

Solution of dispersion relations for planar waveguides in the case of complex roots

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A method for calculating the complex roots of a nonlinear equation is described whereby the solution of the problem is reduced to quadratures. Applications of the method to the investigation of dispersion relations for various open waveguide structures with a complex dielectric permittivity are discussed. The possibilities of the prismatic excitation of modes corresponding to the roots of the dispersion relations on different Riemann sheets are analyzed. Solutions are obtained for the inverse problems of reconstructing complex mode propagation constants and determining the parameters of films that guide waveguide and leaky modes. The solution is based on processing of the angular dependence of the reflection coefficient in a prismatic excitation scheme. © 1998 American Institute of Physics. [S1063-7842(98)01604-3]

INTRODUCTION

The rigorous determination of complex roots of dispersion relations is of fundamental importance in the electrodynamic theory of open-ended waveguides. Despite the long history of this problem, a satisfactory solution has yet to be found for it. This dilemma accounts for the several alternative computational approaches in use, including various interpolation^{1–4} and gradient^{5,6} methods. Their common shortcoming is the need to specify a sufficiently accurate zeroth approximation for the root and to calculate the derivatives of the dispersion relations, which poses a rather complex problem. Moreover, smoothness of the functions involved in the equations is essential for convergence, but unfortunately they suffer discontinuities at branch cuts. Another fundamental requirement is nondegeneracy of the roots.

Here we propose a method, free of these limitations, for rigorously calculating the complex roots of dispersion relations for planar waveguides having an arbitrary distribution of the complex dielectric permittivity. The method is an elaboration of previously published results.⁷ It is based on a contour integration technique and can be used to find all the roots of a nonlinear equation $f(u)=0$ in the domain of analyticity of the function $f(u)$.

1. METHOD FOR CALCULATING THE COMPLEX ROOTS OF NONLINEAR EQUATIONS

Let us suppose that it is required to find the roots of the equation $f(u)=0$ in a simply connected, closed domain G of the complex variable u bounded by the contour C . We also assume that the function $f(u)$ is analytic in this domain. The total number of roots m (taking their multiplicity into account) can be determined on the basis of the argument principle,⁸ whereby m is equal to $1/2\pi$ times the total variation of the argument of the quantity $W=f(u)$ in traversing

the contour C . We assume initially that all the roots are nondegenerate. If $m=1$, then by calculating the integrals $I_c^{(0)}$ and $I_c^{(1)}$ numerically, where

$$I_c^{(k)} = \frac{1}{2\pi i} \oint_C \frac{u^k du}{f(u)},$$

and invoking the residue theorem, we find the value of the root $u_1 = I_c^{(1)}/I_c^{(0)}$. If $m>1$, then by successively shrinking the domain and calculating the variations of the argument of W , we obtain a domain G_1 that is bounded by a contour C_1 and contains $m-1$ roots. For the excluded root we obtain

$$u_1 = \frac{I_{c_1}^{(1)} - I_c^{(1)}}{I_{c_1}^{(0)} - I_c^{(0)}}.$$

Repeating the process, we find all the roots in succession. We note that the calculation of the variation of the argument of W reduces to the calculation of the number of crossings of the boundaries of the coordinate quadrants. This operation can be executed in parallel with the accumulation of integral sums, enhancing the computational efficiency of the method.

We now generalize the computational scheme to the case involving a double root u_0 . We treat this situation as the limiting case when $u_1 \rightarrow u_2 \rightarrow u_0$, where u_1 and u_2 are simple roots. We assume that two roots are present in the domain G . We introduce integrals $I_c^{(2)}$ and $I_c^{(3)}$ in addition to $I_c^{(0)}$ and $I_c^{(1)}$. Using the residue theorem, we arrive at the system of four equations

$$I_c^{(k)} = u_1^k [f'(u_1)]^{-1} + u_2^k [f'(u_2)]^{-1} \quad (k=0,1,2,3) \quad (1)$$

in the four unknowns u_1 , u_2 , $f'(u_1)$, and $f'(u_2)$. Its solution has the form

$$u_{1,2} = a/2 \pm \sqrt{(a/2)^2 - b}, \quad (2)$$

$$a = \frac{I_c^{(1)}I_c^{(2)} - I_c^{(0)}I_c^{(3)}}{[I_c^{(1)}]^2 - I_c^{(0)}I_c^{(2)}}, \quad (3)$$

$$b = \frac{[I_c^{(2)}]^2 - I_c^{(3)} I_c^{(1)}}{[I_c^{(1)}]^2 - I_c^{(0)} I_c^{(2)}}. \quad (4)$$

