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Solution of the Equation for Wave Propagation in Layered Slabs with Complex Dielectric Constants

Abstract: A numerical procedure for solving the eigenvalue equation $u'' = [V(x) - E]u$, where $V(x)$ is complex, is described. The number of eigenvalues, and their approximate location, can be determined by contour integration in the complex trial eigenvalue plane. Some general features of the solutions, and an example, are given.

1. Introduction

In this paper we show how to count and find the solutions of the equations for electromagnetic wave propagation along a dielectric slab whose complex dielectric constant is an arbitrary bounded function of one rectangular coordinate. These equations must be solved to find a quantitative description of the modes which propagate in injection lasers,[1] devices in which population inversion and negative absorption coefficients are achieved in a thin layer near a p-n junction by injecting carriers across the junction. They apply also to a variety of other structures. A very simple three-layer model is illustrated schematically in Fig. 1.

We simplify the problem by considering the dielectric to be of infinite extent in the y and z directions. If the wave propagates in the z direction, then the electric and magnetic fields can be independent of y. There are two classes of such fields which satisfy Maxwell's equations.[2] For one class, the transverse electric or TE modes, the solution has the form

$$\mathcal{E}_y(x, z, t) = u(x) \exp(iKz - i\omega t), \tag{1.1}$$

where $\mathcal{E}_y$ is the y-component of the electric field, K is the complex propagation constant, and ω is the angular frequency of the radiation. The x- and z-components of the electric field and the y-component of the magnetic field vanish in this case. For the other class of solutions, the transverse magnetic (TM) modes, the roles of electric and magnetic field are interchanged. We consider only the TE modes in the body of this paper, since they lead to a simpler differential equation, but briefly consider the TM modes in Appendix 1.

The time-averaged intensity of the wave [Eq. (1.1)] varies as exp (Gz), where $G = -2\,\mathrm{Im}(K)$ is the gain constant. If the real and imaginary parts of K have opposite signs, the mode is a growing mode and the radiation is amplified on traversing the medium.

If Eq. (1.1) is substituted in Maxwell's equations,[2] we find that $u(x)$ must satisfy

$$u''(x) + [(\omega^2/c^2)\kappa(x) - K^2]u(x) = 0, \tag{1.2}$$

where $\kappa(x)$ is the complex dielectric constant, which is related to the index of refraction $n(x)$ and the absorption coefficient $\alpha(x)$ by

$$\kappa(x) = [n(x) + \tfrac{1}{2}ic\omega^{-1}\alpha(x)]^2. \tag{1.3}$$

For convenience we rewrite Eq. (1.2) in the form

$$u''(x) = [V(x) - E]u(x). \tag{1.4}$$

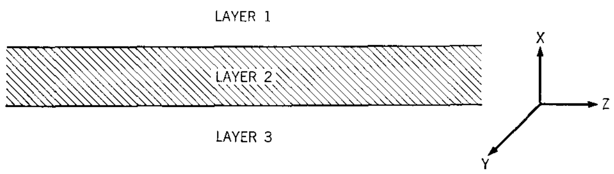

Figure 1 Cross section of a simple three-layer dielectric slab. The complex dielectric constant takes on different values in each of the three layers.

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This equation would be equivalent to the one-dimensional Schrödinger equation if the potential

$$V(x) = -(\omega^2/c^2)\kappa(x) = -[c^{-1}\omega n(x) + \tfrac{1}{2}i\alpha(x)]^2 \quad (1.5)$$

were real. In our case both V and the eigenvalue $E = -K^2$ are complex.

We want to find absolutely square integrable solutions of Eq. (1.4) which are continuous and have continuous derivatives. Because E and V are complex, the procedures required are somewhat different from those used in the real case.[3] Furthermore, the solutions $u(x)$ will also be complex, and we cannot use node counting to label them. In the following section we give the numerical procedure used to solve Eq. (1.4) provided a reasonably good trial eigenvalue is known. An alternative procedure is described in Appendix 2. In Section 3 we show how to determine the number of solutions in a given region of the complex trial eigenvalue plane and how to find suitable trial eigenvalues. Some general properties of the solutions of Eq. (1.4) are summarized in Section 4. In Section 5 we consider a particular example to show how the solutions evolve as the imaginary part of the potential varies.

