Differential transfer-matrix method for solution of one-dimensional linear nonhomogeneous optical structures

Sina Khorasani
School of Electrical and Computer Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332-0250, and Department of Electrical Engineering, Sharif University of Technology, P.O. Box 11365-9363, Tehran, Iran

Khashayar Mehrany
Department of Electrical Engineering, Sharif University of Technology, P.O. Box 11365-9363, Tehran, Iran

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We present an analytical method for solution of one-dimensional optical systems, based on the differential transfer matrices. This approach can be used for exact calculation of various functions including reflection and transmission coefficients, band structures, and bound states. We show the consistency of the WKB method with our approach and discuss improvements for even symmetry and infinite periodic structures. Moreover, a general variational representation of bound states is introduced. As application examples, we consider the reflection from a sinusoidal grating and the band structure of an infinite exponential grating. An excellent agreement between the results from our differential transfer-matrix method with other methods is observed. The method can be equally applied to one-dimensional time-harmonic quantum-mechanical systems. © 2003 Optical Society of America

1. INTRODUCTION

The analytical solution of one-dimensional (1-D) wave-propagation problems in arbitrary nonhomogeneous quantum and optical systems has been studied in numerous reports. The existing known approaches include the transfer-matrix function,1 the iterative eigenfunction expansion method,2 and the domain integral equation method.3 There exist also approximate approaches, including semiclassical4 and the famous WKB5 methods. The transfer-matrix function has the capability to analyze 2-D-dimensional problems; however, the structure has to be artificially placed in a virtual rectangular tube with infinite potential barriers. The iterative eigenfunction expansion method and the domain integral equation method both require elaborate numerical computations and cannot be applied only by analytical methods. The semiclassical methods, though analytically simple, are too approximate and fail in correct derivation of lower-order modes. There is therefore still a need for development of a mathematical approach capable of solving 1-D problems analytically with less effort.

The solution of the wave equation is studied for nonhomogeneous layered media with piecewise constant profiles of refractive index through the well known transfer-matrix method6–8 (TMM). In the standard TMM,6,8 the up- and down-traveling plane waves in layers are matched to those of adjacent layers, in compliance with the continuity of the total electromagnetic field and its derivative, and the resulting equations are written in matrix form with each layer having its own reference of position. The TMM has been recently improved7 to include the effect of interface conductivity (which appears as discontinuities in the derivative of electric field), and the same reference for addressing the position has been employed in all layers.

In this paper, a new analytical method is described for calculation of the scalar wave function in 1-D optical systems. Here, we take the benefit of having the same reference of position in the improved TMM,7 while neglecting the presence of conducting interfaces through setting the interface conductivities to zero. As discussed below, this has enabled us to evolve the transfer matrices into differential forms. Our formalism can be used for derivation of reflection and transmission coefficients of the system, as well as its bound states. The proposed method is mathematically exact within the validity range of the 1-D approximation of the realistic physical system. We demonstrate the compatibility of the WKB method with our approach and discuss improvements under even symmetry and infinite periodic structures. We show the applications to several examples and also present a variational form for the bound states. In both cases, an excellent agreement is observed, as discussed below.

2. FORMULATION

The propagation of a scalar TE polarized electromagnetic wave in a 1-D nonhomogeneous time-harmonic system is given by
\[
\frac{\partial^2}{\partial x^2} A(x) + k^2(x) A(x) = 0, \tag{1}
\]

in which \( A(x) \) and \( k(x) \) represent the field amplitude and wave vector, respectively. We further accept that either \( k(x) \) or \( jk(x) \) are real and positive with \( j = \sqrt{-1} \); this condition corresponds to lossless media. For the moment, we limit ourselves to TE polarized waves, since the treatment of TM modes is slightly different.

We propose a solution to Eq. (1) of the form

\[
A(x) = A^+(x) \exp[-jk(x)x] + A^-(x) \exp[+jk(x)x], \tag{2}
\]

with \( A^+(x) \) and \( A^-(x) \) as unknown functions, associated with the forward and backward waves, to be determined.