Forming Taylor expansions of the function $f(u)$ and its derivatives, we obtain

$$f'(u_1) = -\frac{1}{2}f''(u_1)\Delta u - \frac{1}{6}f'''(u_1)(\Delta u)^2 + O[(\Delta u)^3], \quad (5)$$

$$f'(u_2) = \frac{1}{2}f''(u_1)\Delta u + \frac{1}{6}f'''(u_1)(\Delta u)^2 + O[(\Delta u)^3], \quad (6)$$

$$f''(u_2) = f''(u_1) + f'''(u_1)\Delta u + O[(\Delta u)^2], \quad (7)$$

where $\Delta u = u_2 - u_1$. The application of Eqs. (5)–(7) reduces Eqs. (1) to the form

$$I_c^{(0)} = -\frac{2}{3} \frac{f'''(u_1)}{f''(u_1)} + O(\Delta u),$$

$$I_c^{(1)} = \frac{2}{f''(u_1)} + u_1 I_c^{(0)} + O(\Delta u),$$

$$I_c^{(2)} = \frac{4u_1}{f''(u_1)} + u_1^2 I_c^{(0)} + O(\Delta u),$$

$$I_c^{(3)} = \frac{6u_1^2}{f''(u_1)} + u_1^3 I_c^{(0)} + O(\Delta u).$$

It follows from these expressions that $a^2/4 \rightarrow b$ and $u_1 \rightarrow u_2 \rightarrow u_0 = a/2$ in the limit $\Delta u \rightarrow 0$. For $m > 2$ it is necessary once again to shrink the domain. If $m-2$ roots are contained in the domain G_1 , the values of the two excluded roots can be calculated from Eqs. (2)–(4) after the substitution $I_c^{(k)} \rightarrow I_c^{(k)} - I_{c_1}^{(k)}$. For the double root we again obtain $u_0 = a/2$.

All not more than twofold-degenerate roots of the equation $f(u)=0$ can be found by combining the above-described computational schemes. The case of l -fold degeneracy ($l > 2$) can be treated analogously by computing the integrals $I_c^{(k)}$, where $k=0,1,\dots,2l-1$. The corresponding expressions are rather cumbersome and will not be written out here, particularly in view of the fact that the roots of the dispersion relations for planar waveguides are not degenerate as a rule, and only in rare situations encountered in the investigation of anisotropic waveguides and systems of coupled waveguides are they twofold degenerate.

2. SOLUTION OF THE DISPERSION RELATIONS

We consider a waveguide formed by a layered medium, which has a complex dielectric permittivity, is contained in the domain $-d \leq y \leq 0$, and is surrounded by homogeneous media with dielectric constants $\varepsilon_g (y > 0)$ and $\varepsilon_s (y < -d)$. The dispersion relation for modes whose fields are exponential functions of the time and the coordinate z , $\exp(i\omega t - ihz)$ has the form^{7,9}

$$F_\nu = i\psi(0)\nu + \psi'(+0) = 0, \quad (8)$$

where $\psi(y)$ has the meaning of the component E_x for the TE modes and H_x for the TM modes, $\nu = \sqrt{k_0^2 \varepsilon_g - h^2}$, and $k_0 = 2\pi/\lambda_0$ is the wave number in vacuum.

In the derivation of Eq. (8) we have chosen the functional dependence $\psi(y) = \psi(0)\exp(-i\nu y)$, $y \geq 0$. We use a stratification method to specify the quantities appearing in Eq. (8), representing the waveguide by a set of n homogeneous layers.¹⁰ In this case the quantities $\psi'(+0)$ and $\psi(0)$ can be calculated from the recursion relations⁷

$$\psi_{j+1} = \psi_j K + \psi'_j S, \quad (9)$$

$$\psi'_{j+1} = (\varepsilon_{j+1}/\varepsilon_j)^T (\psi'_j K - \psi_j \nu_j^2 S), \quad (10)$$

$$\psi_1 = 1, \quad (11)$$

$$\psi'_1 = i\nu_1(\varepsilon_2/\varepsilon_1)^T, \quad (12)$$

where $S = \sin(\nu_j \Delta y_j)/\nu_j$, $K = \cos(\nu_j \Delta y_j)$, $\nu_j = \sqrt{k^2 \varepsilon_j - h^2}$, $\varepsilon_1 = \varepsilon_s$, $\varepsilon_{n+2} = \varepsilon_g$, $\psi_{n+2} = \psi(0)$, $\psi'_{n+2} = \psi'(+0)$, ε_j and Δy_j are the permittivity and thickness of the j th layer, $T=0$ for TE modes, and $T=1$ for TM modes; the field in the domain $y < -d$ is represented as $\psi(y) = \exp[i\nu_i(y+d)]$.