2. Calculation of solutions

The numerical method is essentially that described in Ref. 3 except that here all numbers are complex rather than real. It is assumed that $V(x)$ approaches constant values as x goes to $+\infty$ or $-\infty$. We take a finite x interval (x_1, x_N) so large in both directions that our results will approximate those for an infinite interval if we assume V to be equal to V_1 for $x < x_1$, and V_N for $x > x_N$. Then, imposing the condition that the solution be bounded for all x gives the solution outside the (x_1, x_N) interval,

$$u(x, E) = u_1 \exp [(V_1 - E)^{\frac{1}{2}}(x - x_1)] \quad \text{for} \quad x < x_1, \quad (2.1)$$

and

$$u(x, E) = u_N \exp [-(V_N - E)^{\frac{1}{2}}(x - x_N)] \text{ for } x > x_N, \quad (2.2)$$

where we take the square root whose real part is positive. Regarded as a function of the complex variable E, $u(x, E)$, with $x < x_1$ is an analytic function of E in the complex plane except for points on the branch cuts

$$\begin{aligned} \operatorname{Re} E &\geq \operatorname{Re} V_1, \\ \operatorname{Im} E &= \operatorname{Im} V_1. \end{aligned} \quad (2.3)$$

For $x > x_N$, the same situation holds for the branch cut

$$\begin{aligned} \operatorname{Re} E &\geq \operatorname{Re} V_N, \\ \operatorname{Im} E &= \operatorname{Im} V_N. \end{aligned} \quad (2.4)$$

For $x < x_1$ or $x > x_N$, $u(x, E)$ is sinusoidal with constant amplitude for all E on the branch cut, Eq. (2.3) or (2.4), respectively. The analytic continuation of $u(x, E)$ in E past a branch cut is unbounded in x for large $|x|$, hence is not an acceptable solution.

To derive difference equations in the quantities $u_i = u(x_i, E)$ and $V_i = V(x_i)$, where $x_i = x_1 + (i-1)h$, $i = 0, 1, \cdots, N+1$, we use the approximation

$$u_i'' \approx (y_{i-1} - 2y_i + y_{i+1})/h^2, \quad (2.5)$$

where

$$y_i \equiv [1 - h^2(V_i - E)/12]u_i. \quad (2.6)$$

At points where V is continuous, the error in this approximation is $-h^6 u_i^{(6)}/240$ (See Ref. 3). Where V is discontinuous, we replace it by its average, $(V_l + V_r)/2$, where "l" and "r" denote values approached from the left and right, respectively. The error is $h^3(u_l^{(3)} - u_r^{(3)})/6$ at such points. Boundary conditions are obtained from Eqs. (2.1) and (2.2), giving

$$\begin{aligned} y_0 &= y_1 \exp [-h(V_1 - E)^{\frac{1}{2}}], \\ y_{N+1} &= y_N \exp [-h(V_N - E)^{\frac{1}{2}}]. \end{aligned} \quad (2.7)$$

From these, we get the difference equations

$$\begin{aligned} C_1^* y_1 - y_2 &= 0, \\ -y_{i-1} + C_i y_i - y_{i+1} &= 0, \quad i = 2, 3, \cdots, N-1, \\ -y_{N-1} + C_N^* y_N &= 0, \end{aligned} \quad (2.8)$$

where

$$\begin{aligned} C_i &= 2 + h^2(V_i - E)/[1 - h^2(V_i - E)/12], \\ C_1^* &= C_1 - \exp(-h\sqrt{V_1 - E}), \\ C_N^* &= C_N - \exp(-h\sqrt{V_N - E}). \end{aligned} \quad (2.9)$$

These are N linear equations in the y_i's which we wish to solve for the values of E for which non-zero eigenvectors $\{y_i\}$ exist.

