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Serov, Valeri S.; Shestopalov, Youri V.; Kristensson, Gerhard; Lundin, Richard

1998

Total number of authors:
4

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Valeri S. Serov, Youri V. Shestopalov,

Gerhard Kristensson, and Richard Lundin

Department of Electroscience
Electromagnetic Theory
Lund Institute of Technology
Sweden
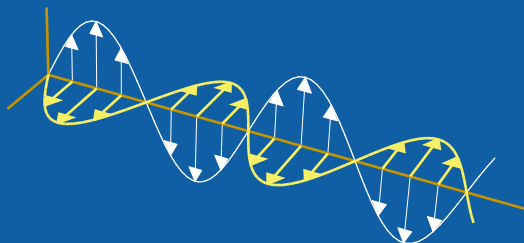
Valeri S. Serov and Youri V. Shestopalov

Department of Computational Mathematics and Cybernetics
Moscow State University
199899 Moscow
Russia

Gerhard Kristensson and Richard Lundin

Department of Electroscience
Electromagnetic Theory
Lund Institute of Technology
P.O. Box 118
SE-221 00 Lund
Sweden

Abstract

In this paper we give an introduction to the mathematical foundations of the optical waveguide design. A survey of the main results of the spectral theory of the Schrödinger operator on the line having compactly supported potential, with particular emphasis on the case of piece-wise constant potential is presented. This theory is then applied to the optical waveguide design problem of a piece-wise constant permittivity.

1 The optical waveguide design problem

1.1 Preliminaries

We here consider the problem of waves propagation in inhomogeneous planar waveguide as it is stated in *e.g.*, Ref. 10.

The medium inside the waveguide is assumed to be stratified in x-direction. The Maxwell equations for the wave propagation are

$$\begin{cases} \nabla \times \boldsymbol{E} = -\mu_0 \dfrac{\partial \boldsymbol{H}}{\partial t} \\[2mm] \nabla \times \boldsymbol{H} = \epsilon \dfrac{\partial \boldsymbol{E}}{\partial t} \end{cases}$$

The electric field $\boldsymbol{E}$ satisfies the hyperbolic equation

$$\nabla^2 \boldsymbol{E} + \nabla \left(\frac{\nabla \epsilon}{\epsilon} \cdot \boldsymbol{E} \right) - \mu_0 \epsilon \frac{\partial^2 \boldsymbol{E}}{\partial t^2} = \boldsymbol{0} \tag{1.1}$$

We consider time harmonic transverse electric (TE) waves polarized in the y-direction and propagating in the positive z-direction, *i.e.*,

$$\boldsymbol{E} = \boldsymbol{e}_y \phi(x, \lambda) \exp[i(\beta z - \omega t)] \tag{1.2}$$

where ω is the angular frequency and β and λ are the longitudinal and transversal wave numbers, respectively, satisfying the relation

$$k_0^2 - \beta^2 = \lambda \tag{1.3}$$

Here $k_0 = \omega \sqrt{\mu_0 \epsilon_0}$ is the wavenumber in the external region (free space). Substitution of (1.2) into (1.1) yields the equation for $\phi(x, \lambda)$

$$\left(-\frac{d^2}{dx^2} + q(x) \right) \phi(x, \lambda) - \lambda \phi(x, \lambda) = 0, \tag{1.4}$$

where

$$q(x) = k_0^2 \left(1 - \frac{\epsilon(x)}{\epsilon_0} \right), \qquad -\infty < x < \infty \tag{1.5}$$

Hence, the existence of the solutions of the form (1.2) is reduced to the analysis of the spectral properties of the Schrödinger operator

$$H \overset{\text{def}}{=} -\frac{d^2}{dx^2} + q(x)$$

with real-valued potential $q(x)$. In our case the potential $q(x)$ has compact support, say, the segment $[0, L]$, and belongs to the space $L^\infty(\mathbb{R})$. It is well known (see, e.g., Refs. 3, 8) that in this case H is a self-adjoint operator in $L^2(\mathbb{R})$ and the spectrum is formed in the following way: the set $[0, \infty)$ is an absolutely continuous spectrum without positive eigenvalues, i.e., for every $\lambda > 0$ equation (1.4) has bounded solutions which at the same time are the unique solutions to the Lippmann-Schwinger equation

$$\phi^\pm(x, \lambda) = e^{\pm ix\sqrt{\lambda}} \pm \int_x^{\pm\infty} \frac{\sin\sqrt{\lambda}(t-x)}{\sqrt{\lambda}} q(t)\phi^\pm(t, \lambda)dt \tag{1.6}$$