In the special case of a homogeneous thin-film waveguide ($n=1$), Eq. (8) with allowance for Eqs. (9)–(12) reduces to the form

$$F_\nu = \left[\nu_1 \left(\frac{\varepsilon_2}{\varepsilon_s} \right)^T + \nu \left(\frac{\varepsilon_2}{\varepsilon_g} \right)^T \right] \cos(\nu_2 d) + i \left[\nu_2 + \frac{\nu_1 \nu}{\nu_2} \left(\frac{\varepsilon_2}{\varepsilon_s \varepsilon_g} \right)^T \right] \sin(\nu_2 d) = 0. \quad (13)$$

It is convenient to choose $u = \nu_1$ as the unknown in Eqs. (8) and (13). Then $\nu_j = \sqrt{k_0^2(\varepsilon_j - \varepsilon_s) + u^2}$ ($j=2,\dots,n+2$; $\nu_{n+2} = \nu$). According to Eqs. (8)–(13), the function $F_\nu(u)$ is bounded (in a finite part of the complex plane) and invariant with respect to the choice of signs of ν_j ($j < n+2$); the only source of nonanalyticity of the function is the presence of branch points and branch cuts of the function $\nu(u)$. The nonanalyticity is eliminated by working with the product

$$f(u) = F_\nu(u) F_{-\nu}(u), \quad (14)$$

which is an entire function of the variable u (Ref. 9). The roots of Eq. (14) coincide with those of Eqs. (8) and (13) corresponding to two branches of the function $\nu(u)$ (e.g., the branches $\text{Im } \nu \leq 0$ and $\text{Im } \nu \geq 0$). We note that for $\nu \neq 0$ Eq. (14) and the equation $F_{\pm\nu}(u) = 0$ have roots of identical multiplicity. Indeed, the multiplicity of the roots increases if the system of equations $F_\nu(u) = 0$, $F_{-\nu}(u) = 0$ holds, from which, according to (8), it follows that $\psi(0) = 0$ and $\psi'(+0) = 0$ ($\nu \neq 0$). In this case the solution of the Cauchy problem for the differential equation describing the mode field gives $\psi(y) \equiv 0$ and $\psi'(y) \equiv 0$, contradicting conditions (11) and (12). The case $\nu = 0$, on the other hand, can be analyzed separately. We also note the implication of Eqs. (8)–(12), that if $d \neq 0$, then the quantity $|W|$ grows exponentially as $|u| \rightarrow \infty$. In this case the number of roots of Eq. (14) is $m = O(r)$ in the limit $r \rightarrow \infty$, where r is the radius of the circle C (Ref. 9), i.e., when G is interpreted as the entire complex plane, the number m is unboundedly large. But if

