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Padé approximate solution for wave propagation in graded-index metamaterials

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Abstract
A new approximate solution for wave propagation in graded-index media is developed whereby the exact wave propagation equation is replaced by any one of a sequence of higher-order (m, n) Padé approximant operators. The resulting formulations may be discretized by common numerical schemes and solvable by existing numerical techniques. The accuracy of this approximate calculation of the wave propagator is demonstrated in comparison with the exact result. We then employ the resulting method to investigate wave propagation in metamaterials with graded-index profiles which change according to a hyperbolic tangent function along the propagation direction.

Keywords: Padé approximant operators, wave propagation, graded-index metamaterials

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Electromagnetic (EM) metamaterials, a new class of artificial composite materials, have recently attracted intensive interest due to their potential for new applications such as negative refraction, inverse Doppler effect, and radiation tension instead of pressure [1, 2], as well as the electromagnetic cloaking of arbitrary shaped objects [3]. In addition, there has been growing research interest in the propagation behavior of EM waves in metamaterials with material properties which change during the propagation direction.

There exist analytical and numerical approaches to investigate wave propagation in optical structures incorporating metamaterials with graded-index profiles such as the invariant embedding method [4] and the finite difference time domain (FDTD) method [5, 6]. While the analytical methods are currently limited to low-dimensionality problems, the FDTD method is well known as a time-consuming method, especially for three-dimensional structures. Efforts to find more efficient methods for large computational problems are thus very imperative. In this paper, we present a new approximate solution for wave propagation whereby the exact wave propagation operator is approximated by any one of a sequence of higher-order (m, n) Padé approximant operators. The resulting formalism offers a substantial advantage in terms of an accurate and efficient solution of high-dimensionality wave propagation problems.

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2. Formulation

For isotropic metamaterials we assume that their optical properties can be described by the effective dielectric permittivity and the effective magnetic permeability. Furthermore, with EM fields that are periodic in time according to an $\exp(-\mathrm{i}\omega t)$ dependency we can obtain the scalar wave equations for the electric field (E_y) and the magnetic field (H_x) components from Maxwell's equations as follows [7]:

$$\frac{\partial^2 E_y}{\partial z^2} + \frac{\partial^2 E_y}{\partial x^2} + \frac{\partial^2 E_y}{\partial y^2} - \frac{1}{\mu}\frac{\partial \mu}{\partial z}\frac{\partial E_y}{\partial z} + \omega^2 \mu\varepsilon E_y = 0 \quad (1)$$

or

$$\frac{\partial^2 H_x}{\partial z^2} + \frac{\partial^2 H_x}{\partial x^2} + \frac{\partial^2 H_x}{\partial y^2} - \frac{1}{\varepsilon}\frac{\partial \varepsilon}{\partial z}\frac{\partial H_x}{\partial z} + \omega^2 \mu\varepsilon H_x = 0 \quad (2)$$

Table 1. Most useful low-order Padé approximants for wave propagator in terms of the operator $X = \frac{P}{Q^2}$.

Order	Expression: Padé	Expression: Modified Padé
(1, 1)	$\dfrac{X}{1-X}$	$\dfrac{X}{1-\dfrac{1}{1+\mathrm{i}\beta/2}X}$
(2, 2)	$\dfrac{X-2X^2}{1-3X+X^2}$	$\dfrac{X-\left(1+\dfrac{1}{1+\mathrm{i}\beta/2}\right)X^2}{1-\left(2+\dfrac{1}{1+\mathrm{i}\beta/2}\right)X+\dfrac{1}{1+\mathrm{i}\beta/2}X^2}$
(3, 3)	$\dfrac{X-4X^2+3X^3}{1-5X+6X^2-X^3}$	$\dfrac{X-\left(3+\dfrac{1}{1+\mathrm{i}\beta/2}\right)X^2+\left(1+\dfrac{2}{1+\mathrm{i}\beta/2}\right)X^3}{1-\left(4+\dfrac{1}{1+\mathrm{i}\beta/2}\right)X+\left(3+\dfrac{3}{1+\mathrm{i}\beta/2}\right)X^2-\dfrac{1}{1+\mathrm{i}\beta/2}X^3}$

where $\varepsilon = \varepsilon(\omega, z)$ and $\mu = \mu(\omega, z)$ are the frequency-dependent electric permittivity and magnetic permeability, respectively. These equations describe the propagation of EM waves through a medium of which the constitutive parameters vary along the propagation direction z-axis.