According to the transfer-matrix method, \(^\text{6-8} \) if \( k(x) \) is piecewise constant equal to \( k_1 \) and \( k_2 \) for \( x < X \) and \( x > X \), respectively, the functions \( A^\pm(x) \) would be also constants equal to \( A_1^\pm \) or \( A_2^\pm \). In this case, one has

\[
A_0 = Q_{1 \rightarrow 2} A_1,
\]

in which \( A_0 = [A^+_1 \ A^-_2] \) and

\[
Q_{1 \rightarrow 2} = \begin{bmatrix}
\frac{k_2 + k_1}{2k_2} & \frac{k_2 - k_1}{2k_2} \\
-\frac{k_2 - k_1}{2k_2} & \frac{k_2 + k_1}{2k_2}
\end{bmatrix}
\]

is the transfer matrix from layer 1 to layer 2. This transfer matrix resembles the wave-amplitude transmission matrix\(^\text{6,7} \) in microwave engineering, where the determinant equals the ratio between impedances in both sides of the junction. In contrast, by direct inspection of Eq. (4) one can verify that \( |Q_{1 \rightarrow 2}| = k_1/k_2 \).

As stated above, this approach follows the modified TMM\(^\text{7} \) in which the same reference is used for addressing the position in all layers. This special treatment of transfer matrices enables us to proceed with the analytical calculations, mainly because of the solution form prescribed in Eq. (2), which requires a single reference at \( x = 0 \).

Now if \( k(x) \) is an analytic function of \( x \), one can write

\[
A(x + dx) = Q_{x \rightarrow x + dx} \cdot A(x), \tag{5}
\]

where \( A(x)' = [A^+(x) \ A^-(x)] \). Equivalently,

\[
dA(x) = (Q_{x \rightarrow x + dx} - I) \cdot A(x) = U(x) \cdot A(x) dx, \tag{6}
\]

in which \( I \) is the identity matrix. Also differentiating Eq. (4) results in

\[
U(x) = \frac{1}{2k(x)} \frac{dk(x)}{dx} \begin{bmatrix}
-1 + j2k(x)x \\
-1 - j2k(x)x
\end{bmatrix}
\exp[+j2k(x)x] - \begin{bmatrix}
1 \\
1
\end{bmatrix}
\exp[-j2k(x)x], \tag{7a}
\]

which can be equally rewritten as

\[
U(x) = \frac{1}{2k(x)} \begin{bmatrix}
I - j2k(x)x \\
I + j2k(x)x
\end{bmatrix}
\exp[+j2k(x)x] - \begin{bmatrix}
I \\
I
\end{bmatrix}
\exp[-j2k(x)x], \tag{7b}
\]

in which the first term represents the phase accumulation along the propagation path, and the second term represents the interaction between up- and down-traveling waves. Below, we observe that the second expression can be neglected under the assumption of gradual variations for \( k(x) \).

However, Eq. (6) has a solution of the form

\[
A(x_2) = \exp[\int_{x_1}^{x_2} U(x) dx] A(x_1) = \exp(M) \cdot A(x_1)
\]

\[
= Q_{x_1 \rightarrow x_2} \cdot A(x_1), \tag{8}
\]

in which \( \exp(M) \) is defined as

\[
\exp(M) = I + \sum_{n=1}^{\infty} \frac{1}{n!} M^n. \tag{9}
\]

It thus can be easily observed that \( \exp(0) = I \) and \( \exp(M)^{-1} = \exp(-M) \). Meanwhile, the transfer matrix \( Q_{x_1 \rightarrow x_2} \) has the properties

\[
Q_{x \rightarrow x} = I, \tag{10a}
\]

\[
Q_{x_2 \rightarrow x_3} \cdot Q_{x_1 \rightarrow x_2} = Q_{x_1 \rightarrow x_3}, \tag{10b}
\]

\[
Q_{x_2 \rightarrow x_3} = Q_{x_1 \rightarrow x_2}^{-1}, \tag{10c}
\]

\[
|Q_{x_1 \rightarrow x_2}| = k(x_1)/k(x_2). \tag{10d}
\]

Equation (10a) is directly followed by Eqs. (7)–(9), and the validity of Eqs. (10b) and (10c) originates from the definition of transfer matrices. Equation (10d) holds, since the determinant of the basic transfer matrix as given by Eq. (4) is \( |Q_{1 \rightarrow 2}| = k_1/k_2 \).