The iteration-variation method of Löwdin[4] is applied to the system of equations (2.8). To obtain the iteration formulas, consider the more general problem of finding the eigenvalues of

$$\mathbf{M}\mathbf{v} = 0 \quad (2.10)$$

where $\mathbf{M}$ is a matrix whose elements are all analytic functions of E in some open region R of the complex E-plane, and $\mathbf{v}$ is a nonzero vector. Assuming the existence of a trial solution of the form $\mathbf{v} = (1, \mathbf{v}_r)$ which satisfies all but the first of Eqs. (2.10), we can write

$$\mathbf{M}\mathbf{v} = \begin{cases} \mathbf{M}_{11} + \mathbf{M}_{1r}\mathbf{v}_r = f(E), & (2.11) \\ \mathbf{M}_{r1} + \mathbf{M}_{rr}\mathbf{v}_r = 0. & (2.12) \end{cases}$$

where $\mathbf{M}_{1r}$ and $\mathbf{M}_{r1}$ are, respectively, the first row and column of $\mathbf{M}$ with the first element, M_{11}, deleted, and $\mathbf{M}_{rr}$ is the submatrix of $\mathbf{M}$ obtained by deleting the first row and column of $\mathbf{M}$. Thus, $f(E)$ is defined as the result of solving Eq. (2.12) for $\mathbf{v}_r$ and substituting the solution in Eq. (2.11). If we further restrict E to a region where $\det \mathbf{M}_{rr} \neq 0$,

$$f(E) = M_{11} - \mathbf{M}_{1r}\mathbf{M}_{rr}^{-1}\mathbf{M}_{r1}. \tag{2.13}$$

The zeros of $f(E)$ give all eigenvalues except those for which $v_1 = 0$. In order to use the Newton-Raphson method[5] to find the zeros of $f(E)$, we derive a formula for the derivative of $f(E)$. Multiplying Eqs. (2.11) and (2.12) on the left by $\mathbf{v}^{\mathrm{T}} = (1, \mathbf{v}_r^{\mathrm{T}})$, [T denotes transpose] we get

$$f(E) = \mathbf{v}^{\mathrm{T}}\mathbf{M}\mathbf{v}. \tag{2.14}$$

Using the fact that $\mathbf{M}$ is symmetric, we get

$$df/dE = \mathbf{v}^{\mathrm{T}}(d\mathbf{M}/dE)\mathbf{v} + 2(d\mathbf{v}^{\mathrm{T}}/dE)\mathbf{M}\mathbf{v}. \tag{2.15}$$

The last term of Eq. (2.15) is zero since the first element of $(d\mathbf{v}^{\mathrm{T}}/dE)$ is zero and all elements of $\mathbf{M}\mathbf{v}$ are zero except the first. Hence, the Newton-Raphson correction to a trial eigenvalue E is

$$E^* - E = \frac{-f(E)}{df(E)/dE} = \frac{-\mathbf{v}^{\mathrm{T}}\mathbf{M}\mathbf{v}}{\mathbf{v}^{\mathrm{T}}(d\mathbf{M}/dE)\mathbf{v}}. \tag{2.16}$$

The basic procedure for finding the eigenvalues is as follows: With a trial eigenvalue E, an arbitrary value is selected for y_1 and the recurrence relation, Eq. (2.8), is applied with increasing i, yielding $y_1, y_2, \cdots, y_m$. These are normalized by dividing each by y_m and replacing the respective y's by the result. Similarly, starting with an arbitrary y_N, Eq. (2.8) is applied with decreasing i and the resulting series of values, $y_N, y_{N-1}, \cdots, y_m$, is normalized by dividing by the value obtained for y_m. In this manner, a trial solution is obtained which satisfies all difference equations except the m^{th}. Letting this m^{th} difference equation assume the role of Eq. (2.11) and letting $y_m = v_1 = 1$, we have

$$f(E) = -y_{m-1} + C_m y_m - y_{m+1}. \tag{2.17}$$

This is a measure of the mismatch in the difference $y_m - y_{m-1}$ as given by the inward and outward integration. From Eq. (2.15), and the definition of the matrix elements given in Eqs. (2.8) and (2.9), we get

$$df(E)/dE = -h^2 \sum_{i=1}^{N} u_i^2 - \frac{h}{2}\left[\frac{y_1^2 \exp[-h(V_1 - E)^{\frac{1}{2}}]}{(V_1 - E)^{\frac{1}{2}}} + \frac{y_N^2 \exp[-h(V_N - E)^{\frac{1}{2}}]}{(V_N - E)^{\frac{1}{2}}}\right]. \tag{2.18}$$

We use Eqs. (2.17) and (2.18) in the correction formula of Eq. (2.16) to obtain a correction to the trial eigenvalue E.