We now start to solve these equations numerically and investigate the propagation of EM waves through a graded-index metamaterial structure. The transition between negative and positive index media was ignored in this paper. We choose a graded-index profile for both the permittivity and the permeability to make sure that their first derivative terms are non-zero. For simplification purposes, we only consider equation (1) as those for equation (2) are equivalent. Equation (1) can be rewritten as

$$Q\frac{\partial E_y}{\partial z} - \frac{\partial^2 E_y}{\partial z^2} = PE_y \tag{3}$$

where $P = \nabla_\perp^2 + \omega^2\mu\varepsilon = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \omega^2\mu\varepsilon$ and $Q = \frac{1}{\mu}\frac{\partial\mu}{\partial z}$.

We may formally rewrite equation (3) in the form

$$\frac{\partial E_y}{\partial z} = \frac{P}{Q - \frac{\partial}{\partial z}}E_y. \tag{4}$$

Equation (4) suggests the following recurrence relation

$$\left.\frac{\partial}{\partial z}\right|_{n+1} = \frac{P}{Q - \left.\frac{\partial}{\partial z}\right|_n}. \tag{5}$$

This recurrence relation is the well-known form in the area of guided-wave optics which results in either the real or the modified Padé approximant operators depending on its initial value [8–11]. If equation (5) is used to replace the first derivative of fields with respect to z with an expression containing only the operator P, then a propagator of the following form is obtained:

$$\frac{\partial E_y}{\partial z} \approx \frac{N}{D}E_y. \tag{6}$$

where N and D are polynomials in P.

2.1. Real Padé approximant operators

In case the initial value of $\frac{\partial}{\partial z}|_0 = 0$ is used, this gives us a real Padé (m, n) approximant-based wave propagation formula as follows:

$$\frac{\partial E_y}{\partial z} \approx Q\frac{A(m)}{B(n)}E_y \tag{7}$$

where $A(m)$ and $B(n)$ are polynomials in $X = \frac{P}{Q^2}$. The most useful low-order Padé (m, n) approximant operators are shown in table 1.

If equation (7) is compared with a formal solution of equation (1) written in the well-known form

$$\frac{\partial E_y}{\partial z} = Q\left(\frac{1}{2} - \sqrt{\frac{1}{4} - X}\right)E_y, \tag{8}$$

we obtain the approximation formula

$$\frac{1}{2} - \sqrt{\frac{1}{4} - X} \approx \frac{A(m)}{B(n)}. \tag{9}$$

Since the operator X has a real spectrum, it is useful to consider the approximation of $\frac{1}{2} - \sqrt{\frac{1}{4} - X}$ by the Padé approximant operators. Figure 1 shows the absolute values of $\frac{1}{2} - \sqrt{\frac{1}{4} - X}$ and the most useful low-order Padé (m, n) approximant operators with respect to X. It is shown that the real Padé (m, n) approximations are a good fit to the exact solution of the wave equation. Furthermore, it is clearly seen that the higher order of the approximation Padé (m, n) is, the more accurate approximation to wave propagator is obtained. However, if the denominator of the real approximation Padé (m, n) formula approaches zero, its absolute value approaches ∞ as clearly seen in figure 2. Physically, the real Padé approximant operators incorrectly propagate evanescent modes. To circumvent this problem, we introduce modified Padé approximant operators as follows.

2.2. Modified Padé approximant operators

By sharing the same idea with the real Padé approximant operators but using a different initial value we obtain the

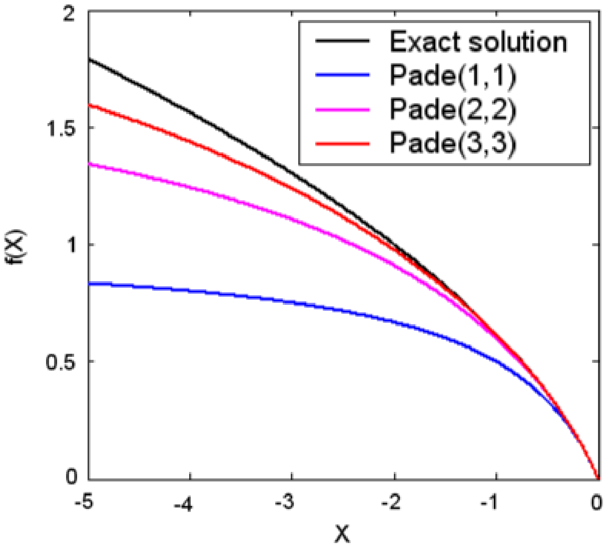

Figure 1. The absolute values of $f(X) = \frac{1}{2} - \sqrt{\frac{1}{4} - X}$ and the most useful low-order Padé approximant operators.

modified Padé approximant operators. Here, we derive this initial value for the specific problem that we are considering here.

