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The one-way wave equation and its invariance properties

Luc Leviandier

Thales Research & Technology, Campus de Polytechnique, 91767 Palaiseau, France
and

LAUM, CNRS, Université du Maine, Av. O. Messiaen, 72085 Le Mans, France

E-mail: luc.leviandier@thalesgroup.com and luc.leviandier@univ-lemans.fr

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Abstract

The harmonic wave equation in inhomogeneous media is exactly split into coupled first-order equations with respect to a principal direction of propagation according to the Bremmer scheme. The resulting one-way wave equation is shown not to conserve energy flux for dimensions two and three against the general belief in one-way wave propagation or parabolic equation literature. Conservation of energy flux is only ensured in the high frequency limit. On the other hand, a simple invariant is found that may be seen as a generalization of the Snell law to arbitrary, non-stratified, media. Similarly, the reciprocity property is not fully ensured in general and the time-reversal symmetry is ensured for propagating fields. Besides, in the one-way wave equation, the additional term to the standard parabolic equation is shown to strengthen mode coupling. The analysis encompasses the evanescent waves.

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1. Introduction

Wave propagation in inhomogeneous media is often characterized by a principal direction of propagation. This is true, for example, for natural waveguides, either atmospheric or oceanic, where rough geophysical stratification favours acoustic or electromagnetic wave propagation in the horizontal direction. It is of course also true for acoustic propagation in ducts or slabs or for electromagnetic propagation in optical fibres or any kind of waveguides. It is then appealing to split the global field into forward and backward propagating fields obeying coupled first-order equations [1]. When the longitudinal dependence of the medium is weak, it is even possible to decouple these two waves and to consider a first-order propagation equation that is much easier to integrate than the initial second-order equation since the outgoing radiation condition is automatically satisfied [1–4]. More precisely, the three-dimensional scalar wave

field φ with angular frequency ω in the celerity field $c(x, y, z)$ obeys, apart from the sources, the Helmholtz equation

$$(\partial_{xx}^2 + \partial_{yy}^2 + \partial_{zz}^2 + k^2(x, y, z))\varphi = 0,$$

where we have introduced the wavenumber $k = \omega/c(x, y, z)$. Due to the preferred or principal direction of propagation, which we choose to be x , this equation reads better as

$$(\partial_{xx}^2 + Q)\varphi = 0, \quad (1)$$

where

$$Q(x) = k^2 + \partial_{yy}^2 + \partial_{zz}^2 = k(x_\perp, x)^2 + \nabla_\perp^2 \quad (2)$$

is the Helmholtz operator acting on functions of transverse coordinates $x_\perp = (y, z)$ and parametrically depending on the principal direction x . When the medium is invariant by translation along the x direction, the harmonic wave propagation equation is exactly factored into two one-way wave equations that are of first order in x , $\partial_x \phi = \pm i Q^{1/2} \phi$. The square root operator appearing in each of these equations is generally evaluated using spectral methods, for example a modal decomposition. When the medium is no more invariant by translation in the x direction but slowly varying with x , it is appealing to modify the previous method in order to retain the ease of integration of the first-order equation. This leads on the one hand to the forward coupled modes theory [1] and on the other hand to the so-called parabolic equation methods [2, 3] (also known as the beam propagation method in optics). In the latter case, the square root operator is made explicit using paraxial approximation. This approximation consists of polynomial or preferably Padé expansions of the infinitesimal generator [5], or of the propagator itself [6], with respect to some *ad hoc* small parameter. An alternative is to construct a square root Helmholtz operator using standard or Weyl symbols of pseudo-differential operator calculus [7]. The coefficients of the one-way wave equation obtained are then updated along the x direction. It has long been recognized that this procedure was ineffective for severe range dependence of the medium, and various methods have been proposed to correct the parabolic equation. In particular, many attempts have been made to add terms in the equation that ensure the conservation of energy flux, without this constraint being theoretically justified [8–11]. The origin of the corrected one-way equations obtained is an analogy with the WKB solution in the one-dimensional case [11]. An alternative method [12–14] to derive improved one-way wave equations, still with claimed energy flux conservation, is to resort to the Foldy–Wouthuysen (FW) transformation, initially developed in order to derive relativistic corrections to the Schrödinger equation, from the Dirac or Klein–Gordon equations. A similar method has been developed for one-dimensional propagation [15], exhibiting WKB corrections at high orders. It is worth noting that the conservation of energy flux has also been claimed in the context of forward coupled modes theory [16].

In the one-dimensional case, Bremmer [17] has developed an approach in which the global field is decomposed into two forward and backward propagating components. Two first-order coupled equations are asymptotically obtained by describing the wavenumber of the medium as being the limit of a staircase function and considering all the successive reflections and transmissions at the risers of the staircase. Several authors [18–20] have outlined a generalization of this procedure in higher dimensions. In particular, a theory that extends the concept of Bremmer series to a dimension higher than 1, in which the splitting operator at the source of the derivation remains largely arbitrary, has been derived and the convergence discussed [21]. Incidentally it is common practice in wave propagation in the inhomogeneous media literature to consider that such a decomposition, expression (3), of a wave into forward and backward components is arbitrary (see for example a discussion in [22]). Arguments establishing the uniqueness of such a decomposition on physical grounds in one dimension

will be presented elsewhere. In section 2, the approach of Bellman and Kalaba is pursued in order to derive in higher dimensions the complete set of first-order equations for the two components of the wave field. The essential properties verified by the wave field, invariance by time reversal, conservation of energy flux and reciprocity are recalled in the present context. The issue of energy flux conservation in the resulting one-way wave equation is addressed in section 3. An invariant of this equation, close to but different from the energy flux, is presented in section 4. Time-reversal invariance and reciprocity of the one-way equation are discussed in section 5. The one-way wave operator is decomposed on a modal basis in section 6 and issues of energy conservation and mode coupling strength are discussed in this context. Explicit correction terms for the small angle and high frequency limit are given and compared to those given by other approaches. A general discussion of the results is presented in section 7.