The present method is essentially the one used by Hartree[6] except that here the correction to the trial eigenvalue, obtained from Eqs. (2.16) through (2.18), may differ from Hartree's depending on how one approximates the derivatives and integral in the latter.

It has been shown in the real case[3] that it is important to keep m, the matching point, away from nodes in the desired solution, and experience has indicated that selecting m near a maximum of the solution gives a better rate of convergence and more accuracy. Therefore, the program selects an optimal m on each iteration by integrating inward and outward to $i = N/2$. Then, m is set at the point where the modulus of the solution is greatest and the inward or outward integration is continued from $i = N/2$ to m. During the iterations on E, it is important for the program to check that it does not cross one of the branch cuts. This can occur when the corrections have inadvertently started converging towards inadmissible solutions on the analytic continuation of $f(E)$ past the branch cut or when the correction has overshot its mark in attempting to converge to an admissible solution lying near a branch cut. In either case, the correction is reduced in magnitude, but not direction, and several further attempts at convergence are carried out.

3. Counting and locating solutions

The procedures described in the previous section show how to find the solution to Eq. (1.4) when a good trial eigenvalue is known. Most of the solutions can be found by a systematic variation of trial eigenvalues, but there is no guarantee that all the solutions will be found in this way. In fact, in the example to be given in Sec. 5, some of the solutions were missed until the procedure to be described here was used. We find that it is easy to count the number of solutions in any specified region of the complex trial eigenvalue plane, and to locate the position of each solution with arbitrary accuracy.

Our method is based on the theorem that for a function $F(E)$, analytic in an open region containing a closed simple curve C except for a finite number of points inside C where it may have poles of finite order, the difference between the number of zeros, N, and poles, P, inside C is given by[7]

$$Z - P = \frac{1}{2\pi i}\oint \frac{dF(E)/dE}{F(E)}\,dE = \frac{1}{2\pi}\oint d(\arg F(E)), \tag{3.1}$$

where the integral is taken around C. For the purpose of counting eigenvalues we modify our definition of $F(E)$. We now rescale only the result of the inward integration by a factor chosen to make it match y_m from the outward integration. Letting $\bar{y}_N, \bar{y}_{N-1}, \cdots, \bar{y}_m$ designate the result of the inward integration, we let

$$y_i = \bar{y}_i y_m / \bar{y}_m, \qquad i = m, m+1, \cdots, N, \tag{3.2}$$

$$F(E) = -y_{m-1} + 2y_m - y_{m+1} + h^2(V_m - E)u_m, \tag{3.3}$$

and define

$$g(E) = \bar{y}_m. \tag{3.4}$$

Note that the formula for the derivative, Eq. (2.18), no longer applies because y_m is not kept equal to one, but the present $F(E)$ still has the sought-for eigenvalues as its zeros.

The poles of $F(E)$ coincide with the zeros of $g(E)$, and their number is

$$P = \frac{1}{2\pi} \oint d(\arg g(E)), \tag{3.5}$$

since $g(E)$ has no poles. Adding Eqs. (3.1) and (3.5) gives

$$Z = (2\pi)^{-1} \oint d[\arg F(E)g(E)] \tag{3.6}$$

for the number of zeros of $F(E)$ within the contour. In the calculation, a closed curve C is given and $F(E)$ and $g(E)$ are computed for values $E_1, E_2, \cdots$, of E around C. The change in phase of $F(E)$ $g(E)$ for any successive pairs of E's is taken to be between $-\pi$ and $+\pi$, and the intervals between successive E's are adjusted during the calculation to keep the magnitude of the phase change smaller than a fixed quantity. In our work, this upper limit was 0.8 radians. After a complete circuit, Eq. (3.6) is calculated to yield Z, the number of zeros within C.

In the computer program for counting solutions, provision is made for a rectangular contour C, subdivided into a variable number of rectangular subcontours. Care must be taken that none of the regions or contours contains points on the branch cuts of Eq. (2.3) or (2.4). The number of solutions is evaluated in each of the internal rectangles. In this way it is possible both to count the solutions and to obtain an estimate of their location. More accurate estimates can be obtained by further subdivision of the rectangles which contain one or more solutions.