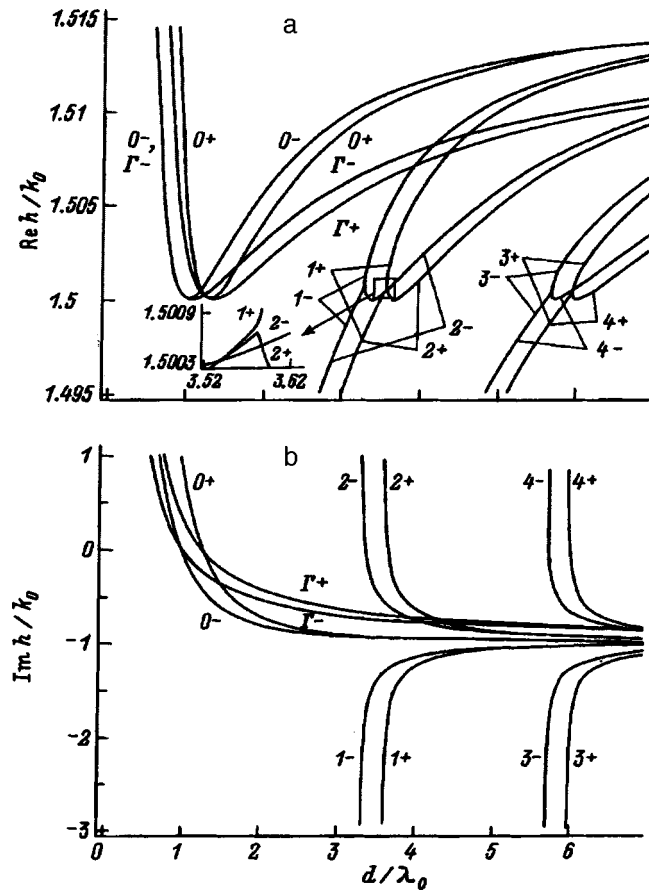


FIG. 1. Dispersion curves for the modes of a homogeneous waveguide and an inhomogeneous waveguide. a) $\text{Re } h/k_0$; b) $\text{Im } h/k_0$.

$d=0$, we infer from (13) that $m=2$ for $T=1$, $m=0$ for $T=0$ and $\varepsilon_g \neq \varepsilon_s$, and $m=1$ for $T=0$ and $\varepsilon_g = \varepsilon_s$.

Using the method described in Sec. I, we have obtained solutions of Eq. (14) for several waveguide structures. Typical plots of $h = \sqrt{k_0^2 \varepsilon_s - \nu_1^2}$ ($\text{Re } h \geq 0$) as a function of d/λ_0 are shown in Figs. 1a and 1b. They have been obtained for TE-polarized modes of a homogeneous waveguide with $\varepsilon_s = 2.25 - i3 \times 10^{-6}$, $\varepsilon_2 = 2.295225 - i3.03 \times 10^{-6}$, and $\varepsilon_g = 1$. The “+” and “-” signs in the figures identify curves pertaining to $\text{Im } \nu \geq 0$ and $\text{Im } \nu \leq 0$, respectively. Curves $1\pm$ and $3\pm$ correspond to $\text{Im } \nu_1 > 0$, $\text{Re } \nu_1 > 0$. Curves $1+$ and $3+$, for which $\text{Re } \nu > 0$, correspond to leaky waves exiting from the waveguide into the two open domains $y > 0$ and $y < -d$, while curves $1-$ and $3-$ ($\text{Re } \nu < 0$) correspond to waves which are leaky only in the domain $y < -d$. The inequality $\text{Re } \nu_1 < 0$ holds for curves $0\pm$, $2\pm$, and $4\pm$. The indicated curves in Fig. 1a have points of tangency with the line $\text{Re } h/k_0 = 1.5$. These points correspond to critical thicknesses $d = d_k$ (k denotes the symbol enumerating the curves). For $d > d_k$ we have $\text{Re } \nu < 0$ and $\text{Im } \nu_1 > 0$ ($k = 0-, 2-, 4-$) or $\text{Re } \nu > 0$ and $\text{Im } \nu_1 < 0$ ($k = 0+, 2+, 4+$). In this case curves $0-, 2-,$ and $4-$ describe the usual dispersion curves for waveguide modes, whereas curves $0+, 2+,$ and $4+$ correspond to waves leaking from the waveguide into the domain $y > 0$. For $d < d_k$ we have $\text{Re } \nu > 0$ and $\text{Im } \nu_1 > 0$ ($k = 0-, 2-, 4-$) or $\text{Re } \nu < 0$ and $\text{Re } \nu > 0$ ($k = 0+, 2+, 4+$). In this case curves $0-, 2-,$

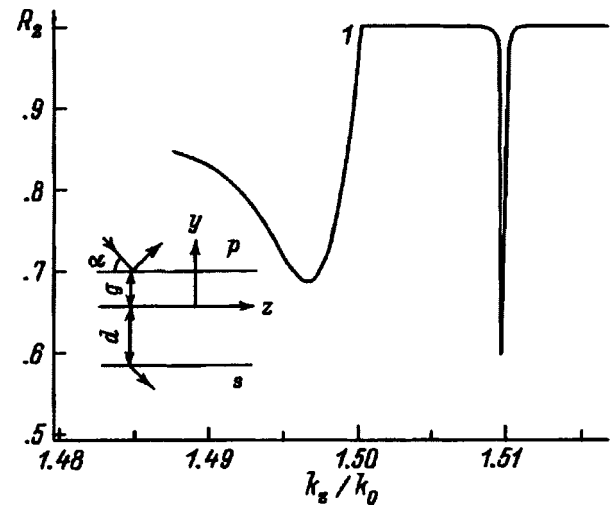


FIG. 2. Schematic diagram of the prismatic excitation device and graph of the reflection coefficient of the exciting wave versus the z -component of its wave vector for $\varepsilon_p = 3.811$.

