment (FISHMAN, 1993).

The fundamental, Helmholtz scattering problem is, however, global: in general, the determination of the wave field at a given point requires the computation of the wave field everywhere in the relevant domain. This issue is discussed in greater computational detail in (FISHMAN *et al.,* 1997), where the need to incorporate marching (one-way) methods into the solution algorithm, for the inherently two-way, "elliptic wave propagation" problem for large-scale ocean, atmospheric, and seismic wave propagation problems, is clearly appreciated. The simplest, and most obvious, approach is to recast the original Helmholtz equation in its first-order (initial-value) formulation given in Eq. (2) in (FISHMAN, 1993). The subsequent simultaneous marching of the wave field and its normal derivative provided the impetus for the development of the so-called "marching elliptic methods" (FISHMAN *et al.,* 1997), which generally require (1) the back propagation of a backward wave field component and (2) the knowledge of both the wave field and its normal derivative on the initial plane. The first requirement leads to an ill-posed problem, requiring a regularization that effectively filters out the evanescent portion of the spectrum or a stability requirement that ultimately limits the spatial resolution. The second requirement leads to non-independent initial data. Thus, the simplest, and most obvious, way to incorporate one-way wave equation modeling into the two-way Helmholtz model will not be appropriate for the complex environments encountered. What is needed is an approach for the "elliptic wave propagation" problem that can exploit marching (one-way) methods as much as possible, in a well-posed manner, while formulated in terms of the correct initial data.

Given the basic scattering picture of the wave propagation problem, it is reasonable to require that any appropriate one-way marching approaches must explicitly incorporate the kinematically correct physics of the envisioned scattering experiment. This is accomplished through the application of directional wave field decomposition. Directional wave field decomposition essentially decomposes the total wave field into right- and left-traveling components, which represent the exact, physical, decoupled, one-way wave fields in a transversely-inhomogeneous environment (the half spaces), while only providing for a coupled, mathematical representation of the total wave field in a generally-variable environment (the transition region). This, in effect, kinematical scattering transformation defines the right- and left-traveling wave field components in terms of the total wave field, its normal derivative, and the square-root (and inverse square-root) Helmholtz operators, as expressed in Eqs. (3), (4), and (7) in (FISHMAN, 1993). This, then, results in an equivalent Helmholtz formulation given in Eq. (5) in (FISHMAN, 1993). In transversely-inhomogeneous regions, this coupled system decouples into the independent, one-way wave equations in terms of the square-root Helmholtz operator, as illustrated in Eq. (6) in (FISHMAN, 1993). While the kinematically correct scattering picture has been explicitly incorporated, this reformulation is still ill-posed for marching in the range direction and requires non-independent initial data. While you cannot simultaneously march the total wave field and its normal derivative in the range direction, in a well-posed manner, neither can you simultaneously march the right- and left-traveling wave field components in the range direction, in a well-posed manner. So far, only the geometrically correct picture of the scattering experiment has been explicitly incorporated into the mathematical formulation; it remains to construct the well-posed, one-way approaches with the correct initial data.

Two complementary, well-posed, one-way reformulations, of the two-way Helmholtz wave propagation problem, accounting for the correct initial data, will be considered: (1) the construction and application of the generalized Bremmer coupling series and (2) the exact, well-posed, one-way reformulation of two-way, Helmholtz-type, wave propagation problems. Both of these approaches start from the fundamental scattering problem.

In his original formulation, Bremmer considered a right-traveling wave field impinging upon a scattering block imbedded in a homogeneous background (BREMMER, 1951). The analysis was restricted to the one-dimensional case. Decomposing the "block" into, for example, homogeneous sections (piecewise-constant modeling), and accounting for the detailed local scattering (reflection and transmission) at all of the encountered interfaces and the exact, one-way wave propagation within the sections, the total wave field is written as a series of terms, ordered by the total number of reflections suffered during the path. The first term, representing all transmissions and zero reflections, corresponds to the WKB approximation, although the series is distinct from the high-frequency asymptotic series, even converging under appropriate conditions. Terms representing an even number of reflections correspond to a transmitted component of the total wave field, while terms representing an odd number of reflections correspond to a reflected component of the total wave field. Moreover, this wave field series was shown to correspond to a wave field decomposition based on the assumed environmental model chosen in the sectional (block) decomposition. In starting with the incoming (right-traveling) wave field, and following the local scattering and subsequent, exact, one-way wave propagation throughout the block, the Bremmer series is well-posed and consistent with the correct initial data.