4. General properties of the solutions

In this section we summarize some properties of the solutions of Eq. (1.4). We shall assume that the potential $V(x)$ is bounded, and that it approaches constant values V_+ and V_- as x approaches $+\infty$ and $-\infty$, respectively. The trial solutions of Eq. (1.4) are analytic functions of the trial eigenvalue E everywhere except on the branch cuts of Eqs. (2.3) and (2.4). When $V_+ = V_-$, these branch cuts coincide. The branch cuts give the continuous eigenvalues of our problem, i.e., those values of E for which the eigenfunctions $u(x)$ of Eq. (1.4) are bounded but are not absolutely square integrable.

Absolutely square integrable solutions of Eq. (1.4) exist only for a discrete set of eigenvalues; there may not be any such solutions. If we assume that such a solution u_i exists, with eigenvalue E_i, then

$$u_i''^*(x) = [V^*(x) - E_i^*]u_i^*(x) \tag{4.1}$$

is the complex conjugate of Eq. (1.4). If we multiply Eq. (1.4) by u_i^*, multiply Eq. (4.1) by u_i, subtract the two products, and use Green's theorem and the fact that the absolutely square-integrable solutions vanish as $|x| \longrightarrow \infty$, we find[8]

$$\mathrm{Im}\ E_i = \left[\int_{-\infty}^{\infty} [\mathrm{Im}\ V(x)]u_i^*(x)u_i(x)\,dx\right] \times \left[\int_{-\infty}^{\infty} u_i^*(x)u_i(x)\,dx\right]^{-1}. \tag{4.2}$$

When the potential is real, this reproduces the familiar result that the eigenvalues are real. It is also easy to show in a similar way that two solutions u_i and u_j belonging to different eigenvalues E_i and E_j are orthogonal,[8]

$$\int_{-\infty}^{\infty} u_i(x)u_j(x)\,dx = 0, \qquad E_i \neq E_j. \tag{4.3}$$

If E_i is an eigenvalue not too close to other eigenvalues, and if it has only one associated solution $u_i(x)$, then we can give the first- and second-order perturbations $\delta_1 E_1$ and $\delta_2 E_i$ of the eigenvalue, and the first-order perturbation $\delta_1 u_i$ of the eigenfunction, which result from a small change δV in the potential. We find:

$$\delta_1 E_i = \int_{-\infty}^{\infty} \delta V(x)u_i^2(x)\,dx/N_i, \tag{4.4}$$

$$\delta_2 E_i = \sum_j{}' (E_i - E_j)^{-1} \times \left(\int_{-\infty}^{\infty} \delta V u_i(x)u_j(x)\,dx\right)^2 \Big/ N_i N_j, \tag{4.5}$$

$$\delta_1 u_i(x) = \sum_j{}' (E_i - E_j)^{-1} u_j(x) \int_{-\infty}^{\infty} \delta V u_i u_j\,dx/N_j, \tag{4.6}$$

where the primed sums are over all the solutions except the i^{th}, and

$$N_i = \int_{-\infty}^{\infty} u_i^2(x)\,dx. \tag{4.7}$$

In the interesting case in which V is real and δV is purely imaginary, the first-order changes in both the eigenvalue and the eigenfunction are purely imaginary, and the second-order change in the eigenvalue is real. In this case the real parts of the eigenvalues of two neighboring, strongly interacting solutions approach each other and can cross, a result quite different from the usual one for real V and δV. We find an example of this behavior in the following section.

5. An example

To illustrate the nature of the solutions of the wave equation (1.4), we consider a specific example which arose in connection with experimental observations of high-order transverse modes in the radiation patterns of injection lasers with a high-resistance layer.[9] The optical model for our example has five layers, of which the two outermost are infinitely thick. In all layers the index of refraction n and the absorption coefficient α are constant. The index values and the thicknesses of the layers are given in the first two rows of Table 1. We vary the absorption coefficients in the layers to see how the solutions depend on the magnitude of the imaginary part of the potential. The absorption coefficients for three cases are also given in Table 1. The potential itself is found from Eq. (1.5) once n and α are given in each layer. These examples are of interest because the layers are many wavelengths thick, and thus there are many solutions. In such cases the procedures we have described are particularly useful.