2. Equations for the forward and backward components of the field

Following the Bremmer scheme [17], the global wave field φ is decomposed into forward φ^+ and backward φ^- components with respect to the x coordinate:

$$\varphi = \varphi^+ + \varphi^-. \quad (3)$$

In order to set up the equations satisfied by φ^+ and φ^- , the medium is approximated by transverse slabs in which wavenumber k and thus operator Q do not depend on x and whose thickness tends towards zero. In each of these slabs, equation (1) exactly factorizes in

$$\partial_x \varphi^\pm = \pm iK \varphi^\pm, \quad (4)$$

where the square root operator K is defined by

$$K = Q^{1/2}. \quad (5)$$

In order to study later on the energy conservation issue, we consider for simplicity a medium with perfectly reflecting, possibly irregular, boundaries. In the absence of dissipation, i.e. for real wave number k , Q is a Hermitian operator whose positive (respectively negative) eigenvalues correspond to propagating (respectively evanescent) modes. The square root operator K is chosen so that its eigenvalues are either real positive or imaginary positive. This ensures the proper signs in equation (4), assuming a time dependence $\exp(-i\omega t)$. In the staircase approximation, $K(x)$ is approximated by a piece-wise constant operator. Naming x_n , $n = -\infty, +\infty$, the abscissas of the slab interfaces, this approximation reads as $K(x) = K(x_n) = K_n$ for $x_n \leq x < x_{n+1}$. We consider the propagation of the two components of the field between x_0^+ , just to the right of the 0th interface, and x_1^+ , just to the right of the first interface. Between x_0^+ and x_1^- , just to the left of the first interface, the medium is uniform along the x direction so that, using (4),

$$\begin{cases} \varphi^+(x_1^-) = e^{iK_0 \delta x} \varphi^+(x_0^+) = (1 + iK_0 \delta x) \varphi^+(x_0^+) + O(\delta x^2) \\ \varphi^-(x_1^-) = e^{-iK_0 \delta x} \varphi^-(x_0^+) = (1 - iK_0 \delta x) \varphi^-(x_0^+) + O(\delta x^2) \end{cases}, \quad (6)$$

where $\delta x = x_1 - x_0$ is the slab thickness. At the first interface, the global field must satisfy the continuity of φ as well as that of its normal derivative. For example in the purely acoustic case, with no variation of the zeroth-order medium density, this corresponds to the continuity of pressure and normal velocity respectively. These continuity relations read as

$$\begin{cases} \varphi^+(x_1^+) + \varphi^-(x_1^+) = \varphi^+(x_1^-) + \varphi^-(x_1^-) \\ K_1 \varphi^+(x_1^+) - K_1 \varphi^-(x_1^+) = K_0 \varphi^+(x_1^-) - K_0 \varphi^-(x_1^-) \end{cases}. \quad (7)$$

The Taylor expansions of the operator $K(x_1)$ and of the fields $\varphi^\pm(x_1^+)$ read as

$$\begin{cases} \varphi^\pm(x_1^+) = \varphi^\pm(x_0^+) + \varphi_x^\pm \delta x + O(\delta x^2) \\ K_1 = K_0 + K_x \delta x + O(\delta x^2) \end{cases}, \quad (8)$$

where the subscript x stands for the derivation with respect to x (which, unless specified, will be the convention adopted in this paper). Inserting (6) and (8) into system (7), the first-order term is easily solved in φ_x^\pm . Dropping the subscript 0 for K , one obtains

$$\partial_x \begin{pmatrix} \varphi^+ \\ \varphi^- \end{pmatrix} = \begin{pmatrix} iK - \frac{1}{2}K^{-1}K_x & \frac{1}{2}K^{-1}K_x \\ \frac{1}{2}K^{-1}K_x & -iK - \frac{1}{2}K^{-1}K_x \end{pmatrix} \begin{pmatrix} \varphi^+ \\ \varphi^- \end{pmatrix}. \quad (9)$$

This first-order equation was derived by Bremmer in the one-dimensional case, where the operator K is scalar, $K(x) = k(x)$. Surprisingly, it seems that it has never been rigorously derived in higher dimension using operator formalism and continuity arguments. The approach was sketched by various authors [18, 20] who obtained the transmitted terms. In generalizing the Bremmer series to multi-dimension, de Hoop [21] introduced an ansatz that leads, as a possible choice, to the wave splitting equation in the acoustic-pressure normalization

$$\begin{pmatrix} \varphi \\ \varphi_x \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ iK & -iK \end{pmatrix} \begin{pmatrix} \varphi^+ \\ \varphi^- \end{pmatrix}, \quad (10)$$

where the second row is largely arbitrary while it is here demonstrated by summing the two rows of (9). The same assumption is the basis of the derivation of first-order coupled mode theories; see for example [1, 16]. The splitting given by (10) has often been presented as a possible choice amongst others, possibly infinitely numerous; see for example [1, 21, 23]. An early attempt to derive a parabolic equation from a wave splitting approach [19] uses the splitting (10) with operator K replaced by a scalar. This scalar is either a reference wave number k_0 , leading, when neglecting the backscattered field, to the standard parabolic equation, or the wave number $k(x)$, which is the approximation obtained by neglecting the transverse Laplacian in equation (2), leading to a modified small angle parabolic equation (see below). Besides, other systems of coupled first-order equations than system (9) have been derived, but without the two components of the field being interpreted as forward and backward ones; see for example [24]. These systems not being suitable to derive one-way equation will not be further discussed here.

System (10) has a useful and expected property with respect to time reversal. In order to write it down, it is necessary to differentiate propagating modes from evanescent ones. According to the discussion following definition (5), the operator K reads as $K = K_p + iK_e$ where K_p and K_e are Hermitian operators defined on orthogonal subspaces on which the wave field vector is divided up into propagating and evanescent components, $\varphi = \varphi_p + \varphi_e$.