In his multidimensional generalization of the Bremmer series approach, de Hoop started from the equivalent Helmholtz formulation in Eq. (5) in (FISHMAN, 1993), treating (1) the exact, diagonal, one-way component of the matrix operator as the principal part of the scattering/propagation process and (2) the remaining, local scattering (reflection and transmission), coupling component as a perturbation (DE HOOP, 1996). Introducing the one-way Green's functions (propagators) associated with the principal part of the Helmholtz operator, transforming to an equivalent integral equation formulation, and appropriately iterating then result in a Born-Neumann series representation for the wave field components. As in Bremmer's original one-dimensional construction, this generalized Bremmer coupling series is well-posed and consistent with the initial data. By following the "multiples" in the original wave field, this approach effectively "traces" the wave constituents, providing the "wave tracing" extension of the geometrical method of "ray tracing."

While the generalized Bremmer coupling series approach follows the detailed, local scattering and propagation of the wave field in the medium, the exact, well-posed, one-way reformulation of Helmholtz-type wave equations directly addresses the scattering from the global block through the introduction of a scattering matrix in terms of the block reflection and transmission operators, as illustrated in Eq. (8) in (FISHMAN, 1993). Invariant imbedding techniques (FISHMAN, 1993) then enable the derivation of the scattering (reflection and transmission) operator equations, transforming a two-point, boundary-value problem on the wave field into an initial-value problem on the scattering operators. This is the key step in the construction of the well-posed marching method. The resulting system of operator Riccati equations is given in Eqs. (11)-(17) in (FISHMAN, 1993). Subsequent transformation from the scattering picture, in terms of the right- and left-traveling wave field components, to the boundary-value picture, in terms of the total wave field and its normal derivative, then naturally introduces the DtN operators, and the one-way wave equations appropriate for marching the total wave field. A DtN operator simply transforms wave field data into normal derivative data on a "boundary," which, in this case, is the front face of the appropriate transition region. The two, fundamental, scattering block solutions, from the original scattering block decomposition, are then "glued" together to account for the block multiple scattering.

The final result of the construction is summarized in Eqs. (2)-(11) in (FISHMAN *et al.,* 1997), with the corresponding fundamental solution (propagator) represented by a product integral in Eqs. (15) and (16). Equations (2), (3), and (6)-(10) are essentially equivalent to an exact factorization of the Helmholtz equation in the general case. The one-way wave equations (2) and (3), for the total wave field, generalize the one-way wave equation (6) in (FISHMAN, 1993) to the range-dependent case. This exact reformulation of the Helmholtz radiation problem is a particular mathematical realization of a double-sweep method. The original, two-way Helmholtz equation, which is ill-posed for the simultaneous marching of the total wave field and its normal derivative in the range direction, is transformed into one-way equations, on the DtN operators and the total wave field, which are successively marched, in a well-posed manner, in opposite directions, to solve the two-way problem. The initial, equivalent, scattering picture establishes the physical content of the reformulation expressed in Eqs. (2)-(11). The first sweep, constructing the DtN operators as expressed in Eqs. (6)-(9), effectively solves a series of "fictitious internal scattering problems" that the wave field encounters on propagating into the block. The solution of these internal scattering problems exactly decouples the wave field components, leading to the one-way wave equations. The solution of the block multiple-scattering problem, which establishes the initial total wave field, is given in Eq. (11) concisely in terms of the DtN operators, and accounts for all of the reflections between the two blocks. The subsequent, one-way marching procedure, in Eqs. (2) and (3) of the second sweep, is well-posed because the solution of the internal scattering problems, encountered by the propagating wave field, eliminates the ill-posed back propagation required to simultaneously march the total wave field and its normal derivative. Moreover, the initial data is consistent with the final, one-way wave equations.