From equation (4) we can derive the relevant form as follows:

$$-\frac{2}{Q}\frac{\partial}{\partial z} = \frac{-\frac{4P}{Q^2}}{2 - \frac{2}{Q}\frac{\partial}{\partial z}}. \tag{10}$$

This equation may be rewritten by

$$f(Y) = \frac{Y}{2 + f(Y)} \tag{11}$$

where $f(Y) = -\frac{2}{Q}\frac{\partial}{\partial z}$ and $Y = -\frac{4P}{Q^2}$.

Equation (11) suggests the recurrence relation

$$f_{n+1}(Y) = \frac{Y}{2 + f_n(Y)} \qquad \text{for } n = 0, 1, 2, \ldots. \tag{12}$$

Lu [12] has proved that equation (12) can provide a good approximation to $\sqrt{1+Y} - 1$ with the initial value of

$$f_o(Y) = \mathrm{i}\beta \qquad \text{where } \beta > 0 \text{ is a damping parameter.} \tag{13}$$

Subsequently, our modified Padé approximant operators are obtained from the same recurrence formula (5) with a different initial value of $\frac{\partial}{\partial z}|_0 = -\mathrm{i}\frac{\beta}{2}Q$. The most useful low-order modified Padé approximant operators are also shown in table 1.

The absolute value and real part of the modified Padé (1, 1) approximant of $\frac{1}{2} - \sqrt{\frac{1}{4} - X}$ are also depicted in figure 2. It is seen that the modified Padé (1, 1) (with $\beta = 2$) allows a more accurate approximation to the true wave equation than the real Padé (1, 1) operator. Furthermore, the real one incorrectly propagates evanescent modes as its denominator gradually approaches zero. In contrast, the modified Padé operator could give waves propagating in evanescent regions the desired damping as shown in the same figure.

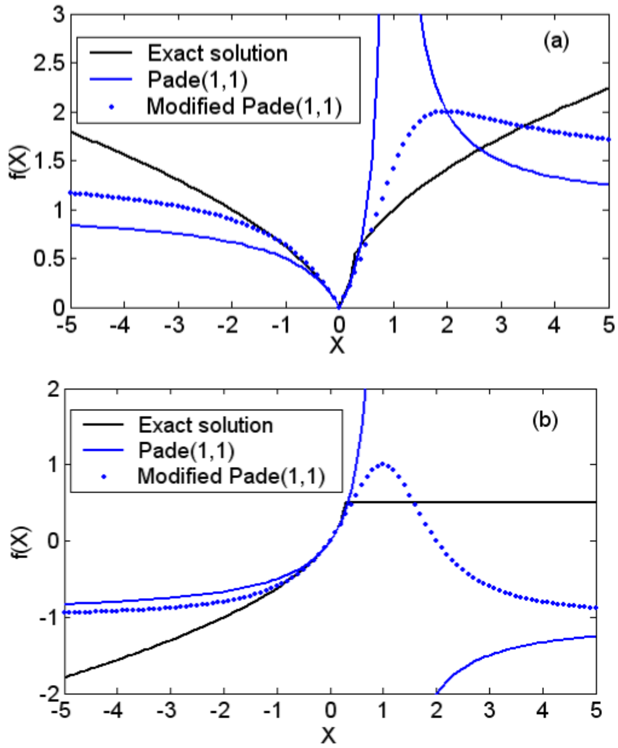

Figure 2. The absolute values (a) and real part (b) of $f(X) = \frac{1}{2} - \sqrt{\frac{1}{4} - X}$, the most useful low-order real and complex Padé approximant operators.

