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One-Way Large Range Step Methods for Helmholtz Waveguides

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A useful approach for long range computation of the Helmholtz equation in a waveguide is to re-formulate it as the operator differential Riccati equation for the Dirichlet-to-Neumann map. For waveguides with slow range dependence, the piecewise range-independent approximation is used to derive a second-order range stepping method for this one-way re-formulation. The range marching formulas are exact for each range-independent piece and a large range step is possible if the range dependence is gradual. Based on a fourth-order conservative exponential method for linear evolution equations, a fourth-order method that admits even larger range steps is developed for the one-way re-formulation. Numerical examples are used to demonstrate the improved accuracy of the fourth-order method.

1. INTRODUCTION

For acoustic, electro-magnetic, and seismic wave propagation problems of practical interest, it is often necessary to solve the governing equation in a domain that has length scales much larger than the typical wavelength. Very often, boundaries and different medium properties lead the waves to propagate in some preferred direction. The length scale along the waveguide is typically very large. The transverse length scale is much smaller, but still much larger than the characteristic wavelength. For example, the ocean surface and the relatively slow speed of sound in water (compared with the seabed) effectively force the sound waves to propagate in horizontal directions. Low-frequency sound waves in the ocean could travel hundreds and even thousands of kilometers in the horizontal (i.e., range) direction.

Standard numerical techniques such as the finite difference and finite element methods lead to a system of equations with a very large number of unknowns and are not very practical for these large-scale problems. The boundary integral equation method [7, 27] can be very useful when it is applicable, but it is restricted to cases in which the medium properties

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are constants. Fortunately, for many long range wave propagation problems, the medium properties have very gradual variations in the main propagation direction. The purpose of this paper is to develop an efficient numerical method for Helmholtz waveguides by taking advantage of this feature.

Consider the simple model of a 2-dimensional Helmholtz equation

$$u_{xx} + u_{zz} + \kappa^2(x, z)u = 0 \tag{1}$$

in the strip $0 < z < 1$, where x is the range variable (for the main propagation direction). Homogeneous and x-independent boundary conditions are assumed at $z = 0$ and $z = 1$. Furthermore, the wavenumber κ is x-independent for $x \le 0$ and $x \ge L$, for some L. A radiation condition is imposed at $x = L$ so that only waves propagating towards $+\infty$ are allowed for $x > L$. Our problem is characterized by the existence of three distinct length scales

$$\frac{1}{\kappa} \ll 1 \ll L.$$

Namely, the typical wavelength $O(1/\kappa)$ is much smaller than the transverse length scale (normalized as 1), which is still much smaller than the range distance L. We also assume that the dependence of κ on the range variable x is gradual in the sense that the variation of κ over a typical wavelength is small compared with κ itself.

Exact one-way re-formulations [9, 21] turn the Helmholtz equation boundary value problem into "initial" value problems with the range variable x (along the waveguide) acting as the usual "time" variable. A simple one-way re-formulation is based on the Dirichlet-to-Neumann (DtN) map. Let u be an arbitrary solution of the Helmholtz equation satisfying the boundary conditions at $z = 0$ and $z = 1$, and the radiation condition at $x = L$. The DtN operator $Q(x)$ maps u (at a fixed x, as a function of z) to its x derivative. We have $u_x = Q(x)u$ and

$$\frac{dQ}{dx} = -\left[\partial_z^2 + \kappa^2(x, z)\right] - Q^2. \tag{2}$$

A numerical implementation for such a one-way re-formulation requires relatively little computer memory (since it is independent of L). Meanwhile, the total computation time is linearly proportional to L. For long range waveguide problems where $L \gg 1$, the one-way re-formulations are particularly useful.

Notice that the DtN map is often associated with the exact boundary condition at an artificial boundary introduced to truncate the original unbounded domain [12, 13, 22, 15, 23]. As a special case, the radiation condition here can be given at $x = L$ (since κ is x-independent for $x \ge L$) as $u_x = Q(L)u$, where $Q(L) = i\sqrt{\partial_z^2 + \kappa^2(L, z)}$ for a properly defined square root operator. In this paper, the DtN map is not just used for an artificial boundary condition, it is defined at different values of x and used as the main tool for solving the Helmholtz equation.

The main objective of this paper is to develop numerical methods for discretizing the Riccati equation (2), such that a large step size can be used when the x dependence of κ is weak. In a step where κ is x-independent, our methods reproduce the exact relationships between the operators at the two end points of the step. For the general x-dependent case, a second-order method is derived based on approximating κ in each step by its value at the

midpoint (still a function of z). We also develop a fourth-order "large range step" method based on a fourth-order method for linear evolution equations.

In Section 2, we present the necessary background of exact one-way re-formulations of the Helmholtz equation and compare them with the related approximate one-way Helmholtz equation. A second-order method is derived in Section 3. The operator formulas of Section 3 are further discretized with two methods in Section 4. The full matrix approach approximates the operators by matrices directly based on a fourth-order finite difference method for the z variable. A more efficient approach is to use the truncated local eigenfunction expansion where the operators are represented by matrices of much smaller sizes. A fourth-order large range step method is presented in Section 5. Numerical examples are given in Section 6 to illustrate the capacity of the methods. Finally, we end this paper with some conclusions in Section 7.

2. ONE-WAY RE-FORMULATIONS

Fishman [9] first developed a one-way re-formulation based on wave-field decomposition and the scattering operators. The wave field is decomposed as $u = u^{(+)} + u^{(-)}$ and the condition $u_x = iB(x)[u^{(+)} - u^{(-)}]$ is required, where $B(x) = \sqrt{\partial_z^2 + \kappa^2(x, z)}$ is the square root operator which can be defined based on the eigenvalues and eigenfunctions of the transverse operator $\partial_z^2 + \kappa^2$ (see, for example, [21]). The one-way re-formulation based on the DtN map is simpler [10, 11, 21, 14]. Substituting $u_x = Q(x)u$ into the Helmholtz equation, we have

$$\left[\frac{dQ}{dx} + Q^2 + \partial_z^2 + \kappa^2(x, z)\right]u = 0.$$

Since the above is true for any solution of the Helmholtz equation (satisfying the boundary conditions at $z = 0$ and $z = 1$, and the radiation condition at $x = L$), we obtain Eq. (2) for Q.