For the Helmholtz radiation problem, the one-way wave equations provide for the, in principle, exact marching of the total wave field to both the right and left of the source. Once the DtN operators have been determined and the initial total wave field subsequently constructed, a single sweep (marching) in the range direction completely accounts for all of the internal reflections and transmissions normally associated with the multiple sweeps in the generalized Bremmer coupling series. The DtN operators contain all of the relevant information in the range-dependent problem, which accounts for their role in the exact reflecting boundary conditions in Eqs. (4) and (5) in (FISHMAN *et al.,* 1997).

To summarize, to this point, two complementary, formal operator approaches, to the well-posed incorporation of one-way (marching) methods into two-way, Helmholtz-type wave propagation problems, have been briefly discussed. The generalized Bremmer coupling series approach focuses on the square-root Helmholtz propagation operator, the one-way wave equation in terms of this operator, and the corresponding fundamental wave field solution (propagator), essentially the exponential of this operator (FISHMAN and MCCOY, 1984a, 1984b, 1984c; FISHMAN *et al.,* 1987). This approach follows the local wave scattering within the medium, essentially tracing the wave constituents, resulting in a multiple-sweep computational algorithm ("wave tracing"). The DtN operator reformulation focuses on the DtN propagation operator, the one-way wave equation in terms of this operator, and the corresponding fundamental wave field solution (propagator), essentially the product-integral associated with the exponential of this operator (FISHMAN *et al.,* 1997; FISHMAN, 2002). This approach constructs the scattering operators for the global block, incorporating the complete internal scattering information into the DtN operator, resulting in a single-sweep computational algorithm on the total wave field.

The task, now at hand, is to construct explicit representations of these formal propagation operators, formal one-way wave equations, and corresponding, formal fundamental solutions (propagators).

3 Phase space and path integral methods

3.1 Homogeneous medium

Before addressing the general, explicit operator constructions, it is useful to see how much insight can be obtained with a minimal effort. In other words, just what can be learned from the simplest possible case, namely, the homogeneous half space? The specific forms, of the one-way wave equation, path integral representation of the propagator, and marching computational algorithm, follow directly from Fourier (optics) analysis.

The one-way wave equation, given in Eq. (3) in (FISHMAN *et al.,* 1987), establishes that, even in the homogeneous case, the wave equation is nonlocal. This is the price paid for decomposing the two-way, local equation into its independent, one-way forms. The phase space path integral representation, given in Eq. (8) in (FISHMAN *et al.,* 1987), follows from a Hankel function identity, and immediately results in the marching computational algorithm given in Eq. (12) in (FISHMAN *et al.,* 1987). The prominent role of the square-root function is noted. While the homogeneous half space is a trivial case, the forms of these constructions will turn out to be remarkably robust, essentially holding true all the way through the generally-variable environment case corresponding to the DtN operator.

3.2 Classical waves, quantum mechanics, and microlocal analysis

At the simplest level, the initial problem is to provide the proper meaning for an operator that is a nontrivial function of two non-commuting operators. The square-root Helmholtz operator is the specific example. Subsequently, the exponential of this operator must be explicitly constructed. Both of these constructions have a long history in the development of both quantum mechanics and microlocal analysis, and it is, ultimately, the correspondences between the classical wave propagation problem, quantum mechanics, and microlocal analysis that are exploited to construct the appropriate mathematical framework.

In the quantum mechanical context, the obvious correspondences, between the time-independent (fixed-energy), multidimensional, Schrödinger equation of non-relativistic quantum mechanics and the fixed-frequency, multidimensional, scalar, Helmholtz equation, which is ubiquitous in classical wave propagation modeling, have been known since the first appearance of the quantum mechanical wave equation more than seventy-five years ago. Since then, these correspondences have been repeatedly noted and (at least superficially) exploited in virtually every applied classical field, including acoustics, electromagnetics, optics, and seismics. This, however, is initially misleading. At the simplest level, the relevant one-way wave equation is the one-way Helmholtz equation, in terms of the formal, square-root Helmholtz operator, given in Eq. (11) in (FISHMAN, 2002). Thus, the appropriate correspondence in quantum mechanics is not with the time-independent Schrödinger equation, but, rather, with the time-dependent Schrödinger equation corresponding to a Hamiltonian that is a nontrivial function of two non-commuting operators (in this case, the square root of the transverse Helmholtz operator). In this correspondence, the global, principal propagation, or range, coordinate is the "time-like" variable.