In order for \( \exp(A) \exp(B) = \exp(B) \exp(A) = \exp(A + B) \), the necessary and sufficient condition is that \( [A, B] = 0 \).

3. ADDITIONAL CONSIDERATIONS

A. Constant Wave Vector

In this case, \( k(x) = k \) corresponds to a homogeneous medium. Therefore the vector \( A(x) \) would be also independent of \( x \). In other words, for any \( x_1 \) and \( x_2 \), \( Q_{x_1 \rightarrow x_2} = I \). However, this condition is automatically satisfied by Eqs. (7) and (8), by taking \( \frac{dk(x)}{dx} = 0 \).
B. Single Interface Across Two Homogeneous Media

In this case, the wave vector \( k(x) \) is given by

\[
k(x) = \begin{cases} 
  k_1 & x < X \\
  k_2 & x > X 
\end{cases}
\]  

\( (11) \)

Therefore the parameter \( dk(x)/dx \) is nonzero only at the interface \( x = X \), being singular. According to the discussions in the previous subsection, one has

\[
Q_{x_1 < x_2} = \begin{cases} 
  I & x_1 < x_2 < X \\
  \text{Q}_{x_2} & X < x_2 < x_1 \\
  \text{I} & X < x_1 < x_2 
\end{cases}
\]  

\( (12) \)

with \( \text{Q}_{x_2} = \exp(M) \) and

\[
M = \begin{bmatrix} 
  \int_{k_1}^{k_2} (-1 + j2kX) \frac{dk}{2k} & \int_{k_1}^{k_2} \exp(\text{j}2kX) \frac{dk}{2k} \\
  \int_{k_1}^{k_2} \exp(-j2kX) \frac{dk}{2k} & \int_{k_1}^{k_2} (-1 - j2kX) \frac{dk}{2k} 
\end{bmatrix}.
\]  

\( (13) \)

In derivation of Eq. (13) we notice that the integrals running from \( x_1 < X < x_2 \) are nonzero where \( dx/k(x)/dx \) is singular, i.e., at the interface \( x = X \). Subsequently, the integrals can be evaluated by a change of variables from \( x \) to \( k \).

Unfortunately, it is not possible to evaluate the off-diagonal elements of \( M \) analytically. However, in the case that \( X = 0 \), Eq. (13) can be simplified as

\[
M = \frac{1}{2} \ln \begin{bmatrix} 
  k_1 \\
  k_2 
\end{bmatrix} \begin{bmatrix} 
  1 & -1 \\
  -1 & 1 
\end{bmatrix}.
\]  

\( (14) \)

This matrix has the property

\[
M^n = \ln^{n-1} \begin{bmatrix} 
  k_1 \\
  k_2 
\end{bmatrix} M,
\]  

so that

\[
\exp(M) = I + \frac{1}{2} \sum_{n=1}^{\infty} \frac{1}{n!} \ln^n \begin{bmatrix} 
  k_1 \\
  k_2 
\end{bmatrix} \begin{bmatrix} 
  1 & -1 \\
  -1 & 1 
\end{bmatrix}
\]  

\( (15) \)

Expanding and simplifying Eq. (15) gives

\[
\begin{bmatrix} 
  k_2 + k_1 & k_2 - k_1 \\
  2k_2 & 2k_2 \\
  2k_2 & 2k_2 
\end{bmatrix}.
\]  

\( (16) \)

The result is in agreement with Eq. (4) when \( X = 0 \).

C. Reflection and Transmission Coefficients

In this subsection, we derive the reflection and transmission coefficients of a nonhomogeneous medium placed in the region \( X_1 < x < X_2 \) and bounded by vacuum. We consider two cases: when a down-traveling plane wave is incident upon the medium from the lower boundary \( x = X_1 \), and when an up-traveling wave is incident upon it from upper boundary \( x = X_2 \). Furthermore, we identify the lower and upper vacuums with the indices 1 and 2, respectively.