Numerical computation for the above re-formulation was reported in [21]. This re-formulation is an example of the invariant imbedding or Riccati method for two point boundary value problems of ordinary differential equations [2], with the only difference being that the matrices are replaced by operators. The Riccati equation for Q should be solved for decreasing x with an initial condition that matches the exact radiation condition at $+\infty$. Since $\kappa(x, z)$ does not depend on x for $x \geq L$, the initial condition of Q can be given at $x = L$ as $Q(L) = i\sqrt{\partial_z^2 + \kappa^2(L, z)}$. The reflection operator at $x = 0$ can be constructed from $Q(0)$, leading to the solution of back-scattered waves for given incident waves from $-\infty$. To find the wave field for $x > 0$, a naive approach is to use the "evolution" equation $u_x = Q(x)u$ in a second sweep. This is not practical since Q must be remembered for all x. For stability reasons, (2) cannot be solved for increasing x to reproduce the solution obtained in the first sweep. This difficulty can be avoided by introducing the fundamental solution operator Y satisfying $Y(x)u(x, z) = u(L, z)$ and

$$\frac{dY}{dx} = -YQ. \tag{3}$$

The modified first sweep is now to solve Q and Y together from $x = L$ to $x = 0$. The initial condition at $x = L$ is $Y(L) = I$, where I is the identity operator. When $Y(0)$ is calculated, the solution at $x = L$ can be generated by a simple multiplication with the "starting field"

$u(0, z)$, namely,

$$u(L, z) = Y(0)u(0, z).$$

The approach can be further modified to find the solutions at other selected range locations [21]. This re-formulation produces the exact solution of the Helmholtz equation and can be used for arbitrary range dependence. The numerical procedure requires $O(n^3)$ operations for each range step, where n is the number of points used to discretize z. It is possible to speed it up to $O(m^3)$ operations, where m is the number of modes used in a local eigenfunction expansion. Usually, m is slightly larger than the number of propagating modes in the waveguide. When a typical finite difference method is used for discretizing z, we have $n \approx 10m$.

In [21], for the step from x_1 to $x_0 = x_1 - h$, the numerical scheme replaces dQ/dx at the midpoint $x_{1/2} = (x_0 + x_1)/2$ by $(Q_1 - Q_0)/h$ and approximates the Riccati equation for $x_0 < x < x_1$ by

$$\frac{Q_1 - Q_0}{h} = -\frac{1}{2}(Q_0 Q_1 + Q_1 Q_0) - \left[\partial_z^2 + \kappa^2(x_{1/2}, z)\right], \tag{4}$$

where $Q_j \approx Q(x_j)$. This is a second-order method and a small range step size h is necessary even in a range-independent region. In this paper, we develop large range step methods for the DtN re-formulation to take advantage of the weak range dependence of the waveguide. The method developed in Section 3 also approximates $\kappa(x, z)$ on the interval (x_0, x_1) by $\kappa(x_{1/2}, z)$, but it finds the exact solution of the equation

$$\frac{dQ}{dx} = -Q^2 - \left[\partial_z^2 + \kappa^2(x_{1/2}, z)\right].$$

If κ happens to be x-independent on the interval (x_0, x_1), this method produces no error in this step. Therefore, when κ varies with x slowly, we can use a step size larger than that used with the method based on (4), for a given required accuracy. The method developed in Section 5 allows us to use even larger range steps. It is a fourth-order method for the general x-dependent κ and it still gives exact solutions when κ is x-independent.

Before we proceed to develop numerical methods for the operator equations (2) and (3), it is worthwhile to compare our approach with the widely used *approximate* one-way methods. For weakly range-dependent waveguides, under the assumption that the wave field is dominated by the outgoing component (towards $+\infty$), the Helmholtz equation is often approximated by the following one-way Helmholtz equation,

$$u_x \approx i\sqrt{\partial_z^2 + \kappa^2(x, z)}\,u. \tag{5}$$

A large class of "parabolic" equations [17, 16, 18, 26, 28, 3, 5, 6] are further approximations of (5). The exact evolution equation should be $u_x = Q(x)u$, where Q satisfies the Riccati equation (2). Thus, Eq. (5) is the result of $Q(x) \approx i\sqrt{\partial_z^2 + \kappa^2(x, z)}$, say obtained from (2) by ignoring the term dQ/dx. When κ is x-independent, (5) is truly valid. However, this range-independent problem is not difficult, since it can be simply solved by the method of separation of variables. When (5) is used for weakly range-dependent problems, it often gives useful approximations to the outgoing component of the wave field. The main

advantage of (5) and its further approximations is that they can be solved efficiently by marching forward in x. However, when the one-way Helmholtz equation is used in a long range calculation, the accuracy is questionable, even when the range dependence is weak. On the contrary, the exact one-way re-formulations give exact solutions of the Helmholtz equation (including the back-scattered waves) in principle. Approximations are introduced only when the operator equations (say, (2) and (3) for Q and Y) are solved numerically.

Despite the differences between the *exact* one-way re-formulations and the *approximate* one-way Helmholtz equation, there is a common desire to use a large range step size when they are solved numerically. For the one-way Helmholtz equation, the original approach [5] is based on the Crank–Nicolson method and a rational approximation of the square root operator. This second-order method requires a small range step size even for range-independent problems. On the other hand, consider a typical step from x_0 to $x_1 = x_0 + h$; the solution of the one-way Helmholtz equation can be approximated by

$$u(x_1, z) \approx e^{ih\sqrt{\partial_z^2 + \kappa^2(x_{1/2}, z)}} u(x_0, z). \tag{6}$$

This formula is exact if $\kappa(x, z)$ is x-independent on the interval (x_0, x_1). Therefore, a large range step can be used when the range dependence is weak. One possible approach for evaluating (6) is to use the eigenvalues and eigenfunctions of the operator $\partial_z^2 + \kappa^2(x_{1/2}, z)$. The split-step Padé method [6] approximates $\exp\{ih\sqrt{\partial_z^2 + \kappa^2(x_{1/2}, z)}\}$ directly by an operator rational function and it is much more efficient. An alternative method based on higher order generalizations of the Crank–Nicolson method is presented in [19]. Both these methods allow a much larger range step in a weakly range-dependent region compared with the method in [5].

3. PIECEWISE EXACT SOLUTIONS

In this section, we develop a second-order method that approximates the waveguide by pieces of range-independent segments and uses the exact solutions for each piece for marching Q and Y in the range. This is similar to the coupled mode method [24, 25, 4, 8, 1], but the one-way re-formulation allows us to avoid the large linear system (for the coefficients of the modes in all pieces) appearing in the coupled mode method.

On the interval (x_0, x_1), the Riccati equation for Q is approximated by

$$Q' = -Q^2 - \left[\partial_z^2 + \kappa^2(x_{1/2}, z)\right], \tag{7}$$

where $x_{1/2} = x_0 + h/2 = (x_0 + x_1)/2$. For a given initial condition $Q_1 \approx Q(x_1)$, the exact solution of (7) is used to obtain $Q_0 \approx Q(x_0)$. For this purpose, we explore the relationship with the Helmholtz equation and consider the associated equation

$$u_{xx} + u_{zz} + \kappa^2(x_{1/2}, z)u = 0 \tag{8}$$

on (x_0, x_1). Since the interval (x_0, x_1) corresponds to a range-independent segment, we can decompose the wave field as right- and left-going waves

$$u = u^{(+)} + u^{(-)},$$

where $u^{(+)}$ and $u^{(-)}$ satisfy

$$u_x^{(+)} = iB_{1/2}u^{(+)}, \qquad u_x^{(-)} = -iB_{1/2}\,u^{(-)},$$

where $B_{1/2} = \sqrt{\partial_z^2 + \kappa^2(x_{1/2}, z)}$. Let $\tilde{R}_1$ be defined by

$$u^{(-)}(x_1, z) = \tilde{R}_1 u^{(+)}(x_1, z);$$

it is easy to obtain from $u_x(x_1, z) = Q_1 u(x_1, z)$ and the above relationship that

$$\tilde{R}_1 = [iB_{1/2} + Q_1]^{-1}[iB_{1/2} - Q_1]. \tag{9}$$

Similarly, we define $\hat{R}_0$ by

$$u^{(-)}(x_0, z) = \hat{R}_0 u^{(+)}(x_0, z)$$

and obtain

$$Q_0 = iB_{1/2}[I - \hat{R}_0][I + \hat{R}_0]^{-1}. \tag{10}$$

Compare the definitions of $\tilde{R}_1$ and $\hat{R}_0$ and notice that

$$u^{(+)}(x_1, z) = e^{ihB_{1/2}}u^{(+)}(x_0, z), \qquad u^{(-)}(x_1, z) = e^{-ihB_{1/2}}u^{(-)}(x_0, z);$$

we obtain

$$\hat{R}_0 = e^{ihB_{1/2}}\tilde{R}_1 e^{ihB_{1/2}}. \tag{11}$$

The formulas (9), (11), and (10) reveal the exact relationship between Q_0 and Q_1 for Eq. (7).