In the quantum mechanical literature, formal operator representation methods, rooted in phase space, were developed, starting from the classical Hamiltonian, and accounting for the operator-ordering issue. These formal representations were adapted for the construction of the square-root Helmholtz operator in the classical setting. A detailed presentation of these constructions, along with a discussion of the subtle differences between the "quantization" and the square-root Helmholtz operator construction problems, are given in (FISHMAN and MCCOY, 1984a, 1984c; FISHMAN *et al.,* 1987), where many literature citations can be found. Moreover, the operator construction procedures, in the quantum mechanical development, enable for the propagator, or fundamental solution of the wave equation, to be expressed by a formal, phase space, path integral representation, supplementing the long history of the role of path integrals in quantum mechanics initiated by Feynman in 1948. The phase space, path integral constructions were immediately adapted for the classical wave propagation formulations, the details of which are discussed in (FISHMAN and MCCOY, 1984b, 1984c; FISHMAN *et al.,* 1987).

Furthermore, the formal operator construction methods from the quantum mechanical literature, which were adapted for the classical formulations, are naturally associated with the development of pseudodifferential and Fourier integral operators from the mathematical theory of microlocal analysis. This theory, developed over the past half century, provides a rigorous mathematical foundation for much of the formal asymptotic calculations found in applied wave propagation modeling, and directly addresses the characterization and approximation of the operators occurring in the general quantum mechanical formulations. The pseudodifferential and related Fourier integral operators provide the primary tools for the quantization and, subsequent, representation of classical dynamical systems (see the references cited in (FISHMAN *et al.,* 1987, 2000), for example). The final result is that the formal, one-way Helmholtz wave equation (11) in (FISHMAN, 2002) can be explicitly written in the form of Eq. (12), with the propagator expressed as a phase space path integral, as given in Eqs. (14) and (15). The principal quantity of interest is the square-root Helmholtz operator symbol, which is explicitly defined through the composition equation (13), supplemented with a right-traveling-wave radiation condition. Equations (12)-(15) in (FISHMAN, 2002) summarize an important mathematical connection between the "factorization, phase space, and path integral approach" to classical wave propagation modeling, quantum mechanics, and the modern mathematical theory of "asymptotics." From this viewpoint, the square-root Helmholtz operator symbol plays a role analogous to that of the classical Hamiltonian in the construction of quantum mechanical theories. It is this three-way interrelationship that provides the driving force behind the current seismic inversion work discussed in (FISHMAN, 2002).

In the simplest case of the square-root Helmholtz operator, the operator has a simple, explicit, formal, functional operator representation. This is no longer true in the general case corresponding to the DtN operator. Nonetheless, the one-way wave equation, corresponding composition-type equation, and path integral representation of the propagator, given, respectively, in Eqs. (12), (13)-(14), and (17)-(18) in (FISHMAN *et al.,* 1997), follow from the general mathematical framework, based on the three-way correspondences, discussed above. The composition-type equation in (13)-(14) provides the explicit statement of the formal operator Riccati equation, while the path integral representation in (17)-(18) correctly accounts for the proper ordering of the infinitesimal propagators in the product-integral definition, in this range-dependent case (see Eqs. (15)-(16) in (FISHMAN *et al.,* 1997)).

For the cases of both the square-root Helmholtz and DtN operators, the subsequent, one-way, phase space, marching computational algorithm is based upon (1) the marching range step (following from the path integral representation), (2) a detailed, uniform, operator symbol analysis (reflecting the study of the appropriate composition-type equation), and (3) Fourier component, or wave number, filtering in phase space (for increased efficiency, decreased computational time, and reduced error). The computational algorithm is discussed in detail in Section II in (FISHMAN *et al.,* 1987). Computing Helmholtz equation wave fields as high (in principle, infinite)-dimensional integrals is in sharp contrast to the more traditional finite-difference and finite-element numerical algorithms.

Reviewing the specific forms of the one-way wave equations, path integral representations, and the marching computational algorithm referenced above, it is apparent that the basic structural forms, appropriate in the homogeneous medium limit, hold up remarkably well in the inhomogeneous environments. The complication is primarily in the increasingly more complex structure associated with the relevant operator symbols.