For $\lambda = 0$ equation (1.4) also has a solution satisfying (1.6) but this solution cannot grow faster than a linear function for $x \to \infty$. Furthermore, the operator H may have a finite number of negative eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_{n_0}$, each of them simple. It means that (1.4) has solutions $\phi_1, \phi_2, \ldots, \phi_{n_0}$ in $L^2(\mathbb{R})$ for $\lambda = \lambda_1, \lambda_2, \ldots, \lambda_{n_0}$, which are the eigenfunctions of H. In this case they say that operator H has bound states. In our case, they correspond to the propagating modes in the optical waveguide. Moreover, eigenfunctions $\phi_1, \phi_2, \ldots, \phi_{n_0}$ decay exponential for $|x| \to \infty$.

If the potential $q(x)$ satisfies the condition

$$\int_0^L q(x)dx \leq 0 \tag{1.7}$$

it then follows from the results of Ref. 8 that the operator H has negative eigenvalues satisfying the following uniquely soluble boundary value problem:

$$\begin{cases} \left(-\frac{d^2}{dx^2} + q(x)\right)\phi(x) = \lambda\phi(x), & x \in (0, L) \\ \phi(0) = 1 \\ \phi(L) = 1 \\ \phi'(0) = -\phi'(L) = \sqrt{|\lambda|} \end{cases} \tag{1.8}$$

and for $x \notin [0, L]$ the eigenfunctions are

$$\phi(x) = \begin{cases} e^{\sqrt{|\lambda|}x} & x < 0 \\ e^{-\sqrt{|\lambda|}x} & x > L \end{cases}$$

It also follows from Ref. 9 that if the potential $q \in C_0^\infty(\mathbb{R})$ and $q \leq 0$, but $q \not\equiv 0$, then for all sufficiently small values $\mu > 0$ the number of negative eigenvalues of the operator

$$H_\mu = -\frac{d^2}{dx^2} + \mu q(x)$$

is exactly equal to 1. In the general case, for arbitrary potential from the Faddeev class, $q(x) \in L_1^1(\mathbb{R})$, the upper estimate for the number $N(q)$ of the negative eigenvalues of the operator H holds [9]

$$N(q) \leq 2 + \int_{-\infty}^{\infty} |x||q_-(x)|\, dx$$

where $q_-(x) = \min(0, q(x))$. In the present case, it is not difficult to obtain the following inequality from the estimate for $N(q)$:

$$N(q) \leq 2 + \frac{L^2}{2} \max |q_-(x)|$$

We consider the problem of reconstruction of the potential $q(x)$ (*i.e.*, the profile function $\epsilon(x)$ in (1.5) from the spectral data (or by the so-called scattering data) of the Schrödinger operator H. Specifically, take the solution $\phi^+(x, k)$ from (1.6) (for $k^2 = \lambda$, $k \in \mathbb{R}$) which has asymptotic behavior e^{ikx} for $x \to \infty$. For $x \to \infty$, this solution has an asymptotic representation

$$\phi^+(x, k) = a(k)e^{ikx} + b(k)e^{-ikx} + o(1)$$

where

$$a(k) = 1 - \frac{1}{2ik} \int_0^L q(t)e^{-ikt}\phi^+(t, k)\, dt$$

$$b(k) = \frac{1}{2ik} \int_0^L q(t)e^{ikt}\phi^+(t, k)\, dt$$

Coefficients $a(k)$ and $b(k)$ are called *spectral data* or *scattering data* and the reflection coefficient in the spectral domain is defined as

$$r(k) = \frac{b(k)}{a(k)} \tag{1.9}$$

It is well-known that it is sufficient to know only the coefficient $r(k)$ in order to reconstruct the potential $q(x)$ when there are no bound states (see Ref. 3, the trace formula). Additional information is necessary in the general case about the negative discrete spectrum.