By taking the complex conjugate (time reversed) of equation (10), and using the fact that $K_{p,e}$ are real operators ($(K_{p,e}\varphi)^* = K_{p,e}\varphi^*$), one obtains

$$\begin{pmatrix} \varphi^* \\ \varphi_x^* \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ iK_p - K_e & -iK_p + K_e \end{pmatrix} \begin{pmatrix} \varphi_p^{*-} + \varphi_e^{*+} \\ \varphi_p^{*+} + \varphi_e^{*-} \end{pmatrix}.$$

On the other hand, applying equation (10) to the field φ^* , we get

$$\begin{pmatrix} \varphi^* \\ \varphi_x^* \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ iK_p - K_e & -iK_p + K_e \end{pmatrix} \begin{pmatrix} \varphi_p^{*+} + \varphi_e^{*+} \\ \varphi_p^{*-} + \varphi_e^{*-} \end{pmatrix}.$$

Hence, comparing the last two systems, it becomes

$$\varphi_p^{\pm*} = \varphi_p^{*\mp} \quad (11a)$$

and

$$\varphi_e^{\pm*} = \varphi_e^{*\pm}. \tag{11b}$$

The time-reversal exchanges the forward and backward components of the propagating field, which is the expected result. On the other hand, the time reversal of the component that is exponentially decaying with x (respectively $-x$) remains decaying with x (respectively $-x$), that is it increases with $-x$ (respectively x).

Another important property of equation (1), or equivalently (9), is related to energy flux conservation. It is convenient to consider in an usual way the wave field as an element of the ensemble L^2_{\perp} of square integrable functions on the transverse coordinates, parameterized by the x propagation coordinate. Using Dirac notations in L^2_{\perp} , such a wave field is represented by the vector $|\varphi(x)\rangle$ parameterized by the x coordinate, with $\langle\varphi(x)| = \langle x_{\perp}|\varphi(x)\rangle$. For classical waves, the energy flux in the x direction is proportional to the imaginary part of the scalar product of the field and its derivative along x :

$$J = \text{Im}(\langle\varphi|\partial_x|\varphi\rangle) = \text{Im}\left(\int \varphi^*(x, x_{\perp}) \partial_x \varphi(x, x_{\perp}) dx_{\perp}\right). \tag{12}$$

For example in acoustics, if φ is the pressure field, according to the Euler law the x component of the velocity is $v_x = (i\rho\omega)^{-1} \partial_x \varphi$ with density ρ . So the energy flux is $\frac{1}{2}(\varphi v_x^* + \varphi^* v_x) = (\rho\omega)^{-1} J$. In the absence of dissipation, the wavenumber $k(x, y, z)$ is real, operator Q is therefore Hermitian and it is straightforward from equation (1) to verify that the energy flux is conservative ($J_x = 0$). This can also be checked directly using (9).

The third property checked by the solutions of equation (1) is reciprocity. Namely, $\varphi_{1,2}$ being two solutions of (1) or equivalently (9), the quantity defined by

$$L(\varphi_1, \varphi_2) = \int (\varphi_2(x, x_{\perp}) \partial_x \varphi_1(x, x_{\perp}) - \varphi_1(x, x_{\perp}) \partial_x \varphi_2(x, x_{\perp})) dx_{\perp}, \tag{13}$$

where the integration is over a section of the waveguide, is independent of the x coordinate of this section.

3. One-way wave operator and energy conservation

We consider a forward propagating wave field in an inhomogeneous medium. If the medium inhomogeneities are weak enough for the doubly reflected waves to be ignored, according to equation (9) the forward propagating wave field satisfies the following one-way wave equation (hereafter, we drop out the $+$ label):

$$\partial_x |\varphi\rangle = \left(iK - \frac{1}{2}K^{-1}K_x\right) |\varphi\rangle. \tag{14}$$

In order for this equation to be tractable, the pseudo-differential operator K must be made explicit. This can be done using the spectral decomposition of the Helmholtz operator (2) and then taking the square roots of the eigenvalues according to the discussion following definition (5). Another possibility is of directly considering some approximation of the square root of the operator Q . Generally, this approximation is the Taylor or Padé approximation with respect to some small parameter, roughly speaking the angle of propagation with the x -axis. By limiting a Taylor expansion to first order, this paraxial approximation applied to equation (4) leads to the well-known parabolic, Schrödinger-type, equation [2, 3] (see below). By extension, methods based upon higher order approximation of the square root operator, leading to first-order equations with differential operators of arbitrary order on the transverse space, are often referred to as ‘parabolic’ equation methods. A large part of the literature on parabolic equations rely upon the rude factorization of the Helmholtz equation,

$\partial_x |\varphi\rangle = \pm iK(x) |\varphi\rangle$. Regarding the staircase approach of the previous section, this equation is obtained by ensuring the continuity of the field, but not of its x derivative. It has long been recognized that this equation does not conserve energy flux. Various strategies have been proposed to correct this equation in order to ensure energy flux conservation, this requirement not being theoretically justified [8–11]. An early approach [8, 9] consists in propagating with the later equation the transformed field $|\chi\rangle = n^{1/2} |\varphi\rangle$, n being the refraction index of the medium and $n = k/k_0$ with k_0 being a reference wavenumber. This is equivalent to propagating the true field according to $\partial_x |\varphi\rangle = (in^{-1/2}Kn^{1/2} - \frac{n_x}{2n}) |\varphi\rangle$, which is equivalent to equation (14) only when the transverse gradient of the wave field vanishes, that is, for axial rather than paraxial propagation. A similar equation, but with a first-order Taylor expansion of the square root operator, was obtained with a splitting approach with $K = k(x)$ in equation (10) [19]. A more recent approach by Godin [10], still developed from the claimed conservation of energy flux, introduces the ansatz $|\psi\rangle = K^{1/2} |\varphi\rangle$ with $|\psi\rangle$ verifying equation (4) and is equivalent to propagating the field according to $\partial_x |\varphi\rangle = (iK - K^{-1/2}K_x^{1/2}) |\varphi\rangle$. This latter equation has wider angle capabilities and frequency range of validity than the previous one but is still an approximation of the equation satisfied by the transmitted wave (zero reflection) in the Bremmer scheme. These various approaches originate from an enlightening formal WKB approximation of equation (1) by Tappert [11], but they do not take into account the non-commuting property of operators K , as considered at various ranges. An alternative method [12–14] to derive corrected one-way equations, still with claimed energy flux conservation, has been to resort to the Foldy–Wouthuysen transformation. The resulting wave equations will be compared with equation (14) for an explicit approximation of the operator K in section 6.