The fundamental solution operator Y satisfying (3) is introduced to map $u(0, z)$ to $u(L, z)$. The initial condition is $Y(L) = I$. On the interval (x_0, x_1), assuming that the Helmholtz equation is approximated by (8), we obtain $u(x_0, z) = (I + \hat{R}_0)u^{(+)}(x_0, z)$ and

$$\begin{aligned} u(x_1, z) &= (I + \tilde{R}_1)u^{(+)}(x_1, z) = (I + \tilde{R}_1)e^{ihB_{1/2}}u^{(+)}(x_0, z) \\ &= (I + \tilde{R}_1)e^{ihB_{1/2}}(I + \hat{R}_0)^{-1}u(x_0, z). \end{aligned}$$

Therefore, we have

$$Y_0 = Y_1(I + \tilde{R}_1)e^{ihB_{1/2}}(I + \hat{R}_0)^{-1}. \tag{12}$$

Notice that $\hat{R}_0$ and $\tilde{R}_1$ used above do not give a good definition for the reflection operator. On the interval (x_0, x_1), we use $\kappa(x_{1/2}, z)$ to approximate $\kappa(x, z)$ and decompose the wave field through the square root operator $B_{1/2} = \sqrt{\partial_z^2 + \kappa^2(x_{1/2}, z)}$. It is appropriate to define the reflection operator at $x_{1/2}$, say $R_{1/2}$, by

$$u^{(-)}(x_{1/2}, z) = R_{1/2}u^{(+)}(x_{1/2}, z).$$

On the other hand, the grid points $x_0, x_1, x_2, \ldots$ correspond to discontinuities of the piecewise range-independent medium. While $\tilde{R}_1$ is defined based on the wave-field decomposition in (x_0, x_1), we must also have an operator, say $\hat{R}_1$, defined based on a wave-field decomposition in (x_1, x_2). Although the total wave field u and its x derivative are ensured to be continuous at x_1, usually, $\tilde{R}_1 \neq \hat{R}_1$. Similarly, the operator $\tilde{R}_0$ defined on (x_{-1}, x_0) is not the same as $\hat{R}_0$.

Since the DtN map is closely related to the reflection operators, it is possible to use the reflection (and transmission) operators in the one-way re-formulation. For a piecewise range-independent medium, the marching formulas for the scattering operators are given in [9]. For the case considered here, the desired formulas are for the pair $(\hat{R}_0, \hat{R}_1)$, or $(\tilde{R}_0, \tilde{R}_1)$, or $(R_{1/2}, R_{3/2})$. These formulas must involve the square root operator at two nearby range-independent segments and the continuity of u and u_x at an interface must be explicitly imposed. In the DtN formulation above, the continuity condition is implicit in the requirement that Q_1 obtained from the previous calculation in (x_1, x_2) be the same Q_1 used to calculate Q_0 in (x_0, x_1).

A slightly different approach is to approximate the Helmholtz waveguide by piecewise range-independent segments using the medium values at x_0, x_1, x_2, etc., and derive operator relationships also at these points. More precisely, we consider

$$u_{xx} + u_{zz} + \kappa^2(x_j, z)u = 0$$

for $(x_{j-1/2}, x_{j+1/2})$, where $x_{j\pm1/2} = (x_j + x_{j\pm1})/2$. Exact solutions in each segment can be written down and continuity conditions at $x_{j\pm1/2}$ are used to match the solutions.

We start with a wave-field decomposition $u = u^{(+)} + u^{(-)}$, where $u^{(+)}$ and $u^{(-)}$ satisfy

$$u_x^{(+)} = iB_j u^{(+)}, \qquad u_x^{(-)} = -iB_j u^{(-)}$$

on the interval $(x_{j-1/2}, x_{j+1/2})$, where $B_j = \sqrt{\partial_z^2 + \kappa^2(x_j, z)}$. At the point x_j, we define the reflection operator R_j by

$$u^{(-)}(x_j, z) = R_j u^{(+)}(x_j, z).$$

For $j = 0$, we write down the solution and its x derivative at $x_{1/2}$ as

$$\begin{aligned} u(x_{1/2}, z) &= e^{ihB_0/2}u^{(+)}(x_0, z) + e^{-ihB_0/2}u^{(-)}(x_0, z) \\ u_x(x_{1/2}, z) &= iB_0\left[e^{ihB_0/2}u^{(+)}(x_0, z) - e^{-ihB_0/2}u^{(-)}(x_0, z)\right]. \end{aligned}$$

For $j = 1$, we use the solution on $(x_{1/2}, x_{3/2})$ and obtain

$$\begin{aligned} u(x_{1/2}, z) &= e^{-ihB_1/2}u^{(+)}(x_1, z) + e^{ihB_1/2}u^{(-)}(x_1, z) \\ u_x(x_{1/2}, z) &= iB_1\left[e^{-ihB_1/2}u^{(+)}(x_1, z) - e^{ihB_1/2}u^{(-)}(x_1, z)\right]. \end{aligned}$$

From the continuity of u and u_x at $x_{1/2}$ and the definitions of R_0 and R_1, we obtain the formulas

$$R_0 = e^{ihB_0/2}(I + T)^{-1}(I - T)e^{ihB_0/2}, \tag{13}$$

where

$$T = B_0^{-1} B_1 (I - X_1)(I + X_1)^{-1} \tag{14}$$

$$X_1 = e^{ihB_1/2} R_1 e^{ihB_1/2}. \tag{15}$$

Equation (13) has the more convenient form

$$X_0 = e^{ihB_0} (I + T)^{-1} (I - T) e^{ihB_0}, \tag{16}$$

where $X_0 = e^{ihB_0/2}\, R_0\, e^{ihB_0/2}$. The reflection operators are related to the DtN maps through the formula

$$iB_j (I - R_j)(I + R_j)^{-1} = Q_j. \tag{17}$$

This can be easily derived by writing down $u_x(x_j, z) = Q_j u(x_j, z)$ through the wave-field decomposition.

Compared with the approach based on the DtN map ((9), (11), and (10)), the method for marching the reflection operator, based on Eqs. (14) and (16), is slightly more expensive, since an extra term of $B_0^{-1} B_1$ is involved in each step.