It is known (see, *e.g.*, Refs. 1, 3) that the function $r(k)$ may be continued to the upper half-plane of the complex variable k as a meromorphic function, whose (finite number of) poles (if they exist) lie on the imaginary axis, *i.e.*, they are equal to ik_1, ik_2, ..., ik_{n_0}; $k_j > 0$, $j = 1, 2, \ldots, n_0$, and they are connected with negative eigenvalues of the operator H by the formulas

$$\lambda_1 = -k_1^2, \qquad \lambda_2 = -k_2^2, \qquad \lambda_{n_0} = -k_{n_0}^2 \tag{1.10}$$

If the reflection coefficient $r(k)$ is a rational function, one can effectively apply the reconstruction technique for $q(x)$ by $r(k)$ developed in Ref. 10, based on Gel'fand-Levitan-Marchenko (GLM) theory (see, *e.g.*, Refs. 4, 6) with the use of reflection kernel in the time domain. This reflection kernel R is associated with the reflection coefficient by the formula

$$R(x + t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} r(k)e^{-ik(x+t)} \, dk - i \sum_{l=1}^{n_0} R_l e^{k_l(x+t)}$$

where k_l are taken from (1.10) and R_l are the residues of the function $r(k)$ at the poles ik_l.

Using the time domain formulation (see, *e.g.*, Ref. 5), one gets the following GLM-type integral equation:

$$K(x, t) + R(x + t) + \int_{-t}^{x} K(x, \tau) R(t + \tau) \, d\tau = 0, \qquad t < x$$

where the function $K(x, t)$ satisfies the conditions

$$K(x, t) = 0, \qquad t > x, \qquad t \leq -x$$

Here, the function $K(x, x)$ is such that

$$2 \frac{d}{dx} K(x, x) = q(x)$$

where $q(x)$ is the sought potential in the Schrödinger operator H. Moreover, the function

$$\Phi(x, t) = \begin{cases} \delta(x - t) + R(x + t) + K(x, t) + \int_{-x}^{x} K(x, \tau) R(t + \tau) \, d\tau, & x \geq 0 \\ \delta(x - t) + R(x + t), & x \leq 0 \end{cases}$$

is the solution to the following wave equation

$$\begin{cases} \dfrac{\partial^2}{\partial x^2} \Phi(x, t) - \dfrac{\partial^2}{\partial t^2} \Phi(x, t) - q(x)\Phi(x, t) = 0 \\ \Phi(x, t) = \delta(x - t), \qquad x < 0, \ t < 0 \end{cases} \tag{1.11}$$

where the potential $q(x)$ is the same as in the Schrödinger operator H.

The Fourier transform of the equation (1.6) with respect to the variable $k \in \mathbb{R}$, $k^2 = \lambda$, $\lambda \geq 0$ yields equation (1.11), where $\Phi(x, t)$ is the Fourier transform of the function $\phi^+(x, k)$. Hence, the equations (1.6) and (1.11) correspond directly to each other only in the case of continuous spectrum. However, the equation (1.11) contains information about the whole spectrum of H due to the results of GLM theory.

1.2 Piece-wise constant permittivity case

The first problem considered in this paper is the reconstruction of the real, piece-wise constant potential $q(x)$ with the support on the interval $[-L, L]$ having the form[1]

$$q(x) = \begin{cases} c_1 & -L < x < 0 \\ c_2 & 0 < x < L \\ 0 & |x| > L \end{cases} \tag{1.12}$$

where c_1, c_2 are, in general, two real different constants. The problem is to determine the values of c_1, c_2, L by the scattering data in the frequency domain. The general uniqueness theorem of the reconstruction of potential from Faddeev class $L_1^1(\mathbb{R})$ is given in Ref. 3 (see also Ref. 7). In order to apply this theorem, one has to know the reflection coefficient $r(k)$, (1.9), for all $k \in \mathbb{R}$ and the negative discrete spectrum. If the potential is a piece-wise constant function, like in (1.12), the problem may be formulated as follows:

What kind of spectral data is sufficient to uniquely reconstruct the constant values c_1, c_2, L in (1.12)?

Stated differently, one must prove that

1) for certain spectral data the required constants are unique

and

2) to construct the appropriate reconstruction procedure.

In Section 2, the problem of piece-wise constant potential is considered as well as the solution of the inverse problem formulated above.

2 Reconstruction by the spectral data

2.1 Dispersion equation one layer

Determination of the propagation constants of the waves in a layer with constant dielectric permittivity may be reduced to the problem of finding (real) roots of a specific dispersion equation [2]. In order to write down this equation in a form convenient for further analysis, let us introduce the normalized (spectral) parameter $y = \beta^2/k_0^2$ corresponding to the propagation constant β and the (non-spectral) parameter $x = k_0 L$ of the problem of waves propagation in a layer having a thickness $2L$, where $\epsilon(\kappa) = \epsilon$, $|\kappa| < L$; $\epsilon(\kappa) = 1$, $|\kappa| > L$; $\epsilon > 1$ is the relative dielectric permittivity of the layer in vacuum; k_0 denotes the vacuum wavenumber, and κ is the coordinate perpendicular to the boundary of the layer.