Using (14), the calculation of the derivative, with respect to x , of the energy flux J defined by (12) leads to

$$J_x = \frac{1}{4}i \langle \varphi | [K^{-1}, R] | \varphi \rangle, \quad (15)$$

with

$$R = K_{xx} - \frac{3}{2}K_x K^{-1} K_x - i[K, K_x], \quad (16)$$

where $[..]$ designates the commutator of the inserted operators. In the course of the derivation of (15), the square root operator K is assumed to be Hermitian (the effect of possible evanescent modes on the behaviour of J will be discussed in the following section). In the one-dimensional case, all the operators are scalar and commute, ensuring the conservation of energy flux of the solution $\varphi(x) = k(x)^{-1/2} \exp(i \int^x k)$ of equation (14), which is in this case the WKB approximate solution [17, 25] of (1). In greater dimensions the operators no longer commute in general as soon as Q and then K depend on x , and the energy flux is no longer conservative.

It is possible to carry out a high frequency asymptotic analysis of the commutators involved in (15). In order to do so, we need an explicit approximation of the operator K . As previously mentioned, the simpler way to do this is to consider the first-order Taylor expansion of $Q^{1/2}$ with respect to some small parameter. For the sake of simplicity, we consider the propagation in two dimensions, with y being the transverse coordinate. Introducing some definitions, the operator Q reads as

$$Q = k_0^2 (1 + \chi), \quad \text{with} \quad \chi = v - p^2, \quad v = n^2 - 1 \quad \text{and} \quad p = \frac{\partial_y}{ik_0}. \quad (17)$$

The scalar operator v describes the amplitude of the medium inhomogeneities, which will be taken small, while the operator p characterizes the grazing angle with respect to the x -axis. We consider waves with small grazing angles so that $\langle \varphi | v | \varphi \rangle$ and $\langle \varphi | -p^2 | \varphi \rangle$ are, for normalized $|\varphi\rangle$, of the same order of magnitude that we call ε . If the medium does not depend on x , the sum of these two terms remains constant along the propagation direction, which corresponds

to the Snell law of refraction in the high frequency limit. The paraxial approximation is then obtained by taking the first-order Taylor series expansion of operator (5) using definitions (17):

$$K = k_0 \left(1 + \frac{1}{2} \chi + \hat{O}(\varepsilon^2) \right), \quad (18a)$$

$$K^{-1} = \frac{1}{k_0} \left(1 - \frac{1}{2} \chi + \hat{O}(\varepsilon^2) \right). \quad (18b)$$

In these expressions and afterwards, we note $\hat{O}(\varepsilon)$ as an operator such that $\langle \varphi | \hat{O}(\varepsilon) | \varphi \rangle / \langle \varphi | \varphi \rangle = O(\varepsilon)$. By neglecting the second term in the right-hand side of equation (14), which means considering equation (4) with $K = K(x)$ as the one-way wave propagation, and neglecting the $O(\varepsilon^2)$ term in (18a), the standard parabolic equation is recovered. This equation reads as $\partial_x \varphi(x, y) = ik_0((n^2 + 1)/2 + \partial_{yy}^2/2k_0^2)$ which is analogous to the time-dependent Schrödinger equation [3].

To asymptotically evaluate expression (15), we need to calculate commutators such as $[p, f]$ and $[p^2, f]$, where f is a scalar. One obtains

$$[p, f] = -i \frac{f_y}{k_0} \quad (19a)$$

and

$$[p^2, f] = -2i \frac{f_y}{k_0} p - \frac{f_{yy}}{k_0^2}. \quad (19b)$$

Introducing the small parameter $\lambda = 1/k_0 L_y$, where L_y is the transverse scale of inhomogeneity, one obtains, using definitions (17), that the commutators of operators f, p, χ are $O(\lambda)$ and then asymptotically cancel in the high frequency limit. Using this property, one obtains after deriving (18a)

$$K_x = k_0 \left(\frac{1}{2} v_x (1 + \hat{O}(\varepsilon)) + \hat{O}(\lambda) \right).$$

In a general way, if an operator A is such that $[\chi, A] = \hat{O}(\lambda)$, then it is easily shown that the relation $[\chi(1 + \hat{O}(\varepsilon)), A(1 + \hat{O}(\varepsilon))] = [\chi, A](1 + \hat{O}(\varepsilon)) + \hat{O}(\lambda^2)$ holds. Using this latter result, the leading order approximation of the commutator of K and K_x is obtained:

$$[K, K_x] = k_0 \left(\frac{1}{2} v_{xy} p (1 + \hat{O}(\varepsilon)) + \hat{O}(\lambda) \right).$$

After some similar but tedious calculations, the complete commutator arising in expression (15) is evaluated:

$$i[K^{-1}, R] = \frac{1}{k_0} \left(\frac{1}{8} (v_y^2)_x + \frac{1}{2} v_{xyy} p^2 + \frac{1}{2} v_{xxy} p \right) (1 + \hat{O}(\varepsilon)) + \hat{O}(\lambda^2). \quad (20)$$

Consequently, by substituting (20) in (15), the x derivative of the energy flux is shown to read as, in the high frequency ($\lambda \rightarrow 0$), low inhomogeneities ($v \rightarrow 0$) and low grazing angle ($\langle \varphi | p | \varphi \rangle \rightarrow 0$) limits,

$$\left. \frac{dJ}{dx} \right|_{\text{lim}} = \frac{1}{8k_0} \text{Re} \left(\langle \varphi | \frac{1}{2} v_y v_{xy} + v_{xyy} p^2 + v_{xxy} p | \varphi \rangle \right). \quad (21)$$

A real part appears in this expression because, in the course of the derivation of (20), non-Hermitian operators such as fp , with f scalar, arise. The departure from hermiticity of this later operator is transferred to the $\hat{O}(\lambda^2)$ term; see equation (??). To discard the resorting to this real part it is necessary to replace in expression (21) terms such as fp by $\frac{1}{2}(fp + pf)$, a step which could have been done from the beginning of the calculation.