In the simplest case, Case 1, the absorption coefficient in each region is taken to be zero. There are eleven solutions for this case, all real, and they have 0, 1, $\cdots$, 10 nodes, respectively. For each solution we calculate

$$K = k - \tfrac{1}{2}iG = (-E)^{\frac{1}{2}}. \tag{5.1}$$

and we order the solutions according to the value of k, as in Table 2. Solution 1 has the largest value of k, and its eigenfunction $u(x)$ has no nodes; solution 11 has the smallest value of k, and has ten nodes. Since the potential is real for Case 1, the eigenvalues are real. They are all negative, and G therefore vanishes for all solutions of Case 1.

Table 1 Optical constants for the multilayer model of Section 5. The thickness, index of refraction n, and absorption coefficient α are given for each of the five layers. The potential $V(x)$ is given by Eq. (1.5) with $\lambda = 2\pi\ c\ \omega^{-1} = 8.33 \times 10^{-5}$ cm.

Constants:	*Layers:*				
	1	2	3	4	5
Thickness [10^{-4} cm]:	∞	8.0	3.2	2.0	∞
Index of refraction n:	3.61	3.63	3.63	3.61	3.58
Absorption coefficient α [cm^{-1}]:					
Case 1	0	0	0	0	0
Case 2	20	200	0	200	250
Case 3	20	200	-1000	200	250

In the physical problem that led to the optical model of Table 1, the middle layer is an active layer in which radiation is generated, and in which the absorption coefficient can be negative. The remaining four layers are absorbing layers. Case 2, the second case for which solutions are given, is one in which the absorption coefficients in the four absorbing layers have attained their full values, but the absorption coefficient α_{act} in the active layer is still zero. In Case 3, the absorption in the active layer attains the value -1000 cm^{-1}.

We find from Table 2 that the introduction of the imaginary part of the potential has two main effects. First, more solutions appear than are present when the potential is real. Second, the order of the k values for the solutions is not preserved. As the imaginary part of the potential varies linearly between Case 2 and Case 3, the order of the k values for solutions 2 and 3 changes. This is an example of the behavior suggested by Eq. (4.5), which shows that an imaginary perturbation to a real potential can cause the real parts of the eigenvalues of two strongly interacting solutions to approach each other.

Table 2 Eigenvalues for the square-integrable solutions of Eq. (1.4) with the potentials of Table 1. Values of G and k, which are related to the eigenvalue E by $E = (\frac{1}{2}G + ik)^2$, are given in cm^{-1}. The values in any row vary smoothly as the potentials is varied linearly from Case 1 to Case 2, and from Case 2 to Case 3, except for solutions 12, 13, and 14. All results were calculated with h, the step size for x, equal to 5×10^{-6} cm.

Solution	*Case 1*[a]:	*Case 2*:		*Case 3*:	
	k	k	G	k	G
1	273 792	273 785	-190	273 782	-196
2	273 754	273 728	-92	273 692	945
3	273 691	273 715	-147	273 711	-182
4	273 602	273 605	-155	273 593	-159
5	273 488	273 486	-141	273 427	-125
6	273 349	273 351	-133	273 350	760
7	273 186	273 189	-144	273 213	-82
8	273 000	273 000	-143	272 953	-22
9	272 792	272 792	-136	272 767	425
10	272 565	272 566	-139	272 625	28
11	272 332	272 329	-134	272 319	30
12[b,c]	–	272 090	-116	272 071	21
13[b]	–	271 927	-122	271 967	-22
14[b,c]	–	271 693	-44	271 730	25

[a] $G = 0$ for all the solutions of Case 1.

[b] Solutions 12, 13, and 14 do not exist for Case 1.

[c] Solution 12 reaches the branch cut when the absorption coefficient α_{act} in layer 3 reaches -436 cm^{-1} as we vary linearly from Case 2 to Case 3. This solution is missing until α_{act} reaches -842 cm^{-1}, where it re-emerges on the other side of the branch cut. The corresponding values of α_{act} are -95 and -864 cm^{-1} for solution 14, which also hits the branch cut.