The dispersion equation for the normalized propagation constant has the form [2, Chapter 6]:

$$\sqrt{y - 1} = \sqrt{\epsilon - y} \tan x \sqrt{\epsilon - y} \tag{2.1}$$

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[1]Note that the support of the potential $q(x)$ is changed compared to Section 1.1.

We consider this equation as a function of y in the semi-open interval $[1, \epsilon)$ for $x \geq 0$ i.e., propagating modes $(\beta^2 > 0)$ in the semi-strip

$$\Omega = \{(x, y) : x \geq 0; \ 1 \leq y < \epsilon\}$$

and rewrite (2.1) in the equivalent form

$$F_1 \equiv y - 1 - (\epsilon - y) \tan^2 u = 0 \qquad (2.2)$$

where

$$u = u(x, y, \epsilon) = x\sqrt{\epsilon - y}$$

The second factor in the second term of (2.1) is a periodic function of u: $\tan^2 u = \tan^2(u + m\pi)$, $m \in Z$ which implies existence of an infinite number of solutions to (2.1). These may be explicitly presented in the form of functions

$$x(y) = x_m(y) = \frac{\arctan p(y) + m\pi}{\sqrt{\epsilon - y}}, \qquad m = 0, 1, 2, \ldots$$

$$p(y) = \frac{\sqrt{y - 1}}{\sqrt{\epsilon - y}}$$

forming the countable family

$$X = \{x_m(y)\}_{m=0}^{\infty}$$

and it is clear that $(x_m(y), y) \in \Omega$ for $y \in [1, \epsilon)$.

The zero element $x_0(y)$ of this family corresponds to the mode which exists for all possible values of the normalized layer's thickness. For higher order elements $(x = x_m(y), m = 1, 2, \ldots)$, the following condition holds:

$$x \geq x_m^0; \qquad x_m^0 = \frac{m\pi}{\sqrt{\epsilon - 1}}$$

so x_m^0 may be interpreted as cut-off values of the normalized layer's thickness. For the principal zero mode this cut-off is equal to zero and this mode may be correctly considered as perturbed with respect to the TEM-mode in free space having propagation constant $\beta = k_0$ which corresponds to $y = 1$ in our notation.

The graphs of $x_m(y)$ are given in Figure 1. It is clear that each element of the family X establishes one-to-one mapping of the semi-interval $\{x = 0, 1 \leq y < \epsilon\}$ onto the infinite semi-interval $\{x \geq x_m^0, y = 1\}$ and hence one can correctly define corresponding inverse functions $y(x) = y_m(x)$, $m = 0, 1, 2 \ldots$, which uniquely determine the propagation constants of the principal and the higher order propagating modes versus the normalized layer's thickness.

The "direct" condition for existence of N propagating modes $(N \geq 1)$, when $\epsilon > 1$ is fixed, is given by the relation

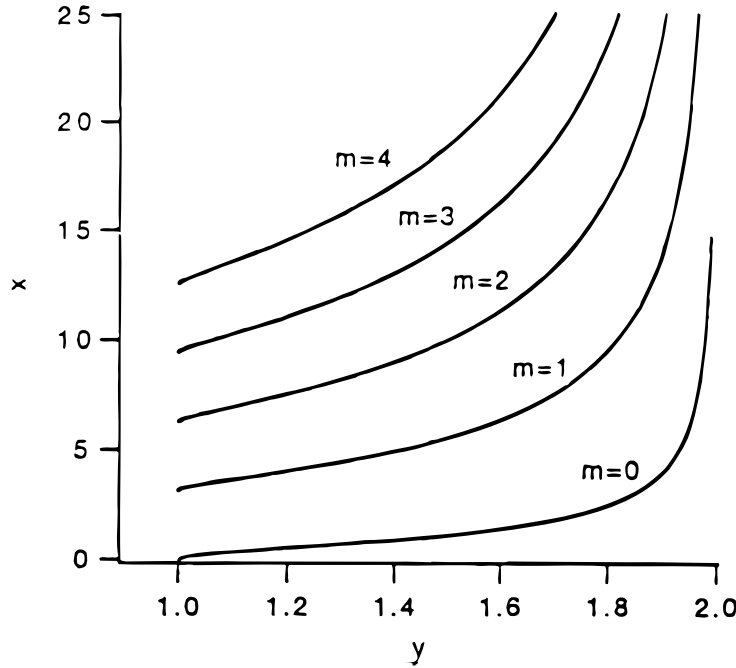$$x_{N-1}^0 \leq x < x_N^0, \qquad N = 1, 2, \ldots$$

Figure 1: The different $x_m(y)$ curves for $\epsilon = 2$.