In most of the waveguides encountered in electromagnetism or acoustics, the longitudinal scale of inhomogeneity L_x is larger than the transverse one. So we define a new small

parameter $\eta = L_y/L_x$. From (12) and (18a), it comes that the energy flux is k_0 to zeroth order in the small parameters. Accordingly, the order of magnitude of the relative change in the energy flux on the horizontal scale length is, after inspection of (21),

$$\frac{1}{J} \frac{dJ}{dx} L_x = O(\lambda^2 \varepsilon^2) + O(\lambda^2 \varepsilon^{3/2} \eta).$$

The first comment on this result is that the energy flux will be conserved by the one-way wave equation (14) only at infinite frequency. This result is different to that obtained in one dimension where the standard WKB solution is known to conserve energy. This is due to the fact that in two or three dimensions the propagation operator does not commute with itself along the propagation direction, unlike for the one-dimensional case where this operator is scalar. The second comment is that a non-zero energy flux variation for the directly transmitted wave is obtained even in the small grazing angle limit. The non-conservation of energy flux at finite frequency is not concentrated nearby the cut-off of modes at normal grazing angles, corresponding to singularities of the operator K^{-1} arising in the one-way wave operator and analogous to the turning points in one dimension. Nevertheless, the effect is expected to be stronger for modes approaching the cut-off since coupling between modes propagating in opposite directions will be more effective.

4. One-way wave invariant

It has been shown in the previous section that the energy flux is not an invariant of the one-way wave equation (14), at finite frequency. We consider in this section the quantity defined by

$$I = \text{Re}(\langle \varphi | K | \varphi \rangle). \quad (22)$$

Using the one-way wave equation (14), we get

$$\partial_x \langle \varphi | K | \varphi \rangle = \langle \varphi | i(K - K^\dagger)K + \frac{1}{2}(K_x - K_x^\dagger K^{-1\dagger} K) | \varphi \rangle, \quad (23)$$

where the superscript \dagger denotes the adjoint operator. The operator K has real positive eigenvalues corresponding to propagating modes and, due to the possible perfect reflecting boundaries we considered in section 2, may also have imaginary positive eigenvalues corresponding to evanescent modes. As in section 2, we use the decomposition $K = K_p + iK_e$. The inverse of K admits the decomposition $K^{-1} = \bar{K}_p - i\bar{K}_e$, where \bar{K}_p (respectively \bar{K}_e) is null on the subspace $L_{\perp e}^2$ (respectively $L_{\perp p}^2$) generated by evanescent (respectively propagating) modes. \bar{K}_p (respectively \bar{K}_e) is further defined by $K_p \bar{K}_p = I_p$ (respectively $K_e \bar{K}_e = I_e$) where I_p (respectively I_e) is the projector onto $L_{\perp p}^2$ (respectively $L_{\perp e}^2$). We then get $K^{-1\dagger} K = I_p - I_e$. Using this result and the decomposition of the wave field vector $|\varphi\rangle = |\varphi_p\rangle + |\varphi_e\rangle$, with $|\varphi_{p,e}\rangle = I_{p,e}|\varphi\rangle$, equation (23) reads as

$$\partial_x \langle \varphi | K | \varphi \rangle = \text{Re}(\langle \varphi_e | K_x | \varphi \rangle) + i(\text{Im}(\langle \varphi_p | K_x | \varphi \rangle) - 2\langle \varphi_e | K_e^2 | \varphi_e \rangle). \quad (24)$$

The derivation with respect to x of the relation $K_p = I_p K I_p$ leads to $I_e K_{p,x} I_e = 0$ and then to $I_e K_x^\dagger I_e = -I_e K_x I_e$. The latter relation corresponds to $\text{Re}(\langle \varphi_e | K_x | \varphi_e \rangle) = 0$. Similarly we get $\text{Im}(\langle \varphi_p | K_x | \varphi_p \rangle) = 0$, so that equation (24) better reads as

$$\partial_x \langle \varphi | K | \varphi \rangle = \text{Re}(\langle \varphi_e | K_x | \varphi_p \rangle) + i(\text{Im}(\langle \varphi_p | K_x | \varphi_e \rangle) - 2\langle \varphi_e | K_e^2 | \varphi_e \rangle).$$

In particular, the x derivative of the quantity I defined by (22) is

$$I_x = \text{Re}(\langle \varphi_e | K_x | \varphi_p \rangle). \quad (25)$$

When there are no evanescent modes, $K_e = 0$, the quantity I is found to be exactly invariant:

$$\frac{dI}{dx} = 0. \quad (26)$$

When the medium bears evanescent modes but these are weakly excited, as in the case of paraxial propagation in slowly varying waveguides, with weak coupling between excited propagative modes and evanescent ones, equation (26) is a very good approximation and the quantity I can still be considered as an invariant.

This invariant, defined by equation (22), is the product of two terms. The first one, $E(x) = \langle \varphi_p | \varphi_p \rangle$, is the energy density of the propagating modes integrated onto a plane orthogonal to the x direction. The second term which is $\overline{k_x}(x) = \langle \varphi_p | K | \varphi_p \rangle / \langle \varphi_p | \varphi_p \rangle$ interprets as the mean value of the wavevector component in the x direction (note that here, the x subscript does not stand for the x derivative of k). For stratified media, i.e. invariant by translation in the x direction, both quantities are constant. Conservation of E follows from the hermiticity of K_p and then expresses the unitarity nature of the propagator acting on propagating modes. Conservation of $\overline{k_x}$ is the finite frequency expression of the Snell law. In fact, any analytic function f provides an invariant $\langle \varphi_p | f(K) | \varphi_p \rangle$ so that all the moments of k_x defined in the same way as $\overline{k_x}$ are invariants. It is then the entire distribution law of k_x so defined that is a propagation invariant. For arbitrary inhomogeneous, unstratified, media, equation (26) shows that there remains one invariant that is the product of the two basic invariants for stratified media:

$$I = E(x) \cdot \overline{k_x}(x) = C^{\text{ste}}. \quad (27)$$

The I invariant for the transmitted wave may be seen as a generalization for arbitrary inhomogeneous media and finite frequency of the Snell law for stratified media.