2.3. *Numerical implementation of Padé-based wave propagation*

One of the most commonly used techniques to numerical deal with equation (7) is the finite difference method. Finite difference equations may be derived from equation (7) by clearing the denominator and centering with respect to z in the usual way:

$$B(E_y^{n+1} - E_y^n) = \frac{Q^n \Delta z}{2} A(E_y^{n+1} + E_y^n). \tag{14}$$

Equation (14) can be solved effectively by a multistep method whereby each component step is treated by the traditional direct matrix inversion (DMI) [11]. However, for large problems requiring huge amounts of memory, it is very slow to establish matrix inversion DMI. In the last decade alternative methods have been proposed to solve matrix inversion effectively by iteration techniques such as Bi-CGSTAB [13]. However, for large three-dimensional problems where the material properties change frequently and which therefore require frequent matrix inversions, this can still be a numerically intensive task. Recently, we reported a different approach by using the new complex Jacobi iterative (CJI) method [14]. There, the wave propagation equation is recast in terms of a Helmholtz equation with a source term. The utility of the CJI technique depends mostly upon its execution speed dominated by the amount of effective absorption (or medium loss). If the medium loss is high, the convergence rate is thus fast.

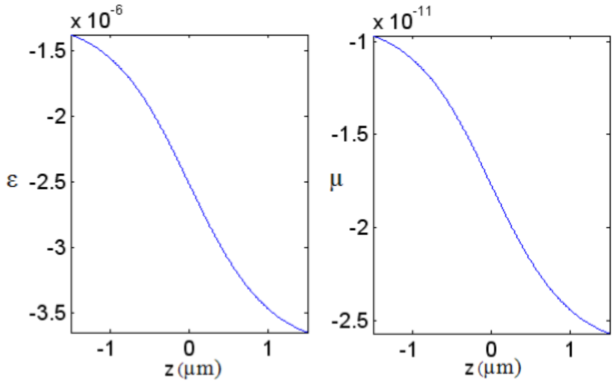

Figure 3. The permittivity and permeability vary along the propagation direction according to a hyperbolic tangent function assumed in this paper.

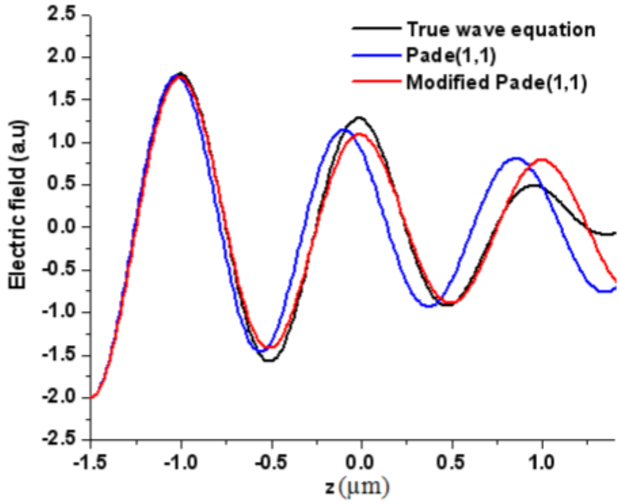

Figure 4. Propagation of electric wave in graded-index structure with positive index profile changing according to hyperbolic tangent function.

3. Example

In order to prove the applicability of this approximant method, we now employ it to study wave propagation in an inhomogeneous negative index metamaterial whereby the effective permittivity and permeability vary according to a hyperbolic tangent function. Of course, our method works equally well for positive index graded materials.

We consider an electric wave propagating in a medium where ε and μ are both always non-zero and are given by the following functions (see figure 3):

$$\begin{aligned} \varepsilon &= -\varepsilon_0\varepsilon_{\mathrm{eff}}(\omega)(\tanh(\rho z)+2), \\ \mu &= -\mu_0\mu_{\mathrm{eff}}(\omega)(\tanh(\rho z)+2), \end{aligned} \tag{15}$$

where ρ ($=10^{+6}$) is a positive parameter ensuring index profiles to be graded and the first derivative of ε and μ are therefore non-zero. We assume a wave with wavelength of $\lambda_0 = 1\ \mu$m propagating in such a medium of $\varepsilon_{\mathrm{eff}}(\lambda_0) = \mu_{\mathrm{eff}}(\lambda_0) = 1$. Figure 4 shows the comparison of the calculated results obtained by the solution from the real Padé operator, the modified Padé operator and the true wave equation (which are solved directly by the finite element method in the commercial software—COMSOL multiphysics [15]). It is seen that the result obtained from the modified Padé operator allows a better agreement to the true wave equation than that of the real one.

4. Conclusions

In this paper, we have derived a new approximate solution for wave propagation in graded-index media based on Padé approximant operators. The resulting formulas allow accurate approximations to the true wave equation. This results in a promising tool to investigate wave propagation in media where the permittivity and the permeability change during propagation direction.

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