4. LOCAL EIGENFUNCTION EXPANSION

When the DtN map Q and the fundamental solution operator Y are solved from $x = L$ to $x = 0$, formulas (9), (11), (10), and (12) are used in the step from x_1 to x_0. For a general step from x_{k+1} to x_k, where k is some integer, the marching formulas follow from (9), (11), (10), and (12) with a trivial index substitution. In this section, we consider its numerical implementation.

A direct approach is to approximate the operators by matrices. Let us consider the following boundary conditions for the Helmholtz waveguide,

$$u(x, 0) = 0, \qquad u_z(x, 1) = 0.$$

If we discretize the z axis by $z_j = j\delta$, for $j = 1, 2, \ldots, n$ and $\delta = 1/(n + \frac{1}{2})$, we could approximate the second-derivative operator ∂_z^2 by the following matrices D_2 and D_4 [21], for second and fourth orders of accuracy, respectively:

$$D_2 = \frac{1}{\delta^2} \begin{bmatrix} -2 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & -2 & 1 \\ & & 1 & -1 \end{bmatrix}, \qquad D_4 = 12 \begin{bmatrix} 10 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & 10 & 1 \\ & & 1 & 11 \end{bmatrix}^{-1} D_2.$$

To implement formulas (9), (11), (10), and (12), it is necessary to find the eigenvalue decomposition for the matrix that approximates $\partial_z^2 + \kappa^2(x_{1/2}, z)$. Namely,

$$D_4 + \begin{bmatrix} \kappa_1^2 & & & \\ & \kappa_2^2 & & \\ & & \ddots & \\ & & & \kappa_n^2 \end{bmatrix} = V \Lambda V^{\mathrm{T}}, \tag{18}$$

where $\kappa_j = \kappa(x_{1/2}, z_j)$, V is the orthogonal matrix of the eigenvectors, and Λ is the diagonal matrix of the eigenvalues. After V and Λ are obtained, the following steps are used to calculate Q_0 and Y_0 from Q_1 and Y_1:

$$\begin{aligned} S &= V^{\mathrm{T}} Q_1 V, \\ P_1 &= (i\sqrt{\Lambda} + S)^{-1}(i\sqrt{\Lambda} - S), \\ P_0 &= e^{ih\sqrt{\Lambda}} P_1 e^{ih\sqrt{\Lambda}}, \\ W &= (I - P_0)(I + P_0)^{-1}, \\ Q_0 &= iV\sqrt{\Lambda} W V^{\mathrm{T}}, \\ Y_0 &= Y_1 V(I + P_1) e^{ih\sqrt{\Lambda}} (I + P_0)^{-1} V^{\mathrm{T}}. \end{aligned}$$

Since Λ is a diagonal matrix, the matrices $\sqrt{\Lambda}$ and $e^{ih\sqrt{\Lambda}}$ are also diagonal matrices which can be easily calculated. Clearly, $O(n^3)$ operations are needed in each range marching step.

Similar to the so-called coupled mode method [24, 25, 4, 8, 1], where the solution of the Helmholtz equation is expanded in a truncated series of x-dependent eigenfunctions of the operator $\partial_z^2 + \kappa^2(x, z)$, the above algorithm for marching the operators Q and Y can be much more efficient, if we consider only the first m eigenvalues and eigenfunctions of $\partial_z^2 + \kappa^2(x, z)$. This approach is very effective, because the Helmholtz waveguide has only a finite number of propagating modes (corresponding to positive eigenvalues of $\partial_z^2 + \kappa^2$) and all the remaining eigenfunctions correspond to evanescent modes that decay exponentially with increasing x for range-independent waveguides. For weakly range-dependent waveguides, the coefficients of the evanescent modes are typically very small. Usually, it is sufficient to choose m slightly lager than the number of propagating modes (i.e., positive eigenvalues of $\partial_z^2 + \kappa^2$).

Let n be the number of points for discretizing z as before and m be the number of retained modes in the truncated local eigenfunction expansion approach; the first step of our method is to calculate the m largest eigenvalues and the corresponding eigenfunctions of $\partial_z^2 + \kappa^2(x_{1/2}, z)$. The fully discretized version corresponds to the computation of the m eigenvalues and m eigenvectors of the matrix in (18). This gives rise to

$$\left(D_4 + \begin{bmatrix} \kappa_1^2 & & \\ & \ddots & \\ & & \kappa_n^2 \end{bmatrix} \right) V_m = V_m \Lambda_m, \tag{19}$$

where Λ_m is the $m \times m$ diagonal matrix of the largest eigenvalues, and V_m is the $n \times m$ matrix of corresponding eigenvectors. Originally the operators Q and Y are approximated by $n \times n$ matrices and $O(n^3)$ operations are required in each step. In the new approach, we look only at the images of these operators acting on the first m eigenfunctions, projected into the subspace spanned by these m eigenfunctions. More precisely, we seek an $m \times m$ matrix S_0, such that

$$Q_0 V_m \approx V_m S_0.$$

Similarly, for the input of this step (x_0, x_1), the operator Q_1 is related to an $m \times m$ matrix S_1. However, S_1, being the result of the calculation of the previous step (x_1, x_2), must be

related to the m eigenfunctions of the operator $\partial_z^2 + \kappa^2$ for $x = x_{3/2}$. But for the remaining calculations of the step (from x_1 to x_0), we need an $m \times m$ matrix for Q_1 related to the eigenfunctions at $x = x_{1/2}$. If $V_m^{(\mathrm{old})}$ is the matrix of m eigenvectors at $x_{3/2}$, the relationship we have is

$$Q_1 V_m^{(\mathrm{old})} \approx V_m^{(\mathrm{old})} S_1, \tag{20}$$

where S_1 is the result of the previous step. We need to find an $m \times m$ matrix S such that

$$Q_1 V_m \approx V_m S.$$

For this purpose, we expand the eigenvectors at $x_{3/2}$ by the eigenvectors at $x_{1/2}$, and then truncate the result. This leads to

$$V_m^{(\mathrm{old})} \approx V_m H.$$

Clearly, the $m \times m$ matrix H is given by

$$H = V_m^{\mathrm{T}} V_m^{(\mathrm{old})}.$$

Equation (20) is then approximated by

$$Q_1 V_m H \approx V_m H S_1.$$

This gives rise to

$$S = H S_1 H^{-1}.$$

This is followed by the computation of P_1, P_0, and W as in the full matrix method with Λ replaced by Λ_m. The matrices P_1, P_0, and W all have the smaller size $m \times m$. The step for Q_0 is replaced by the step for S_0, with $S_0 = i\sqrt{\Lambda_m} W$. Similar considerations apply to the operator Y. We start with Z_1 satisfying

$$Y_1 V_m^{(\mathrm{old})} \approx V_m^{(\mathrm{old})} Z_1$$

and calculate Z_0 for Y_0 satisfying

$$Y_0 V_m \approx V_m Z_0.$$

The relationship between Z_0 and Z_1 is

$$Z_0 = H Z_1 H^{-1} (I + P_1) e^{ih\sqrt{\Lambda_m}} (I + P_0)^{-1},$$

where P_0 and P_1 are $m \times m$ matrices used in the calculation of S_0 for Q_0.