The two quantities I and J asymptotically degenerate at high frequency. With the assumption that no excited mode is at cut-off, the energy flux, neglecting here the coupling between propagating and evanescent fields, reads as

$$J = I + \frac{1}{4} \langle \varphi_p | i[\overline{K_p}, K_{p_x}] | \varphi_p \rangle + \frac{1}{4} \langle \varphi_e | i[\overline{K_e}, K_{e_x}] | \varphi_e \rangle. \quad (28)$$

The third term of this expression shows that a non-zero, but evanescent, energy flux may be associated, for the one-way wave equation, with the evanescent wave field. The first term in expression (28) is $O(k_0)$ while the others are $O(k_0^{-1})$. More precisely, by carrying out the same kind of asymptotic analysis as in the preceding section, the leading term of the second term of expression (28) in the small inhomogeneity, small grazing angle and high frequency limits is $\text{Re}(\langle \varphi | \frac{\nu_{xy}}{8k_0} | \varphi \rangle)$ so that we get

$$J = I(1 + O(\lambda^2 \varepsilon^{3/2} \eta)). \quad (29)$$

The degeneracy of I and J at high frequency may be accounted for by considering a ray tube making an angle θ with the x -axis so that $k_x = \omega \cos \theta / c$. The energy density $E(x)$ is proportional to the square of the amplitude A of the field and to the surface intercepted by the ray tube normally to x . If the section of the ray tube is $d\sigma$, this surface is $d\sigma / \cos \theta$ so that the conservation of $I = k_x(x) \cdot E(x)$ reads as $A^2 d\sigma / c = C^{\text{ste}}$, which results from the transport equation along the ray.

5. Time-reversal invariance and reciprocity

Let φ^+ and φ^- be two wave fields propagating according to reversed one-way wave equations:

$$\partial_x \begin{pmatrix} \varphi^+ \\ \varphi^- \end{pmatrix} = \begin{pmatrix} iK - \frac{1}{2}K^{-1}K_x & 0 \\ 0 & -iK - \frac{1}{2}K^{-1}K_x \end{pmatrix} \begin{pmatrix} \varphi^+ \\ \varphi^- \end{pmatrix}. \quad (30)$$

From this equation, we deduce

$$\varphi^\pm = \frac{1}{2}((1 \mp iK^{-2}K_x)\varphi \mp iK^{-1}\varphi_x). \quad (31)$$

In order to study the time-reversal property of equation (30), we use for K_x the decomposition $K_x = K_x^{(p)} + iK_x^{(e)} + K_x^{(pe)} + K_x^{(ep)}$ where $K_x^{(p)}$ (respectively $K_x^{(e)}$) is defined from $L_{\perp p}^2$ (respectively $L_{\perp e}^2$) on itself and is null on $L_{\perp e}^2$ (respectively $L_{\perp p}^2$). $K_x^{(pe)}$ (respectively $K_x^{(ep)}$) corresponds to the possible coupling between propagating and evanescent modes and is defined from $L_{\perp p}^2$ (respectively $L_{\perp e}^2$) to $L_{\perp e}^2$ (respectively $L_{\perp p}^2$). Using the decomposition $\varphi^\pm = \varphi_p^\pm + \varphi_e^\pm$, and the prescribed decompositions for the operators, equation (31) reads as

$$\begin{aligned}\varphi_p^\pm &= \frac{1}{2}(\varphi_p \mp i \overline{K_p}^2 K_x^{(p)} \varphi_p^* \mp i \overline{K_p}^2 K_x^{(ep)} \varphi_e \mp i \overline{K_p} \varphi_x) \\ \varphi_e^\pm &= \frac{1}{2}(\varphi_e \mp \overline{K_e}^2 K_x^{(e)} \varphi_e \pm i \overline{K_e}^2 K_x^{(pe)} \varphi_p \mp \overline{K_e} \varphi_x).\end{aligned}$$

The time reversed of this equation is, designing by the superscript T the time reversed of an operator,

$$\begin{aligned}\varphi_p^{\pm*} &= \frac{1}{2}(\varphi_p^* \pm i \overline{K_p}^2 K_x^{(p)} \varphi_p^* \pm i \overline{K_p}^2 K_x^{(ep)T} \varphi_e^* \pm i \overline{K_p} \varphi_x^*) \\ \varphi_e^{\pm*} &= \frac{1}{2}(\varphi_e^* \mp \overline{K_e}^2 K_x^{(e)} \varphi_e^* \mp i \overline{K_e}^2 K_x^{(pe)T} \varphi_p^* \mp \overline{K_e} \varphi_x^*).\end{aligned}$$

On the other hand, the decomposition of the time-reversed field φ is

$$\begin{aligned}\varphi_p^{\pm*} &= \frac{1}{2}(\varphi_p^* \mp i \overline{K_p}^2 K_x^{(p)} \varphi_p^* \mp i \overline{K_p}^2 K_x^{(ep)} \varphi_e^* \mp i \overline{K_p} \varphi_x^*) \\ \varphi_e^{\pm*} &= \frac{1}{2}(\varphi_e^* \mp \overline{K_e}^2 K_x^{(e)} \varphi_e^* \pm i \overline{K_e}^2 K_x^{(pe)} \varphi_p^* \mp \overline{K_e} \varphi_x^*).\end{aligned}$$

Comparing the last two systems, it turns that time-reversal relations (11a) and (11b) are recovered if and only if

$$K_x^{epT} = K_x^{ep}, \quad K_x^{peT} = -K_x^{pe}. \quad (32)$$

These properties of the coupling between the propagative and evanescent fields are not verified in general. The one-way equation possibly couples a propagating field in one direction to an evanescent field decaying in the same direction. The time-reversed propagating field then couples, with the corresponding one-way wave equation, to an evanescent field decaying in the opposite direction while the reversed field of an evanescent wave increases in the opposite direction. Thus, the possible coupling between propagative and evanescent parts of the field prevents the one-way equation from satisfying the full invariance by time reversal. Nevertheless, if this coupling is not negligible, the coupling between modes propagating in opposite directions generally also will not be, and the one-way equation solution alone will be a poor approximation of the wave field. For most applications of the one-way equation, like far field propagation in waveguides, the time-reversal invariance property will be approximately well satisfied.