In these cases, one has \( A_1 = 0 \) or \( A_2 = 0 \), respectively. Therefore from the definition of the transfer matrices, it is found that \( R_1 = A_1/(A_1 + A_2) = -q_{21}/q_{22} \) \( T_1 = A_2/(A_1 + A_2) = \Delta/q_{22} \) for the down-traveling wave, and \( R_2 = A_2/(A_1 + A_2) = q_{12}/q_{22} \) \( T_2 = A_1/(A_1 + A_2) = 1/q_{22} \) for the up-traveling wave, where \( q_{ij} \) are elements of \( Q_{x_2} \). Here \( \Delta = |Q_{x_2}| \), which from Eq. (10d) it turns out to be equal to unity.

The expressions for the up- and down-reflection and transmission coefficients simplify considerably when the associated interface coincides with the origin at \( x = 0 \). For instance, we take \( X_1 = 0 \), resulting in \( R_d = (k_1 - k_2)/(k_1 + k_2) \) and \( T_d = 2k_1/(k_1 + k_2) \), being in agreement with well known expressions.

D. Periodic Systems

In a periodic system with the period \( L \), one has \( k(x) = k(x + L) \), and the solutions according to Floquet’s theorem are given by Bloch waves\(^{10} \) as

\[
A(x) = \Phi_{\text{x}}(x) \exp(-j\kappa x),
\]  

\( (17) \)

in which the envelope function \( \Phi_{\text{x}}(x) = \Phi_{\text{x}}(x + L) \) is also periodic. Here, the reader is reminded that the analysis is not valid whenever the field includes an axial TM component, as prescribed in the development of formulation. Comparing the above equation with Eq. (2) and using the periodicity of the envelope function \( \Phi_{\text{x}}(x) \) and \( k(x) \) reveals that

\[
A(x + L) = \begin{bmatrix} 
  \exp(-j[k - k(x)]L) & 0 \\
  0 & \exp(-j[k + k(x)]L) 
\end{bmatrix} \times A(x) = P \cdot A(x).
\]  

\( (18) \)

However, from Eq. (8), one has \( A(x + L) = Q_{x_2} \cdot A(x) \), and therefore the dispersion equation for Bloch states is obtained as

\[
[I - Q_{x_2} \cdot P^{-1}] = 0.
\]  

\( (19) \)

Expanding and simplifying Eq. (19) gives

\[
\exp(-j2\kappa L) - \exp(-j\kappa L)[q_{11} \exp(-j[k(x)]L)] + q_{22} \exp(j[k(x)]L)] + q_{12}q_{21} - q_{12}q_{21} = 0,
\]  

\( (20) \)

where \( q_{ij} \) are the elements of \( Q_{x_2} \). But \( |Q_{x_2}| = k(x + L)/k(x) = 1 \), and Eq. (20) can be solved for \( \exp(-j\kappa L) \) and further simplified as

\[
\cos(\kappa L) = \frac{q_{11}}{2} \exp(-j[k(x)]L) + \frac{q_{22}}{2} \exp(+j[k(x)]L).
\]  

\( (21) \)

The right-hand side depends on \( x \), whereas the left-hand side does not. In order to eliminate this dependence, one can easily integrate both sides from 0 to \( L \), giving rise to the general dispersion equation for Bloch states,
follows that the exponential as given in Eq. (9), since from Eq. (24) it is possible to verify that
\[ J = \frac{1}{2} - \frac{1}{2} \text{Re} \left( -\frac{a_{21}b_{12}}{a_{22}b_{22}} \right) \]  
(29)

which has extrema coinciding with the bounded modes. Moreover, its minima must be independent of the choice of the reference point \( x \). It is also possible to define the closely associated functional
\[ J = \text{Re} \left( \sqrt{-\frac{a_{21}b_{12}}{a_{22}b_{22}}} \right), \]  
(30)