One final effect, briefly explained in the notes to Table 2, is that some of the solutions, in our case solutions 12 and 14, have eigenvalues which reach the branch cuts of Section 2, and then no longer exist, as the absorption in the active layer is varied. In both cases, the solutions eventually reappear on the other side of the branch cut as the active layer absorption is varied further. Thus, the number of solutions of the wave equation depends sensitively on the potential function $V(x)$, and a procedure to count and locate the solutions, as described in Section 3, is essential if all the solutions are to be obtained.

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Appendix 1. Transverse magnetic modes

The second class of solutions of Maxwell's equations for our problem is a superposition of terms of the form

$$\mathcal{H}_y(x, z, t) = u(x) \exp(iKz - i\omega t), \tag{A.1}$$

where $\mathcal{H}_y$ is the y-component of the magnetic field, and the remaining symbols have the same significance as in Eq. (1.1). In this case the equation that $u(x)$ must satisfy is

$$u''(x) - (\kappa'/\kappa)u'(x) + [E - V(x)]u(x) = 0, \tag{A.2}$$

where E and $V(x)$ have the same meaning as in Eq. (1.4). The first derivative can be eliminated if we let

$$u(x) = w(x)[\kappa(x)]^{\frac{1}{2}}, \tag{A.3}$$

and $w(x)$ must then satisfy[2]

$$w''(x) + [E - V(x) + (\kappa''/2\kappa) - (3\kappa'^2/4\kappa^2)]w(x) = 0. \tag{A.4}$$

Although (A.4) has the same form as Eq. (1.4) and can be solved in the same way, it is highly singular near a discontinuity in $\kappa(x)$. For that reason it is preferable to work with the equation

$$(u'/\kappa)' = [V(x) - E][u(x)/\kappa(x)], \tag{A.5}$$

which is equivalent to (A.2). From (A.5) we see that u'/κ is continuous at a discontinuity of $\kappa(x)$, which also follows from the boundary conditions for electric and magnetic fields at a discontinuity in the dielectric constant.

Appendix 2. Alternative solution for the multilayer case

The procedures described in Sec. 2 are applicable to the solution of Eq. (1.4) for any bounded function $V(x)$. If, as in the example of Sec. 5, this function is piecewise constant, then an alternative analytical procedure becomes possible. If the j^{th} layer extends from x_{j-1} to x_j, and if $V(x) = V_j$ in that layer, then we can write as the solution of Eq. (1.4):

$$u(x) = a_j \exp[(V_j - E)^{\frac{1}{2}}x] + b_j \exp[-(V_j - E)^{\frac{1}{2}}x], \quad x_{j-1} \le x \le x_j. \tag{B.1}$$

In the two outermost layers only the exponentially decreasing solution is allowed, and only one of the coefficients is nonzero. We can extend the solution inward from the right, and outward from the left by choosing the a_j and b_j so that both $u(x)$ and $u'(x)$ are continuous at the boundaries between successive layers.

At some matching point x_m, which can be chosen arbitrarily, the inward and outward solutions, $u_{\text{in}}(x)$ and $u_{\text{out}}(x)$, can be compared. If neither piece of the solution vanishes at the matching point, and if the function and its derivative do not join smoothly there, then the correction to the trial eigenvalue E is given by[6]

$$E^* - E = [u'_{\text{out}}(x_m) - u'_{\text{in}}(x_m)][\textstyle\int_{-\infty}^{\infty} u^2(x)\,dx]^{-1}, \tag{B.2}$$

provided the solution has been normalized so that $u_{\text{out}}(x_m) = u_{\text{in}}(x_m) = 1$. If either u_{out} or u_{in} should vanish at x_m, this correction formula cannot be used, and another matching point must be chosen.

Using one point of discontinuity as the matching point, R. A. Willoughby has employed this alternative method in the calculation of solutions for the symmetric three-layer case. The absolute value of the largest eigenvalue so obtained agreed to three significant figures with the one calculated here using $N = 20$ integration points.[10] The analytic procedure requires less computation time if the number of discontinuities is relatively small. However, to permit full generality in the potential function $V(x)$, it was decided to program the finite difference method described here. We are indebted to Dr. Willoughby for proposing this method of solution and for programming it for the symmetric three-layer case.

The procedure described in Sec. 3 for counting the number of solutions in a given region of the trial eigenvalue plane is easily extended to this alternative method of solution.

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