In order to study the reciprocity property of the one-way equation, we consider two wave fields satisfying equation (14). After straightforward calculations, the x derivative of the quantity defined by (13) turns out to be

$$\begin{aligned}L_x &= \int (\varphi_2(x, x_\perp) (-K^2 - \frac{1}{2}K^{-1}R) \varphi_1(x, x_\perp) - \varphi_1(x, x_\perp) (-K^2 - \frac{1}{2}K^{-1}R) \varphi_2(x, x_\perp)) dx_\perp, \\ &= \frac{1}{2} \int (\varphi_1(x, x_\perp) (K^{-1}R) \varphi_2(x, x_\perp) - \varphi_2(x, x_\perp) (K^{-1}R) \varphi_1(x, x_\perp)) dx_\perp\end{aligned}$$

with R given by (16). In general,

$$L_x \neq 0; \tag{33}$$

thus, reciprocity is not ensured by the one-way wave equation. When the evanescent modes are absent, this result would have been deduced from the fact that the verification of two properties among the three (energy flux conservation, time-reversal invariance and reciprocity) implies the satisfaction of the third [26, 27]. It may also be directly deduced from the fact that time-reversal invariance is ensured in this case and that $L(\varphi, \varphi^*)$ is the energy flux of the field φ . The quantity L_x is amenable to the same asymptotic analysis as the energy flux that would show that reciprocity is satisfied in the high frequency, small grazing angles and small inhomogeneity limits.

In the case where there are no evanescent waves ($K_e = 0, K = K^\dagger$), it is possible to find an invariant that plays, with respect to reciprocity, the role of I with respect to energy flux conservation. By considering $L(\varphi_1, \varphi_2^*)$ and replacing operator ∂_x by iK , one gets

$$M(\varphi_1, \varphi_2) = \langle \varphi_2 | iK | \varphi_1 \rangle - \langle \varphi_2 | (iK)^\dagger | \varphi_1 \rangle.$$

Dropping a $2i$ factor, the quantity M reads as

$$M(\varphi_1, \varphi_2) = \langle \varphi_2 | iK | \varphi_1 \rangle. \tag{34}$$

Using equation (14), the invariance of M is directly verified:

$$\frac{d}{dx} M(\varphi_1, \varphi_2) = 0. \tag{35}$$

If evanescent modes are present, the conservation of M is only an approximation, all the more satisfied as the paraxial approximation is.

6. Explicit equations—mode coupling

In the previous sections it has been shown that the one-way wave propagation equation could preserve energy flux only in the high frequency limit, due to the non-commutativity of the operators K^{-1} and K_x . In this section a second consequence of this non-commutativity is addressed, namely the influence on mode coupling. The one-way propagation equation (14) is rewritten as

$$\partial_x |\varphi\rangle = (iP + Q) |\varphi\rangle, \tag{36a}$$

$$P = K + \frac{1}{4}i[K^{-1}, K_x], \quad Q = -\frac{1}{4}(K^{-1}K_x + K_xK^{-1}). \tag{36b}$$

Although a number of results are valid in the general case, for the sake of simplicity of the interpretation, we consider here only propagating modes and neglect the possible evanescent ones. The operator P , being Hermitian and multiplied by i in equation (36a), is a phase-like operator while operator Q , being also Hermitian, is an amplitude-like operator. The local propagating modes $|n(x)\rangle$ with wavenumbers $k_n(x)$ are the eigenvectors of the operator $K(x)$ with eigenvalues $k_n(x)$ and of the operator $Q(x)$ with eigenvalues $k_n(x)^2$; see equation (5). These form an orthogonal base of the set of propagating fields, in which a wave field admits the formal decomposition $|\varphi\rangle = \sum_n a_n |n\rangle$. The operator K , for normalized modes, reads as $K = \sum_n k_n |n\rangle \langle n|$, where $|n\rangle \langle n|$ is the projector on the n th mode. Inserting these decompositions into equation (36a), after a few calculations, leads to

$$a_{nx} = ik_n a_n - \sum_m \langle n | m_x \rangle \left(1 + \frac{(k_m - k_n)^2}{4k_m k_n} \right) a_m - \frac{k_{n_x}}{2k_n} a_n - \sum_m \langle n | m_x \rangle \frac{k_m^2 - k_n^2}{4k_m k_n} a_m. \tag{37}$$

The notation $|m_x\rangle$ for the x derivative of $|m\rangle$ has been preferred to $|m\rangle_x$ to avoid ambiguity when the derivative occurs in a scalar product. System (37) is the standard one-way coupled mode equation system [1, 16]. It is generally derived from the postulated second line of system (10), which has been derived here using the Bremmer approach, as discussed in section 2. The term $\langle n | m_x \rangle$ may be factored to give $\langle n | m_x \rangle (k_n + k_m) / 2k_n$ but the aim here is to isolate the contributions of the various terms of (37). The first line of the right-hand side of equation (37) corresponds to the phase-like part P of the (infinitesimal) propagator and the second line to the amplitude-like part Q . This amplitude-like term ensures the conservation of energy in the high frequency limit, in the same way as the $k(x)^{-1/2}$ amplitude term of the WKB solution does in one dimension. The commutator part of operator P is responsible for the $\langle n | m_x \rangle \alpha_{mn} a_m$ terms in equation (37), with $\alpha_{mn} = (k_m - k_n)^2 / 4k_m k_n$. The coefficient α_{mn} being always positive, the effect of the anti-Hermitian part of $K^{-1} K_x$ is to strengthen the coupling between modes. This reinforcement may be of the same order of magnitude as the main term when the inhomogeneities couple non-neighbouring modes, i.e. at low frequency.