To summarize: the basic mathematical framework, needed for the explicit operator constructions in the classical wave propagation problem, follows from the correspondences between classical waves, quantum mechanics, and microlocal analysis. The primary aim of the pseudodifferential and Fourier integral operator theory is to extend classical Fourier analysis of homogeneous media to inhomogeneous environments. Indeed, this approach can be viewed as a natural extension of the theory of partial differential operators with variable coefficients. The principal focus is on the operator symbol, which contains the complete spectral information in just the appropriate manner to lead immediately to the desired infinitesimal propagator. Essentially, the singular operator (kernel) calculus is replaced by a calculus for well-behaved functions (operator symbols). Moreover, operator symbols are a natural quantity to study. For example, they furnish the "generalized vertical slowness" in geophysics, the natural multidimensional extension of the scattering (reflection and transmission) coefficients in the one-dimensional formulation, and the suitable framework to quantize (semi-) classical theories in quantum physics. While the square-root Helmholtz operator symbol plays a role analogous to that of the Hamiltonian in the quantization of classical dynamical systems, its properties deviate in a significant way from most dynamical Hamiltonians. This, shortly, will be seen to have profound ramifications in the subsequent asymptotic analysis.

At this point, the situation is the following. The constructions of both the square-root Helmholtz operator and the corresponding fundamental solution of the governing, one-way Helmholtz wave equation have now been transformed into the mathematical construction of exact (whenever possible) and uniformly (over phase space) approximate (in general) solutions of the composition equation (13) in (FISHMAN, 2002) for the relevant operator symbol. For the more general case of the DtN operator and corresponding propagator constructions, the relevant composition-type equation is (13)-(14) in (FISHMAN *et al.,* 1997).

Given the important interrelationships between the classical formulation, quantum mechanics, and modern "asymptotics" stressed above, it might be reasonably hoped that the desired, general, uniformly approximate solutions simply could be adapted from the existing quantum mechanical and microlocal analysis literatures.

In the quantum mechanical context, the classical wave field decomposition into both left- and right-traveling components, along with the subsequent (in general, approximate) factorization of the original, two-way Helmholtz wave equation, are most closely related to the approximate diagonalization of the relativistic Klein-Gordon (K-G) wave equation, via a systematic application of the Foldy-Wouthuysen (F-W) transformation (FISHMAN and MCCOY, 1984a, 1984c; FISHMAN *et al.,* 1997). For the K-G case, with time-independent vector and scalar potentials, this diagonalization (factorization) is, in principle, exact, corresponding to the, in principle, exact factorization of the two-way Helmholtz wave equation for transversely-inhomogeneous (range-independent) environments. For the simplest K-G formulation, given in Eq. (31) in (FISHMAN, 1992), it is seen in Eq. (32) that the relevant square-root operator differs from the square-root Helmholtz operator by "only the sign" between the two operator terms inside the square root. Thus, from the purely formal perspective, it might be hoped that the F-W analysis can be applied directly to the Helmholtz equation to produce the desired uniform constructions. Exploiting the connections between quantum mechanics and microlocal analysis, however, reveals that the results of the formal F-W analysis, in relativistic quantum theory, are actually a limiting case of the rigorous mathematical theory. Thus, the question of constructing uniformly approximate representations of the square-root Helmholtz and DtN operator symbols, via a relatively easy adaptation from the existing literatures, is reduced to the applicability of the elliptic pseudodifferential operator calculus (from the rigorous mathematical theory) to the Helmholtz formulation.

From the outset, this modern theory of "asymptotics" is about approximation in a well-defined sense; only part of the solution is retained. The theory of pseudodifferential operators expands the operator symbol in orders of smoothness, essentially resulting in a series of algebraic terms of increasing degree of smoothness. Nested within this smoothness expansion is a dual, implicit, "high-frequency" expansion in terms of a small, dimensionless parameter measuring the medium variation on the wavelength scale. This asymptotic development completely neglects the infinitely-smooth contributions of exponential order (FISHMAN *et al.,* 1997). For hyperbolic wave propagation problems, such as the time-domain, plasma, and Klein-Gordon wave equations, for the corresponding square-root (and, more generally, Dirichlet-to-Neumann (DtN)) operators, there is a rigorous, asymptotic machinery, which is what, ultimately, justifies much of the purely formal operator manipulations. The neglected part of the solution can be shown to be appropriately small in a well-defined sense, resulting in uniform operator symbol approximations for the hyperbolic wave propagation problems (see the discussion surrounding Eqs. (31)-(34) in (FISHMAN, 1992), for example).