To summarize, we list the steps involved for marching Q and Y from x_1 to x_0 in the truncated local eigenfunction expansion approach. The inputs are matrices S_1 and Z_1 corresponding to the projected images of the operators Q_1 and Y_1 on the subspace spanned by

the first m eigenfunctions at $x_{3/2}$, and the outputs are S_0 and Z_0 for operators Q_0 and Y_0 and the eigenfunctions at $x_{1/2}$:

$$\begin{aligned} H &= V_m^{\mathrm{T}} V_m^{(\mathrm{old})}, \\ S &= H S_1 H^{-1}, \\ P_1 &= (i\sqrt{\Lambda}_m + S)^{-1}(i\sqrt{\Lambda}_m - S), \\ P_0 &= e^{ih\sqrt{\Lambda}_m} P_1 e^{ih\sqrt{\Lambda}_m}, \\ W &= (I - P_0)(I + P_0)^{-1}, \\ S_0 &= i\sqrt{\Lambda}_m W, \\ Z_0 &= H Z_1 H^{-1}(I + P_1)e^{ih\sqrt{\Lambda}_m}(I + P_0)^{-1}. \end{aligned}$$

5. FOURTH-ORDER LARGE STEP METHOD

The method developed in the previous sections is based on approximating the Helmholtz waveguide by a stepwise range-independent waveguide. In each step, the wave number κ is approximated by its value at the midpoint (still a function of z), and an exact formula for marching the DtN map step by step is then derived. When the waveguide has a very gradual range (i.e., x) dependence, a large step size is possible. However, the range step size is still limited by the variation of the waveguide in the range direction, since the stepwise approximation leads to only second-order accuracy. In this section, we improve the capacity of our large range step method by introducing a fourth-order method which still gives the exact solution for a range-independent region. Our new method relies on a fourth-order method for linear evolution equations developed in [20].

Consider the following linear evolution equation

$$y_x = \mathcal{A}(x)y, \tag{21}$$

where x is the usual "time" variable and $\mathcal{A}$ is some operator acting on functions of some transverse variable, say z. For a typical step from x_0 to $x_1 = x_0 + h$, the midpoint exponential method is

$$y_1 = e^{h\mathcal{A}(x_{1/2})} y_0, \tag{22}$$

where y_0 is the given approximation of $y(x_0)$, $x_{1/2} = x_0 + h/2$, and y_1 gives a new approximation for the solution at x_1. That is, $y_1 \approx y(x_1)$, where $y(x_1)$ is the exact solution of (21) at x_1. The method (22) is in general a second-order method, but it gives an exact solution if $\mathcal{A}$ is x-independent on the step (x_0, x_1). If the operator $\mathcal{A}$ is skew-self-adjoint (the adjoint operator is simply $-\mathcal{A}$), then the numerical solution, like the exact solution, preserves the L^2 norm, if proper boundary conditions are imposed. Namely,

$$\int |y_1|^2 \, dz = \int |y_0|^2 \, dz.$$

This is a desirable property, especially for the Schrödinger equation, where $\mathcal{A} = i[\partial_z^2 - q(x, z)]$.

A fourth-order method for (21) which retains the good properties of the second-order midpoint exponential method is developed in [20]. It gives

$$y_1 = e^{\frac{h^2}{12}\mathcal{A}'} e^{h\mathcal{A}+\frac{h^3}{24}\mathcal{A}''} e^{-\frac{h^2}{12}\mathcal{A}'} y_0, \tag{23}$$

where $\mathcal{A}$, $\mathcal{A}'$, and $\mathcal{A}''$ are all evaluated at the midpoint $x_{1/2} = x_0 + h/2$. The methods (22) and (23) are useful for evolution equations with highly oscillatory solutions and slowly varying evolution operators. The step size is restricted by the variation of the evolution operator, but is not restricted by the variation of the solution. The fourth-order method gives more accurate solutions, without much increase of computational effort. For the Schrödinger equation with a time-dependent potential, the fact that the derivatives of the operators are functions simplifies the first and third exponential operators to function multiplications.

For the Helmholtz equation (1) and the related Riccati equation (2) of the DtN map, the marching formulas (9), (11), (10), and (12) can also be derived based on (22). Let $v = u_x$; we write down the Helmholtz equation as the system

$$\frac{d}{dx}\begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} 0 & I \\ -B^2 & 0 \end{bmatrix}\begin{bmatrix} u \\ v \end{bmatrix}, \tag{24}$$

where $B = \sqrt{\partial_z^2 + \kappa^2(x, z)}$, and apply method (22) to system (24). This leads to

$$\begin{bmatrix} u_1 \\ v_1 \end{bmatrix} = \exp\left(h \begin{bmatrix} 0 & I \\ -B_{1/2}^2 & 0 \end{bmatrix} \right) \begin{bmatrix} u_0 \\ v_0 \end{bmatrix}, \tag{25}$$

where u_1, v_1 and u_0, v_0 are the approximations of u and v at x_1 and x_0, respectively, and $B_{1/2} = \sqrt{\partial_z^2 + \kappa^2(x_{1/2}, z)}$. From the definition of the DtN map, we have

$$v_1 = Q_1 u_1, \qquad v_0 = Q_0 u_0.$$

Plug the above relationships into (25); we could simplify the result and obtain (9), (11), and (10) and the formula

$$u_1 = (I + \tilde{R}_1) e^{ihB_{1/2}} (I + \hat{R}_0)^{-1} u_0, \tag{26}$$

which gives (12).

Because of its relevance to the fourth-order method later, we give a detailed derivation here. We start with the diagonalization of the 2×2 operator matrix

$$\begin{bmatrix} 0 & I \\ -B^2 & 0 \end{bmatrix} = \begin{bmatrix} I & I \\ iB & -iB \end{bmatrix} \begin{bmatrix} iB & \\ & -iB \end{bmatrix} \begin{bmatrix} I & I \\ iB & -iB \end{bmatrix}^{-1}$$

and evaluate the matrix exponential by

$$\exp\left(h \begin{bmatrix} 0 & I \\ -B^2 & 0 \end{bmatrix} \right) = \begin{bmatrix} I & I \\ iB & -iB \end{bmatrix} \begin{bmatrix} e^{ihB} & \\ & e^{-ihB} \end{bmatrix} \begin{bmatrix} I & I \\ iB & -iB \end{bmatrix}^{-1}.$$

Equation (25) then leads to

$$\begin{bmatrix} I & I \\ iB_{1/2} & -iB_{1/2} \end{bmatrix}^{-1} \begin{bmatrix} u_1 \\ Q_1 u_1 \end{bmatrix} = \begin{bmatrix} e^{ihB_{1/2}} & \\ & e^{-ihB_{1/2}} \end{bmatrix} \begin{bmatrix} I & I \\ iB_{1/2} & -iB_{1/2} \end{bmatrix}^{-1} \begin{bmatrix} u_0 \\ Q_0 u_0 \end{bmatrix}.$$

The inverse matrix above can be easily calculated,

$$\begin{bmatrix} I & I \\ iB & -iB \end{bmatrix}^{-1} = \frac{1}{2}\begin{bmatrix} I & -iB^{-1} \\ I & iB^{-1} \end{bmatrix}.$$