By making a Taylor expansion of the correction terms in equation (36a), as being done in section 3, the phase-like part of the first terms of the series expansion of the infinitesimal operator reads as

$$P \cong k_0 \left((1 + \chi)^{1/2} + \frac{1}{16} \left(p \frac{v_{xy}}{k_0^2} + \frac{v_{xy}}{k_0^2} p \right) \right), \quad (38)$$

while its amplitude part reads as

$$Q \cong -\frac{1}{4} v_x (1 - v) - \frac{1}{8} (p^2 v_x + v_x p^2). \quad (39)$$

Using the Foldy–Wouthuysen (FW) transformation, Wurmser [12, 13] obtained a propagation operator whose first-order correction is of phase-like type and reads as, with our notations, $-\frac{1}{16} \frac{v_{xx}}{k_0^2}$. This term will be of smaller amplitude than the correction term in equation (38) for a slowly range-dependent medium ($\eta \ll 1$) and not so small grazing angles. This result has been obtained by neglecting the ‘endpoint’ contribution of the transformation, of the amplitude type, that is claimed to be justified for weak range dependence. Also using the FW transformation, Khan [14] exhibits a correction term which is of a phase-like operator type and whose first order term is exactly half of the correction term in operator (38). Besides, this author does not exhibit any amplitude-like correction, while, being $O(1/k_0^0)$, this type of correction, operator (39), is in our result the leading order one with respect to the parameter $\lambda = L_y/k_0$. The origin of the apparent discrepancy between the different equations based on FW transformation is not clear to the author. It is emphasized that our results are in accordance with forward coupled modes theory and legitimate the hypothesis at the beginning of its derivation.

7. Discussion and conclusion

The Bremmer approach [17] of wave propagation in one-dimensional inhomogeneous media is easily extended to higher dimensions in the way outlined by Bellman and Kalaba [18]. This leads to coupled equations (9) and provides the basis to describe the propagation of waves in terms of multiple reflection and transmission [21]. Incidentally, it allows a justification for the derivation of coupled mode equations through the derivation of the second line of system (10). For sufficiently slowly varying media in the x direction, the first order infinitesimal propagator (14) gives the general frame for the derivation of one-way wave equations, since an explicit approximation of the square root operator has been given. The method accounts for the non-commutativity of operators, unlike previous works based on the rude extension of

WKB theory [8–11]. The method departs from results arising from the Foldy–Wouthuysen transformation [12–14] but mutually supports results obtained with coupled mode theory. Further comparisons with, and amongst, the results of the FW transformation method would be most valuable.

In sharp contrast to the one-dimensional case, the one-way wave equation is shown to conserve energy flux only in the high frequency limit. Let us consider for example a medium that becomes stratified (range independent) after some distance to the source in the x direction. At finite frequency, it will be necessary to consider all the waves that have been reflected an even number of times in the unstratified medium in order to recover the exact amount of energy flux in the stratified medium. This is somehow reminiscent of what happens for the reflection in the one-dimensional case. Consider a wave coming from region I with constant index and incident on region II whose index varies continuously, or a quantum particle coming from region I with constant potential and entering region II where the potential varies continuously but remains below the total energy of the particle. The reflection coefficient of the wave incident on region II will typically behave as $\exp(-1/\varepsilon)$ with the small parameter ε being the reference wavelength for a classical wave (respectively \hbar for a quantum particle), as reported by Berry and Mount [28] on a case, where the potential presents a single bump, and for which all the mathematical calculations are tractable. When considering only one reflection in the Bremmer scheme this exponential behaviour is recovered, but the amplitude of the exponential, while being close, is not the exact one. This amplitude is recovered when considering all the waves that have been reflected an odd number of times. In this one-dimensional case the successive reflections have a negligible effect on the transmission coefficient for small values of the parameter ε and one may consider the directly transmitted (zero reflection) wave, which is the WKB solution. In higher dimensions, the reflected energy is no longer exponentially decaying with the (inverse) small parameter. It is anticipated that for a small parameter and an arbitrary grazing angle, it will be necessary to take into account multiple reflections in order to recover the correct level of the transmitted wave as described by the de Hoop scheme [21]. These considerations deserve further analytical and numerical investigations.

A way to account for the difference between one and higher dimensions is to observe that, in higher dimensions, the principal direction of propagation, in inhomogeneous media without translational symmetry, is somewhat arbitrary. At finite frequency, for a given direction of propagation x the transmitted wave will be scattered from an inhomogeneity in the whole half-space. With respect to any slightly tilted x' direction, this field will have a non-zero reflected component. The argument is only qualitative since the definition of the transmitted field depends on the chosen direction.

Different to the energy flux at finite frequency, an invariant, as given in (22), has been found for the one-way wave equation. This invariant is the product of the energy in the plane perpendicular to the propagation direction by the average wavenumber in this direction, both quantities being invariant for stratified media. Besides its physical interest due to the fact that it may be seen as a generalization of the Snell law to non-stratified media, this invariant may be useful in the testing of numerical marching algorithms. The invariance of I is exact only if the possible coupling between evanescent and propagating fields may be neglected. Under the same condition, the one-way wave equations are shown to be time-reversal invariant. On the other hand, the reciprocity property, such as energy flux conservation, is only achieved in the high frequency limit.

The added term in the one-way wave equation with respect to the standard ‘parabolic’ one (equations (38) and (39) in the paraxial and high frequency limits), beyond being responsible for the existence of an invariant that differs from the energy flux, is at the origin of strengthening mode coupling. This term has then to be incorporated in its original (asymmetric) form in

one-way models especially for low frequencies and high grazing angles with respect to the principal direction.

These new theoretical results might eventually provide efficient and valuable tools for studying various practical problems in the field of wave propagation in inhomogeneous media. Further numerical configurations will be studied elsewhere.

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