It is not so easy to determine the same type of an "inverse" condition. Assume, for example, that $\epsilon > 1$ is given and it is known the l-th eigenvalue $y_l \in [1, \epsilon)$, $i.e.$, the y-coordinate of a certain point on the curve $x_l(y)$. Then one can determine the corresponding value of x and the number of propagating modes using the "direct" condition. But in the case of ϵ not given, one needs additional information to establish both the number of propagating modes and the parameter x. This (regularizing) information may have different nature and its specification forms the essence of the solution of the inverse problem of reconstructing the layer's characteristics by the spectral data.

One of the possible ways of solving such an inverse problem is to assume that one only knows two different values, y_l and y_k, and the different numbers l, k. Then ϵ may be found as the solution to the equation

$$E(\epsilon) \equiv x_l(y_l) - x_k(y_k) = 0$$

and the value of the normalized layer's thickness x will be determined by the formulas for $x_l(y_l)$ or for $x_k(y_k)$.

It is easy to see that the equation $E(\epsilon) = 0$ has no solutions if $y_l > y_k$ and $l > k$ (see Figure 2 where even in the case $y = y_l = y_k$, the curves for $x = x_m(\epsilon)$, $m = 0, 1, 2, 3$ do not intersect). But if the order of this spectral data and corresponding indices do not coincide, $e.g.$, $y_l < y_k$ and $l > k$, this equation may have a unique solution (the ordinate of the intersection point on Figure 3), which, hence, uniquely determines the values of x and ϵ corresponding to the given spectral data.

This may be considered as the draft of the proof of the existence theorem of the reconstruction of the layer's parameters by more than one value of propagation
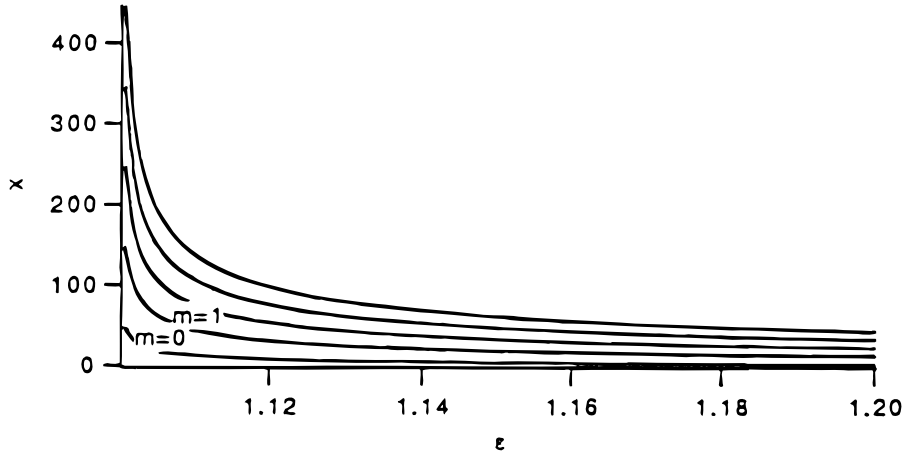
Figure 2: The normalized half-width x as a function of the relative permittivity ϵ for the different modes, for a fixed value of the normalized propagation constant $y = 1.1$.

constants of propagating modes (or, in other terms, by more than one negative eigenvalue of the Schrödinger operator). By using this result, one cannot directly prove the uniqueness of such a reconstruction, but it is necessary to have additional information.

Another possibility to solve the inverse problem in a correct way is to apply the functional approach in the vicinity of the points $(x_m^0, 1)$, $m = 0, 1, 2, \ldots$, by using a kind of parameter differentiation method based on the study of implicit functions determined by the equation (2.2), which is considered in the next section.