If the refractive-index function varies slowly, then \( k(x) \) will also vary gradually. In this case, Eq. (8) can be simplified considerably. If the distance between the starting and ending points \( x_1 \) and \( x_2 \) in Eq. (8) is much larger than \( k(x)^{-1} \), being of the order of local wavelength, then the integrands of the off-diagonal elements of the transfer matrix are much smaller than those of the diagonal ones; here, we further assume that \( k(x) \) is real valued over the integration from \( x_1 \) to \( x_2 \), and its value does not change significantly over this domain. Under these circumstances, the magnitude of the second matrix on the right-hand side of Eq. (7b), expressing the interaction of forward and backward waves, is small compared with the diagonal matrix in the first one. It would be then legitimate to make the approximations
\[ u_{11} \approx +j\frac{dk(x)}{dx}u_{11}, \]  
(32a)
\[ u_{12} \approx u_{21} \approx 0, \]  
(32b)
\[ u_{22} \approx -j\frac{dk(x)}{dx}u_{22}. \]  
(32c)

Comparing Eq. (28) to the results of Subsection 3.C reveals that Eq. (28) consists of the production of two reflection coefficients: the upward reflection coefficient from \( x \) to \( +\infty \) and the downward reflection coefficient from \( x \) to \( -\infty \). However, each of these reflection coefficients has a magnitude less than unity. Therefore the functional
\[ J = \frac{1}{2} - \frac{1}{2} \text{Re} \left( -\frac{a_{21}b_{12}}{a_{22}b_{22}} \right) \]  
(29)

should have minima coinciding with the bounded modes.

E. Bounded Modes

Suppose that a system has bounded eigenmodes so that \( A^-(-\infty) = A^+(+\infty) = 0 \). In this case, solutions exist only for some special values of eigenvalues. From Eq. (8), \( A^+(+\infty) = Q_{-\infty,\infty} \cdot A^-(\infty) \). Therefore the characteristic equation for obtaining eigenvalues would be
\[ q_{22} = 0, \]  
(23)

where \( q_{22} \) is the fourth element of \( Q_{-\infty,-\infty} \). Please notice that Eq. (23) is actually an equation in terms of the propagation constant in the waveguide.

Under even symmetry in bounded modes, one has \( k(x) = k(-x) \), and thus \( k'(x) = -k'(-x) \). In this case, it is possible to verify that
\[ m_{11} = -m_{22} = 2j \int_0^\infty k'(x)x dx, \]  
(24a)
\[ m_{12} = -m_{21} = 2j \int_0^\infty \frac{\sin(2k(x)x)}{2k(x)} k'(x) dx, \]  
(24b)

in which \( m_{ij} \) are the elements of the \( M \) matrix, as defined in Eq. (8). In this case, the transfer matrix \( Q_{-\infty,-\infty} = \exp(M) \) can be greatly simplified by direct expansion of the exponential as given in Eq. (9), since from Eq. (24) it follows that \( M^2 = -\Delta I \), in which \( \Delta = |M| \). Here, one can show that
\[ Q_{-\infty,-\infty} = \cos \sqrt{\Delta} I + \frac{\sin \sqrt{\Delta}}{\sqrt{\Delta}} M. \]  
(25)

From the above, the dispersion equation of bounded modes, Eq. (23), would reduce to the simple expression
\[ m_{11} = \sqrt{\Delta} \cot \sqrt{\Delta}, \]  
(26)
where \( m_{11} \) is defined in Eq. (24a).

F. Variational Extraction of Bounded Modes

According to Eqs. (10b) and (23), it is found that Eq. (23) can be rewritten as either
\[ q_{22} = a_{21}b_{12} + a_{22}b_{22} = 0 \]  
(27)
or
\[ \frac{a_{21}}{a_{22}} \times \frac{b_{12}}{b_{22}} = 1. \]  
(28)

Here, \( a_{ij} \) and \( b_{ij} \) are the elements of the \( Q_{-\infty,\infty} \) and \( Q_{-\infty,-\infty} \), respectively, in which \( x \) is an arbitrary reference point within the medium. Naturally, the solutions of Eq. (28) would be independent of \( x \).
Now, consider a wave propagating in the $+x$ direction at $x_1$. The wave amplitude at $x_2$ is given by

$$A(x_2) = q_{11}A(x_1)\exp[-jk(x_2)x_2]$$

$$= q_{11}A(x_1)\exp[-j[k(x_2)x_2 - k(x_1)x_1]]. \quad (33)$$

But from the above discussions and Eq. (8), we have

$$q_{11} = \exp\left[\int_{x_1}^{x_2} + jk'(x)x\,dx\right]$$

$$= \exp\left[j\int_{x_1}^{x_2} k(x)\,dx - j\int_{x_1}^{x_2} k(x)\,dx \right]. \quad (34)$$