In the case of the Helmholtz-type (the so-called "elliptic") wave propagation problems, however, the discarded part of the solution, in the mathematical asymptotic theory, plays a key role, which must be taken into account. This sharp distinction between the applicability of the mathematical asymptotic analysis in the K-G and Helmholtz cases should not be surprising. Physically, hyperbolic wave equations, such as the K-G, are about the propagation of singularities (i.e., wave fronts), as is microlocal analysis, while the Helmholtz equation is about smoothing, characterized by the nonpropagating, evanescent spectral components. (This is the previously mentioned difference between the square-root Helmholtz operator symbol and most dynamical Hamiltonians. Dynamical Hamiltonians generally correspond to self-adjoint operators, whereas the square-root Helmholtz and DtN operators, for the appropriate one-way wave equations, are not self-adjoint, owing to the "elliptic" part of the wave propagation problem.) Application of the elliptic pseudodifferential operator calculus, to the approximate solution of the Helmholtz, Weyl composition equation (13) in (FISHMAN, 2002), will necessarily result in a nonuniform, singular (over phase space), operator symbol approximation (FISHMAN *et al.,* 1997). This is illustrated in Eqs. (24)-(26) and Figs. (2)-(6) in (FISHMAN *et al.,* 1997), where it is seen that the pseudodifferential operator symbol expansion is appropriate in a properly defined, "outer" phase space region. In the corresponding "inner" phase space region, the neglected terms of exponential order can be of comparable size to, or dominate, the leading, nonsingular, algebraic contribution, and, thus, a properly constructed, uniformly valid, high-frequency operator symbol expansion, for the square-root Helmholtz operator, for example, must account for the appropriate contributions from the infinitely-smooth terms.

Uniformly approximate constructions, of the square-root Helmholtz and DtN operator symbols, inherently require going outside of the elliptic pseudodifferential operator calculus and beyond any of the direct results from quantum mechanics. The desired explicit constructions, in the classical wave propagation problem, do not follow directly from the existing literatures.

3.3 Beyond quantum mechanics and microlocal analysis

Despite the above-mentioned limitations, of the mathematical asymptotic theory and the examples from the quantum mechanical literature, to directly address the classical, one-way wave theory development, results from quantum mechanics can be applied to produce the desired exact and uniformly approximate, operator symbol constructions. This allows, in some sense, for the three-way interrelationships to come "full circle."

The square-root Helmholtz operator symbol can be constructed in terms of spectral (modal) summations and contour integral representations in the complex plane. The general construction procedure extracts the operator symbol from the Helmholtz Green's function, proceeding through the inverse square-root Helmholtz operator symbol and appropriate composition equation, as outlined in Eqs. (16)-(20) in (FISHMAN, 2002). Well-known, exact solution cases from nonrelativistic quantum mechanics (and standard spectral theory) then lead to the construction of exact, square-root Helmholtz operator symbols in several cases. The relationship between the square of the refractive index field, in the classical formulations, and the potential energy function, in the quantum formulation, is well known, and has been discussed, in the present context, in the general case (FISHMAN and MCCOY, 1984b, 1984c; FISHMAN *et al.,* 1987), and in specific cases (Refs. [2] and [45] in (FISHMAN, 1992); Refs. [1], [40], [64], and [66-67] in (FISHMAN *et al.,* 1997); Refs. [4], [28], and [53-58] in (FISHMAN *et al.,* 2000); FISHMAN, 2002).

For the exactly soluble cases, spectral (modal) summation, operator symbol representations follow immediately from the well-known, complex Dunford integral representation, the standard bilinear product Green's function representation, the definition of the operator symbol, and the appropriate composition equation, as discussed in Sections I and II in (FISHMAN *et al.,* 2000) for the case of the focusing quadratic profile. Equations (II.50) and (II.51) represent typical results for this case.