2.2   Local analysis—the method of implicit function

In order to obtain the correct formulation of the problem which solution uniquely determines $y = y(x)$ in the vicinity of the cut-off points x_m^0, $m = 0, 1, 2, \ldots$, we consider equation (2.2), which (locally) determines $y = y(x)$ as an implicit function, and construct $y(x)$ in a vicinity to the right of the point $x = 0$ as the solution to the Cauchy problem

$$\frac{dy}{dx} = \Phi_1(x, y); \qquad \Phi_1(x, y) = -\frac{F_{1x}}{F_{1y}} = \frac{2u^2 g(u)}{x^3(1 + g(u))} \tag{2.3}$$

where

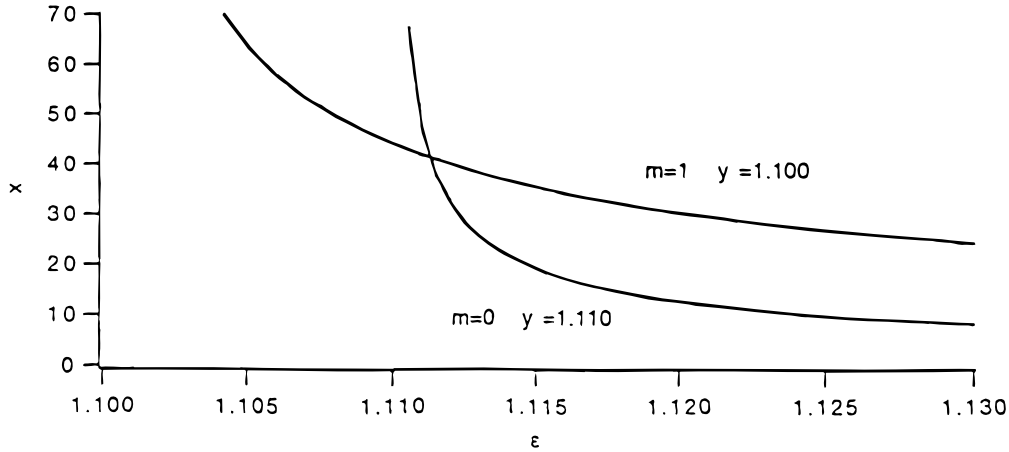$$g(u) = u \tan u$$

with the initial condition

$$y(x_m^0) = 1$$

Figure 3: The half-width x as a function of ϵ for two different modes, assuming fixed and normalized propagation constants.

which follows from the relation

$$F_1(x_m^0, 1) = 0 \qquad (2.4)$$

Here, we assume that $m = 0, 1, 2, \ldots$, and omit the index m which should mark the solution to each of the Cauchy problems (2.3), (2.4). It is easy to see that

$$\frac{d\Phi_1}{dy}(x, y) = -\frac{u^2 + 3g(u)(1 + g(u))}{x(1 + g(u))^2}$$

is continuous in the point $(x_m^0, 1)$ together with F_{1y} and

$$F_{1y}(x_m^0, 1) = 1$$

hence, there exists such $X = X(\epsilon) > 0$ that the Cauchy problem (2.3) and (2.4) — below called Problem 1 — has the unique, continuous solution $y = y(x)$ for $x \in [0, X)$. Analysis of the explicit form of functions $x(y) = x_m(y)$ performed in Section 2.1 shows that the corresponding inverse functions $y(x) = y_m(x)$, which are solutions to Problem 1, are continuous and monotonically increasing for all $x : x > x_m^0$. Therefore, for every fixed value of the permittivity $\epsilon > 1$, $X = X(\epsilon)$ may be taken arbitrarily large. In other words, Problem 1 has unique, continuous solutions $y(x) = y_m(x)$ for all $x > x_m^0$, and $1 < y_m(x) < \epsilon$, $m = 0, 1, 2, \ldots$.

It is not difficult to obtain the (formal) Taylor expansion of the solution to Problem 1 for small values of x. For example, the three first terms of this expansion are as follows:

$$y(x) = y(0) + xy'(x) + 0.5x^2y''(x) + O(x^3) = x_m^0 + x^2(\epsilon - 1)^2 + O(x^3)$$

2.3 One layer with two slabs

Determination of the propagation constants of propagating waves in the layer containing two slabs, *i.e.*, when the dielectric permittivity is a piece-wise constant

function inside the layer:

$$\epsilon(\kappa) = \begin{cases} \epsilon_1 & -L < \kappa < 0 \\ \epsilon_2 & 0 < \kappa < L \\ 1 & |\kappa| > L \end{cases}$$

(κ denotes the coordinate perpendicular to the boundary of the layers) may also be reduced to the problem of finding the (real) roots of the more complicated dispersion equation than the problem considered above (see, *e.g.*, the dispersion equation constructed in Chapter 6 of Ref. 2, for the three-layer rectangular waveguide).