The above two equations give rise to

$$\left[I - iB_{1/2}^{-1}Q_1\right]u_1 = e^{ihB_{1/2}}\left[I - iB_{1/2}^{-1}Q_0\right]u_0, \tag{27}$$

$$e^{ihB_{1/2}}\left[I + iB_{1/2}^{-1}Q_1\right]u_1 = \left[I + iB_{1/2}^{-1}Q_0\right]u_0. \tag{28}$$

Therefore,

$$\left[I + iB_{1/2}^{-1}Q_0\right]\left[I - iB_{1/2}^{-1}Q_0\right]^{-1} = e^{ihB_{1/2}}\left[I + iB_{1/2}^{-1}Q_1\right]\left[I - iB_{1/2}^{-1}Q_1\right]^{-1}e^{ihB_{1/2}}.$$

Since

$$\begin{aligned}\left[I + iB_{1/2}^{-1}Q_1\right]\left[I - iB_{1/2}^{-1}Q_1\right]^{-1} &= \left[I - iB_{1/2}^{-1}Q_1\right]^{-1}\left[I + iB_{1/2}^{-1}Q_1\right] \\ &= \left[iB_{1/2} + Q_1\right]^{-1}\left[-iB_{1/2} + Q_1\right] = \tilde{R}_1, \\ \left[I + iB_{1/2}^{-1}Q_0\right]\left[I - iB_{1/2}^{-1}Q_0\right]^{-1} &= \left[I - iB_{1/2}^{-1}Q_0\right]^{-1}\left[I + iB_{1/2}^{-1}Q_0\right] \\ &= \left[iB_{1/2} + Q_0\right]^{-1}\left[-iB_{1/2} + Q_0\right] = \hat{R}_0,\end{aligned}$$

we obtain $\hat{R}_0 = e^{ihB_{1/2}}\tilde{R}_1 e^{ihB_{1/2}}$ and Eq. (10) for Q_0.

With $\tilde{R}_1$ and $\hat{R}_0$ defined above, we have

$$I + \tilde{R}_1 = I + [iB_{1/2} + Q_1]^{-1}[iB_{1/2} - Q_1] = 2i[iB_{1/2} + Q_1]^{-1}B_{1/2}.$$

Similarly,

$$(I + \hat{R}_0)^{-1} = \frac{1}{2i}B_{1/2}^{-1}[iB_{1/2} + Q_0].$$

From (27), we have

$$[iB_{1/2} + Q_1]u_1 = e^{ihB_{1/2}}[iB_{1/2} + Q_0]u_0.$$

Therefore,

$$\begin{aligned}u_1 &= [iB_{1/2} + Q_1]^{-1}e^{ihB_{1/2}}[iB_{1/2} + Q_0]u_0 \\ &= (I + \tilde{R}_1)B_{1/2}^{-1}e^{ihB_{1/2}}B_{1/2}(I + \hat{R}_0)^{-1}u_0 \\ &= (I + \tilde{R}_1)e^{ihB_{1/2}}(I + \hat{R}_0)^{-1}u_0.\end{aligned}$$

This leads to Eq. (26) and thus Eq. (12).

For the fourth-order method (23), we obtain

$$\begin{bmatrix} u_1 \\ v_1 \end{bmatrix} = H\exp\left(h\begin{bmatrix} 0 & I \\ -\partial_z^2 - \kappa^2 - \frac{h^2}{24}(\kappa^2)_{xx} & 0 \end{bmatrix}\right)H^{-1}\begin{bmatrix} u_0 \\ v_0 \end{bmatrix}, \tag{29}$$

where κ^2 and its first and second derivatives are all evaluated at the midpoint $x_{1/2}$, and

$$H = \exp\left(\begin{bmatrix} 0 & 0 \\ -\frac{h^2}{12}(\kappa^2)_x & 0 \end{bmatrix}\right).$$

It is easy to see that

$$H = \begin{bmatrix} I & 0 \\ -\frac{h^2}{12}(\kappa^2)_x & I \end{bmatrix}, \qquad H^{-1} = \begin{bmatrix} I & 0 \\ \frac{h^2}{12}(\kappa^2)_x & I \end{bmatrix}.$$

If we let

$$\tilde{Q}_j = Q_j + \frac{h^2}{12}\frac{\partial \kappa^2}{\partial x}\bigg|_{x=x_{1/2}} \qquad \text{for } j = 0, 1$$

and

$$\tilde{B}_{1/2} = \sqrt{\partial_z^2 + \left[\kappa^2 + \frac{h^2}{24}\frac{\partial^2 \kappa^2}{\partial x^2}\right]_{x=x_{1/2}}},$$

we obtain

$$\begin{bmatrix} u_1 \\ \tilde{Q}_1 u_1 \end{bmatrix} = \exp\left(h\begin{bmatrix} 0 & I \\ -\tilde{B}_{1/2}^2 & 0 \end{bmatrix}\right)\begin{bmatrix} u_0 \\ \tilde{Q}_0 u_0 \end{bmatrix}. \tag{30}$$

Comparing the above and (25), it is clear that the fourth-order formulas for marching Q and Y should be identical to the second-order ones ((9), (11), (10), and (12)), after the substitution

$$Q_0 \to \tilde{Q}_0, \qquad Q_1 \to \tilde{Q}_1, \qquad B_{1/2} \to \tilde{B}_{1/2}.$$

To summarize, our fourth-order method proceeds from the given Q_1, Y_1 at x_1 to Q_0, Y_0 at $x_0 = x_1 - h$ through the following steps:

1. Calculate $\tilde{Q}_1$ and $\tilde{B}_{1/2}$ by

$$\tilde{Q}_1 = Q_1 + \frac{h^2}{12}\frac{\partial \kappa^2}{\partial x}\bigg|_{x=x_{1/2}},$$

$$\tilde{B}_{1/2} = \sqrt{\partial_z^2 + \left[\kappa^2 + \frac{h^2}{24}\frac{\partial^2 \kappa^2}{\partial x^2}\right]_{x=x_{1/2}}}.$$

2. Calculate $\tilde{R}_1$ by

$$\tilde{R}_1 = \left[i\tilde{B}_{1/2} + \tilde{Q}_1\right]^{-1}\left[-i\tilde{B}_{1/2} + \tilde{Q}_1\right].$$

3. Calculate $\hat{R}_0$ by

$$\hat{R}_0 = e^{ih\tilde{B}_{1/2}}\tilde{R}_1 e^{ih\tilde{B}_{1/2}}.$$

4. Calculate $\hat{Q}_0$ and Y_0 by

$$\tilde{Q}_0 = i\tilde{B}_{1/2}[I - \hat{R}_0][I + \hat{R}_0]^{-1},$$
$$Y_0 = Y_1(I + \tilde{R}_1)e^{ih\tilde{B}_{1/2}}(I + \hat{R}_0)^{-1}.$$

5. Calculate Q_0 by

$$Q_0 = \tilde{Q}_0 - \frac{h^2}{12}\frac{\partial \kappa^2}{\partial x}\bigg|_{x=x_{1/2}}.$$

Therefore, the fourth-order method is achieved with very little extra work (in the first and last steps). The difference with the second-order method is adding and subtracting the derivatives of κ^2 to or from given operators.