By plugging Eq. (33) into Eq. (32) and simplifying, it is found that

$$A(x_2) = A(x_1)\exp\left[-j\int_{x_1}^{x_2} k(x)\,dx \right], \quad (35)$$

which is exactly the WKB solution of Eq. (1).\(^5\)

4. EXAMPLES

In this section we present application examples to assess the validity of the proposed approach. The examples belong to optical structures; however, quantum-mechanical systems can be also analyzed in the same way just by change of dimensions and redefinition of parameters.

A. Reflection from Sinusoidal Grating

Consider the structure shown in Fig. 1. Here we have a sinusoidal grating with the spatial period $L = 0.1375 \mu m$, mean refractive index $n_a = 2$, and modulation amplitude $\Delta n/2 = 0.05$. The grating is obtained by reproduction of the single cosine to 50 times. It is supposed that the structure is illuminated by a normal incident TE light. In Fig. 2, the reflection coefficient of the structure versus wavelength is plotted. We computed the reflection coefficient by two different approaches.

The first is the coupled-mode solution,\(^6,12\) shown as a solid curve, and the next is the solution obtained by the differential transfer-matrix method, shown by a dashed curve. One can observe a reasonable agreement between these two solutions, in justification of our proposed method.

The computation time for the coupled-mode solution has been $\sim 1$ s, whereas it has been $\sim 5$ s for the differential transfer matrix. Please notice that the coupled-mode solution is indeed approximate and suitable only for small modulation indices, whereas the differential transfer-matrix approach is exact. Moreover, the coupled-mode solution for nonsinusoidal gratings usually is hard to derive, whereas our method can solve the system for any other profile at the same efficiency. Please notice that one can still compute the reflection coefficient by dividing the entire grating into many small layers with constant refraction indices and employ the multiplication of corresponding transfer matrices. This approach has been used\(^12\); however, this method is hardly converging and time consuming. We also tested this method and found that the efficiency reduces drastically to 1000 times or even more.

B. Band Structure of Exponential Grating

In this example we consider an infinite grating obtained by periodic reproduction of the exponential profile as shown in Fig. 3. In each period, the refractive index increases exponentially from $n_0 = 1$ to $n_a = 2$. The exact solution of the wave equation for this structure in terms of the Bessel functions is given in Ref. 6, p. 173. The exact frequency dispersion of the grating is shown in Fig. 4 as a solid curve. Here, the first three forbidden frequency gaps can be observed. The band structure is displayed through the reduced-zone scheme so that all gaps occur either at $k = 0$ or $k = k_{\text{max}}$.

The band structure of this grating has been also computed by the differential transfer-matrix method, which is shown in Fig. 4 as dashed lines. The result shows excellent agreement with the exact solution, again confirming the proposed approach.

Please notice that there exists an abrupt fall of the profile of the refractive index from $n_a$ to $n_0$ at $x = nL$, as can be seen in Fig. 3. This discontinuity can be easily included in the computation by multiplying a jump transfer


\(\)
matrix $Q$ from left to the differential transfer matrix $Q_{L^+L^-}$. Here $n(L) = n_s$ and $n(0^+) = n_0$, and Eq. (4) can be used to find the jump transfer matrix $Q_{L^+L^-}$.

5. CONCLUSIONS
A new analytical tool has been presented for an exact solution of linear time-harmonic 1-D optical systems, based on the differential transfer-matrix method. This approach has been based on the generalization of a modified transfer-matrix method. The derivation of reflection and transmission coefficients and bound states have been discussed. The compatibility of this approach with the WKB method and improvements under even symmetry and infinite periodic structures has been shown. A variational form for the bound states has been also presented. Two application examples have been solved and compared with the solutions obtained from other approaches, and in both cases an excellent agreement has been observed. Although the optical interpretation of the method is limited to TE polarization, it is possible to extend the approach to include the TM polarization and even to nonhomogeneous anisotropic media with arbitrary profiles for permittivity and permeability tensors.

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