These obvious operator symbol representations can, however, be complemented by complex, contour integral representations, which are especially appropriate for complex frequency, asymptotic, and analytic continuation applications and extensions. For the specific case of the focusing quadratic profile, the starting point is the imbedding of the desired Helmholtz Green's function in a (time-dependent) Schrödinger formulation in one-higher dimension (i.e., the integral relationship (transmutation) connecting the Helmholtz and Schrödinger equations, known in the path integral literature as the Feynman-Fradkin representation), given by Eqs. (III.11)-(III.13) in (FISHMAN *et al.,* 2000). Repeatedly exploiting the periodicity of the underlying Schrödinger (quantum mechanical) harmonic oscillator solution results in the representations summarized in Eqs. (31) and (32) in (FISHMAN, 2002), and the unification, via analytic continuation arguments, of the focusing (FISHMAN *et al.,* 2000) and defocusing (FISHMAN, 1992) quadratic profile cases presented in (FISHMAN *et al.,* 2000). Figures 2-4 in (FISHMAN, 2002) contain pictorial realizations of the exact, square-root Helmholtz operator symbols for both the focusing and defocusing quadratic profile cases.

For the specific cases of the Dirac delta, discontinuity (two-layer), and three-layer composite profiles, the starting point is the imbedding of the desired Helmholtz Green's function, restricted to the source plane, in a Helmholtz-type formulation in one-lower dimension, expressed through Eqs. (40) and (41) in (FISHMAN *et al.,* 1997). In (FISHMAN, 2002), Eqs. (35)-(37) present specific square-root Helmholtz operator symbol formulas, while Figs. 5-12 illustrate the operator symbol surfaces in the three cases. Particularly striking is the comparison between the exact and pseudodifferential operator expansion constructions presented in Figs. (6)-(7) and (9)-(10), respectively, for the discontinuity and three-layer profile cases. The standard asymptotic results are clearly unable to capture the detailed oscillatory and correct singularity structure associated with the operator symbol surface. Figure 11 illustrates the operator symbol surface transition from the high- to low-frequency limit, for the three-layer profile case.

These contour integral representations, for the square-root Helmholtz operator symbols, have been transformed to corresponding representations for the Helmholtz Green's function on the source plane, establishing new results in both the quantum mechanical and mathematical literatures, and, further, finding application in time-reversal mirror calculations in the context of one-way wave equations (DE HOOP *et al.,* 2003).

While exact operator symbol constructions are quite valuable in illustrating the detailed mathematical theory and providing benchmark cases for approximate operator symbol constructions, the development of an exact, insightful, operator symbol representation for general profiles is quite unlikely. Ultimately, physical applications must depend upon asymptotic results. In (FISHMAN *et al.,* 1997), it is demonstrated how the well-known WKB approximation in quantum theory can be combined with (1) function theoretic arguments from complex and Fourier analysis and (2) matched asymptotic expansion techniques to generate a uniform asymptotic expansion of the square-root Helmholtz operator symbol in the high-frequency limit.

The starting point of the derivation is the operator symbol identity given in Eq. (28) in (FISHMAN *et al.,* 1997). Application of the previously mentioned imbedding of the Helmholtz Green's function, restricted to the source plane, in a Helmholtz-type formulation in one-lower dimension then results in the operator symbol representation given in Eq. (43). In removing the turning, focal, and higher-order singular points, in the lower-dimensional Helmholtz Green's function, from the integration range in the Eq. (43) representation, the construction enables the subsequent application of the WKB approximation to lead to a uniform result. Finally, the application of the stationary phase approximation and the method of matched asymptotic expansions lead to the result summarized in Eqs. (39)-(42) in (FISHMAN, 2002). This uniform, high-frequency, square-root Helmholtz operator symbol approximation recovers the homogeneous medium, pseudodifferential operator, and high-frequency limiting forms, in addition to recovering the pseudodifferential operator expansion appropriate in the "outer" phase space region and both the algebraic and oscillatory, asymptotic branches, of the exact operator symbol, for the defocusing quadratic profile in the high-frequency limit. Figures 7-11 in (FISHMAN *et al.,* 1997) illustrate the range of validity and manner of breakdown for this asymptotic result in a comparison with the exact operator symbol, for the defocusing quadratic profile, for wave numbers ranging over two orders of magnitude. This derivation inherently includes the appropriate contributions from the terms of exponential order (the contributions from the infinitely-smooth part of the kernel) neglected in the application of the elliptic pseudodifferential operator calculus, resulting in a nonsingular, uniform (over phase space) expression, characterized by both an algebraic and an oscillatory (exponential) component.