For a direct numerical implementation based on approximating the operators by $n \times n$ matrices, where n is the number of points used to discretize z, the necessary modification for the fourth-order method is minimal. We start with calculating the eigenvalue decomposition of the matrix corresponding to $\partial_z^2 + \kappa^2 + (h^2/24)(\kappa^2)_{xx}$. That is,

$$D_4 + \begin{bmatrix} s_1 & & \\ & \ddots & \\ & & s_n \end{bmatrix} = V\Lambda V^{\mathrm{T}},$$

where $s_j = \kappa^2(x_{1/2}, z_j) + (h^2/24)(\kappa^2)_{xx}(x_{1/2}, z_j)$, and V and Λ are the matrices of eigenvectors and eigenvalues, respectively. The matrix representations of Q_0, Q_1 and $\tilde{Q}_0$, $\tilde{Q}_1$ are related to each other by the following diagonal matrix:

$$F = \frac{h^2}{12}\,\mathrm{diag}\big[(\kappa^2)_x(x_{1/2}, z_1), \ldots, (\kappa^2)_x(x_{1/2}, z_n)\big].$$

Therefore, after V and Λ are calculated, we proceed as follows:

$$\begin{aligned}
\tilde{Q}_1 &= Q_1 + F,\\
S &= V^{\mathrm{T}}\tilde{Q}_1 V,\\
P_1 &= (i\sqrt{\Lambda} + S)^{-1}(i\sqrt{\Lambda} - S),\\
P_0 &= e^{ih\sqrt{\Lambda}}P_1 e^{ih\sqrt{\Lambda}},\\
W &= (I - P_0)(I + P_0)^{-1},\\
\tilde{Q}_0 &= iV\sqrt{\Lambda}WV^{\mathrm{T}},\\
Y_0 &= Y_1 V(I + P_1)e^{ih\sqrt{\Lambda}}(I + P_0)^{-1}V^{\mathrm{T}},\\
Q_0 &= \tilde{Q}_0 - F.
\end{aligned}$$

For the implementation based on the truncated local eigenfunction expansion, only the first m eigenvalues and eigenvectors are needed,

$$\left(D_4 + \begin{bmatrix} s_1 & & \\ & \ddots & \\ & & s_n \end{bmatrix}\right) V_m = V_m \Lambda_m,$$

where Λ_m is the $m \times m$ diagonal matrix of the m largest eigenvalues and V_m is the $n \times m$ matrix of the corresponding eigenvectors. Similarly, in the previous step (x_1, x_2), we have obtained a matrix of m eigenvectors, denoted by $V_m^{(\mathrm{old})}$, at $x_{3/2}$. Since the operators Q_1 and Q_0 are represented by the $m \times m$ matrices S and S_0 for the subspace spanned by the columns of V_m, it is necessary to calculate a similar matrix representation for the function $(h^2/12)(\kappa^2)_x$. For the diagonal matrix F given above, we look for an $m \times m$ matrix G, such that

$$FV_m \approx V_m G.$$

This leads to $G = V_m^{\mathrm{T}} F V_m$. Therefore, the operators $\tilde{Q}_1$ and $\tilde{Q}_0$ are represented by $S + G$ and $S_0 - G$, respectively. In summary, we have

$$\begin{aligned}
H &= V_m^{\mathrm{T}} V_m^{(\mathrm{old})}, \\
S &= H S_1 H^{-1}, \\
G &= V_m F V_m, \\
\tilde{S} &= S + G, \\
P_1 &= (i\sqrt{\Lambda}_m + \tilde{S})^{-1}(i\sqrt{\Lambda}_m - \tilde{S}), \\
P_0 &= e^{ih\sqrt{\Lambda}_m} P_1 e^{ih\sqrt{\Lambda}_m}, \\
W &= (I - P_0)(I + P_0)^{-1}, \\
\tilde{S}_0 &= i\sqrt{\Lambda}_m W, \\
S_0 &= \tilde{S}_0 - G, \\
Z_0 &= H Z_1 H^{-1}(I + P_1) e^{ih\sqrt{\Lambda}_m}(I + P_0)^{-1}.
\end{aligned}$$

6. NUMERICAL EXAMPLES

To demonstrate the large range step capacity of our method, we consider the following example where κ is given by

$$\kappa^2(x, z) = \kappa_0^2\left[1 + 0.05e^{-20(x/L-0.5)^2}\sin^2(\pi z)\right].$$

We choose $\kappa_0 = 10$ and $L = 10$. The second derivative in z is discretized by a fourth-order finite difference method with $n = 30$.

At $x = 0$, we impose the following starting field:

$$u_0(z) = \sum_{j=1}^{7} \sin(m_j z_0)\sin(m_j z)/\sqrt{\kappa_0^2 - m_j^2} \qquad \text{for } m_j = (j - 1/2)\pi,\ z_0 = 0.65.$$

The wave field at $x = L$ is obtained by $u(L, z) = Y(0)u_0(z)$, where $Y(0)$ is calculated by solving Q and Y from $x = L$ to $x = 0$. Since the range dependence of the waveguide is quite weak, the transmitted wave is not very difficult to calculate. We first use a small range step size $h = 1/128$ to calculate a very accurate solution for reference. After that, we calculate the solution with much larger range steps and then compare them with the more accurate reference solution. In Fig. 1, we plot the approximate solutions of $u(L, z)$ for $h = 1$ and $h = 1/128$. We conclude that reasonably good solutions are already obtained with $h = 1$. In

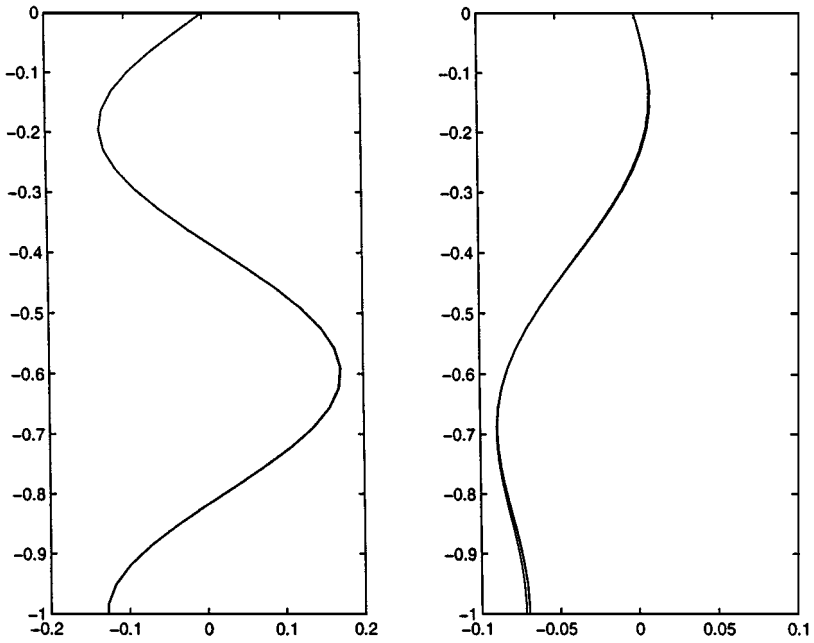

FIG. 1. Comparison of $u(L, z)$ for $h = 1$ and $h = 1/128$.

the following table, we list the relative errors of the numerical solutions of $u(L, z)$ obtained by our fourth-order method with different choices of the range step size. The relative error is calculated using the Euclidean norm for the vector at the n different z values (corresponding to the L^2 norm of functions of z):

Step size h:	1	1/2	1/4	1/8	1/16
Relative error	0.010	0.0049	8.3E-6	2.6E-7	1.6E-8

In contrast, the relative errors of the second-order method are

$$1.04\text{E-}4, \qquad 2.51\text{E-}5, \qquad 6.14\text{E-}6$$

for $h = 1/4$, $1/8$, and $1/16$, respectively.