Before we write down the explicit form of this equation obtained in a similar manner (like equation (2.1)), let us introduce some additional variables:

$$y = \frac{\beta^2}{k_0^2}; \qquad z = \sqrt{\epsilon_1 - y}$$

$$a = \epsilon_1 - \epsilon_2; \qquad b = \epsilon_2 - 1; \qquad (a \geq 0, b \geq 0); \qquad x = k_0 L$$

The dispersion equation for the normalized propagation constant has the form

$$F(x, z, a, b) = 0 \tag{2.5}$$

$$F(x, z, a, b) = A(x, z, a, b)B(x, z, a, b) - C(x, z, a, b)D(x, z, a, b)$$
$$A(x, z, a, b) = G(z - H \tan xz); \qquad B(x, z, a, b) = H - G \tan xG$$
$$C(x, z, a, b) = z(z \tan xz - H); \qquad D(x, z, a, b) = G + H \tan xG$$
$$G = G(z, a) = \sqrt{z^2 + a}; \qquad H = H(z, a) = \sqrt{b - z^2}$$

One of the ways to apply the technique of the local analysis of the solutions to (2.5) is to look for the solution (root) of this equation in the form of implicit function $z = z(x)$ which will be the solution to the Cauchy problem

$$\frac{dz}{dx} = \Phi_0(x, z); \qquad \Phi_0(x, z) = -\frac{F_x}{F_z} \tag{2.6}$$

There are two possibilities to state the initial condition:

$$1) \qquad z(0) = 0$$

which follows from the relation

$$F(0, 0, a, b) = 0$$

and

$$2) \qquad z(0) = \sqrt{b}$$

The latter holds since $F(0, z, a, b) = zGH + zGH = 2zGH = 0$ and $H(\sqrt{b}, a) = 0$.

The first initial condition clearly does not correspond to the physical model and the second one causes a singularity of the right-hand side of (2.6) at the point $(0, \sqrt{b}, a, b)$.

In this case, it turns out that the natural way to formulate the Cauchy problem in the correct way is to consider the sought-for parameter as the function $z = z(a)$. The corresponding Cauchy problem has the form

$$\frac{dz}{da} = \Phi(a, z); \qquad \Phi(a, z) = -\frac{F_a}{F_z} \tag{2.7}$$

with the initial condition

$$z(0) = y_m$$

In order to obtain this initial value one must consider the equation

$$F(x, z, 0, b) = 2z^2(H - z \tan xz) = 0$$

which is equivalent to (2.1), (2.2) and whose roots $y_m = y_m(x, \epsilon)$ for fixed values of $x \geq 0$, $\epsilon > 1$ may be obtained by the methods presented in Section 2.1.

The explicit form for the right-hand side of the Cauchy problem is calculated by equation (2.7) where

$$F_z = A_z B + B_z A - C_z D - CD_z; \qquad -F_a = -A_a B - B_a A + C_a D + CD_a$$

$$A_z B = \frac{1}{GH} \left(H - G \tan xG\right) \left(H(a + 2z^2)\right.$$
$$\left. -2y(b - a - 2z^2) \tan xz - xG^2 H^2(1 + \tan^2 xz)\right)$$

$$B_z A = \frac{-z}{H} \left(z - H \tan xz\right) \left(G + H \tan xG - xGH(1 + \tan^2 xG)\right)$$

$$C_z D = \frac{1}{H} \left(G + H \tan xG\right) \left(2zH \tan xz + 2z^2 - b + xz^2(1 + \tan^2 xz)\right)$$

$$CD_z = \frac{z^2}{GH} \left(z \tan xz - H\right) \left(H - G \tan xG + xH^2(1 + \tan^2 xG)\right)$$

$$A_a B = \frac{AB}{2G^2}; \qquad AB_a = -\frac{1}{2} \left(z - H \tan xz\right) \left(\tan xG + xG(1 + \tan^2 xG)\right)$$

$$C_a D = 0; \qquad CD_a = \frac{C}{2G} \left(1 + xH(1 + \tan^2 xG)\right)$$

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