The uniform asymptotic, operator symbol approximations are the key quantities for applications in direct and inverse wave propagation modeling. The high-frequency, approximate wave theory, based on the uniform, high-frequency operator symbol construction, is quite distinct from geometric, or semiclassical, approximations on the wave field. This is an extremely important point for applications. In this regard, it can be contrasted with the global, uniform, phase-space-based, asymptotic wave field constructions associated with (1) the Maslov, or Lagrangian manifold, method, which effectively exploits the Fourier transform, and (2) the Klauder method based on the coherent-state transform, as discussed in (FISHMAN *et al.,* 1997). Both the Maslov and Klauder approximate wave field constructions are essentially nonuniform, high-frequency (geometric) wave field asymptotics appropriately corrected for the variety of caustic structures inherent in the infinite-frequency approximation. The results are globally uniform wave field representations, in terms of functions, which are still inherently "high-frequency." The wave field approximation based on the uniform, high-frequency, operator symbol construction, on the other hand, is a full path (functional) integral, which, in retaining the "sum over paths" in the phase space, is a full-wave theory, free from caustic structures. Essentially, the phase functional in the path integral is uniformly approximated in the high-frequency limit. The difference between uniform, high-frequency asymptotics directly applied to the wave field and the operator symbol is, roughly, that, in the former case, the classical, high-frequency (geometric) asymptotic wave field is considered as a global solution, while, in the latter case, it is essentially considered as an infinitesimal solution, repeatedly composed to produce a global solution. The key point is that high-frequency approximations on the square-root Helmholtz operator symbol can correspond to accurate wave field regimes well outside of the geometric, or semiclassical, wave field limit. This contention is well supported by numerical computations with the primitive, high-frequency, operator symbol approximation, essentially the leading algebraic (square-root) term in the uniform expansion (FISHMAN *et al.,* 1987; FISHMAN and WALES, 1987; FISHMAN and WALES, 1988).

In so much as they lie outside of the standard mathematical framework, the exact and uniform asymptotic constructions of the square-root Helmholtz operator symbol and the corresponding path integral representations for the propagators are currently of interest to theoretical mathematicians. While in no way providing a complete and rigorous mathematical theory, these explicit constructions, however, do provide a glimpse of what such a theory, for this case, might look like. This reflects the continuing interplay between the classical wave propagation and scattering, quantum mechanical, and modern mathematical asymptotic developments.

3.4 Coordinate space path integral representations

To this point, all of the operator and path integral constructions have been considered in their natural phase space settings. From the path integral purist's perspective, however, the wave theory summarized in the phase space path integral is not entirely satisfactory. Propagation to the right and left of the source must be distinguished, and, further, the one-way, fundamental solution path integral must be applied to the initial wave field corresponding to a point source, which, itself, must be constructed from the DtN operators, as discussed in (FISHMAN *et al.,* 1997). This is a consequence of the introduction of the one-way modeling methods into the two-way Helmholtz formulation. What is, ultimately, desired is a fundamental path integral representation, rooted in the coordinate space, for the Helmholtz Green's function. This returns the emphasis to the full, two-way nature of the wave equation, providing a complementary perspective within the path integral framework. The path integral construction, in terms of a "fixed average-energy" path space, outlined in (DEWITT-MORETTE *et al.,* 1979) provides a starting point. From a more mathematically rigorous viewpoint, this stochastic-based Helmholtz construction, envisioned in (DEWITT-MORETTE *et al.,* 1979), attempts the difficult task of paralleling Wiener's treatment of the diffusion (Schrödinger) equation, and, if successful, should suggest computational algorithms, as well as providing for stochastic interpretations of the relevant pseudodifferential operators appearing in the phase space formulation. The transition from the phase space path integral representation to a suggestive coordinate space representation is illustrated, for the homogeneous medium case, in (FISHMAN and MCCOY, 1984b, 1984c; FISHMAN *et al.,* 1987).

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