Since the waveguide has a very gradual range dependence, the back-scattered waves are quite weak. Based on the DtN map at $x = 0$, i.e., $Q(0)$, we find the reflection operator $R(0)$ and then multiply $R(0)$ on different incident waves to find their corresponding reflected waves. As an example, we consider the back-scattering of the incident wave corresponding to the third propagating mode:

$$u^{(i)}(0, z) = \sin(2.5\pi z).$$

In Fig. 2, the reflected wave calculated by the fourth-order method with $h = 1/8$ is compared with a much more accurate solution obtained with $h = 1/128$. Although the magnitude is only around 10^{-5}, a reasonably accurate solution is already obtained with $h = 1/8$. In contrast, we observe from Fig. 3 that the numerical solution based on the second-order method has a much larger error.

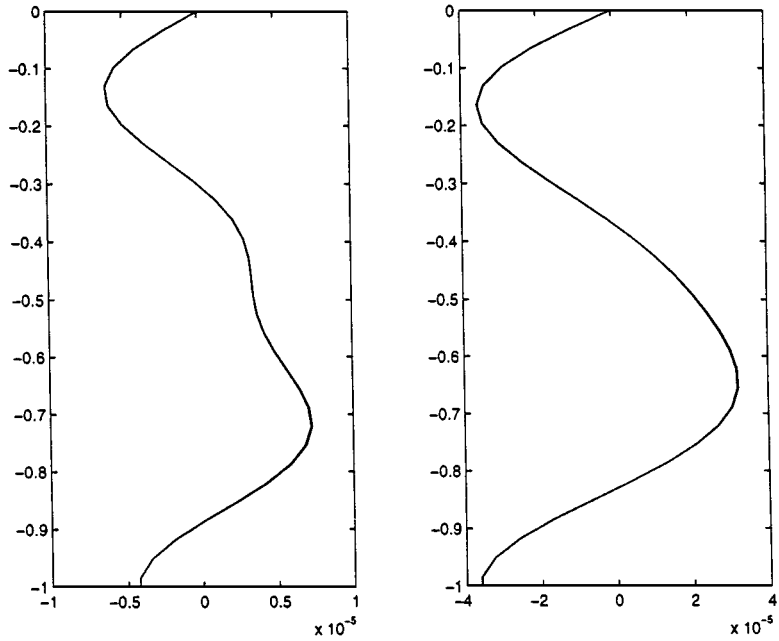

FIG. 2. The reflected wave calculated by the fourth-order method with $h = 1/8$ and $h = 1/128$.

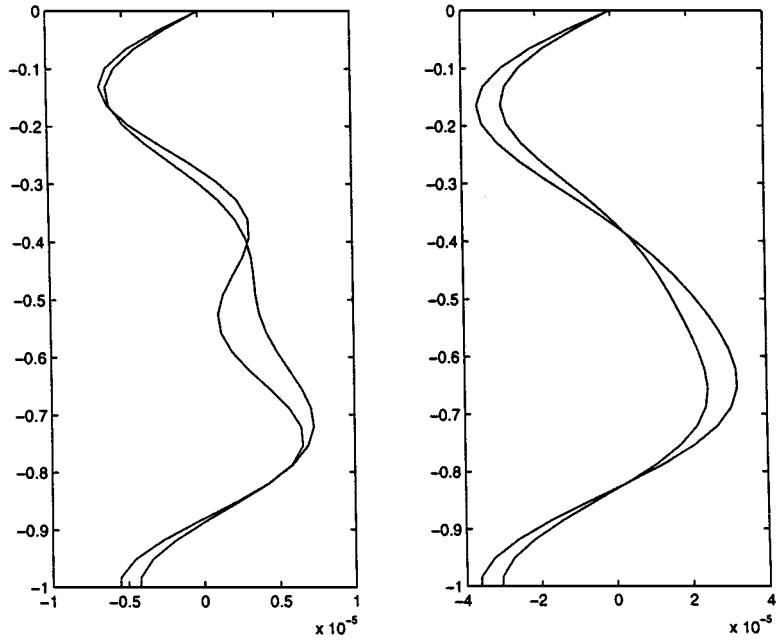

FIG. 3. The reflected wave calculated by the second-order method with $h = 1/8$ and the fourth-order method with $h = 1/128$.

7. CONCLUSION

We have developed large range step methods for Helmholtz waveguides with a particularly large range length scale and a slow variation in the range direction. As in [21], the one-way re-formulation of the Helmholtz equation in terms of the DtN map Q and the fundamental solution operator Y is used. Such a one-way re-formulation is useful when the range length scale is much larger than the transverse length scale of the waveguide, since numerical methods developed based on these one-way re-formulations have memory requirements independent of the total range distance and the computation time is linearly related to the same distance. We notice that for many practical applications, medium properties of the waveguide have a very gradual variation with the range variable, i.e., only very small changes in a typical wavelength. Finite difference and finite element methods fail to take advantage of this feature and a small step size in the range is required even when the waveguide is range-independent. Typically, a few points are always required by these methods in each wavelength to resolve the highly oscillatory wave field. On the other hand, when the waveguide is range-independent, the equation is separable and its exact solution at any range can be written down in terms of the eigenfunctions of the transverse operator. It is quite natural that for nearly separable (slowly varying with range) waveguides, one approximates the waveguide by a piecewise range-independent waveguide and patches the exact solution in each piece together to obtain an approximate solution for the whole waveguide. The coupled mode method [8] uses this approach by solving a global linear system for the coefficients representing the exact solutions in each piece. Our method developed in Sections 3 and 4 also uses the approximation of a piecewise range-independent waveguide. While the coupled mode method uses the local eigenfunction expansion to write down the exact solutions in each piece, we use the same expansion to reduce the operators Q and Y to their images in the eigenfunction space. Since the waveguide supports only a finite number of propagating modes, good approximation is possible when the eigenfunction expansion is truncated with a relatively small number of terms. Because of the one-way re-formulation used in our methods, the operators are marched in the range as an initial value problem, avoiding the large linear system appearing in the coupled mode method.

The drawback of the coupled mode method [8] and our method in Sections 3 and 4 is the low order of accuracy associated with the approximation of a range-dependent waveguide by a piecewise range-independent one. Such an approximation typically leads to a second order of accuracy, so the range step size is still limited by the variation of the waveguide in the range variable. Our method developed in Section 5 is a fourth-order method that preserves the good properties of the second-order method. Namely, for a range-independent piece, the fourth-order formulas for matching Q and Y are still exact. This improved method is related to a fourth-order conservative exponential method developed in [20] for highly oscillatory evolution equations such as the Schrödinger equation. Finally, our fourth-order method requires very little extra work compared with the original second-order method. The advantage of this method is verified by numerical experiments in Section 6.

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