and $4-$ correspond to waves entering the waveguide from the domain $y < -d$ (they grow as $y \rightarrow -\infty$), then leaking from the waveguide into the domain $y > 0$ and decaying as $y \rightarrow \infty$, whereas curves $0+, 2+,$ and $4+$ correspond to waves entering the waveguide from both open domains and growing as $|y| \rightarrow \infty$. A distinctive feature of all these waves is the growth of the field as $z \rightarrow \infty$ ($\text{Im } h > 0$, Fig. 1b). It follows from the above discussion that the sets of curves $(1\pm, 2\pm)$ and $(3\pm, 4\pm)$ correspond to modes having similar properties. The solution of Eq. (14) has shown that increasing d generates new sets $(5\pm, 6\pm), (7\pm, 8\pm), \dots$, analogous to those already mentioned. The indicated prominent characteristics of the behavior of the dispersion relations and the mode fields remain in effect for TM-polarized modes. And they are similar in regard to inhomogeneous waveguides. This statement is illustrated by curves $\Gamma+$ and $\Gamma-$ in Figs. 1a and 1b, which are calculated for TE modes of a waveguide having the index profile $\varepsilon(y) = 2.25 - i3 \times 10^{-6} + (0.045225 - i2.73 \times 10^{-5}) \exp[-(y/d)^2]$, $y \leq 0$; $\varepsilon(y) = \varepsilon_g = 1$, $y > 0$. These curves are analogous to curves $0+$ and $0-$ discussed above. We note, however, that the results here are characteristic of waveguides having a higher permittivity than the surrounding media. The dispersion relations for waveguide media having a lower permittivity (e.g., metal films on dielectric substrates and low-refraction films on high-refraction substrates) exhibit distinct differences. We shall examine them briefly below. We also note that the above-discussed inequalities $\text{Im } \nu_1 > 0$ and $\text{Im } \nu > 0$ correspond to modes whose fields grow exponentially with increasing distance from the waveguide. Such modes do not occur in the complete sets of modes,⁹ making it necessary to ascertain the possibilities of their excitation and practical utilization.

We consider the excitation of modes by means of a prismatic coupler.^{11,12} A schematic diagram of the coupler is shown in Fig. 2. The prism P (which we consider to be unbounded for simplicity) is separated from the waveguide by a buffer layer of thickness g . The prism and the buffer

layer have real permittivities ε_p and ε_g , where $\varepsilon_g < \varepsilon_p$. The structure is excited by a plane wave whose wave vector forms an angle α with the base of the prism. Examining the recursion relations (9) and (10) in the buffer layer, we obtain the following expression for the reflection coefficient of the exciting wave:

$$R = \frac{(1 - \delta)F_\nu - \exp(-2i\nu g)(1 + \delta)F_{-\nu}}{(1 + \delta)F_\nu - \exp(-2i\nu g)(1 - \delta)F_{-\nu}},$$

$$\delta = (\nu/\nu_p)(\varepsilon_p/\varepsilon_g)^T, \quad \nu = \sqrt{k_0^2 \varepsilon_g - k_z^2}, \quad \text{Im } \nu \leq 0,$$

$$\nu_p = \sqrt{k_0^2 \varepsilon_p - k_z^2}, \quad \text{Re } \nu_p \geq 0, \quad k_z = k_0 \sqrt{\varepsilon_p} \cos \alpha. \quad (15)$$

The quantities F_ν and $F_{-\nu}$ can be calculated from Eqs. (8)–(13), where $\nu_j = \sqrt{k_0^2 \varepsilon_j - k_z^2}$ and in accordance with the radiation condition $\text{Re } \nu_1 \geq 0$.

We know that the efficient excitation of waveguide modes characterized by the occurrence of resonance troughs in the $R_2(k_z)$ curve ($R_2 = |R|^2$) takes place under the conditions of weak prism–waveguide coupling:^{11,12}

$$k_z^2 > k_0^2 \varepsilon_g, \quad (16)$$

$$\exp(-i\nu g) \ll 1. \quad (17)$$

According to Eqs. (8)–(13) and (15)–(17), R_2 can differ significantly from unity only if $F_\nu = O[\exp(-2i\nu g)]$. Making use of the fact that the variable k_z in Eq. (15) belongs to the real axis of the Riemann sheet $\text{Re } \nu_1 > 0$, we infer that the stated condition can be satisfied if there is a domain H , defined by the inequality $|k_z - h| < \rho$ (h is the propagation constant of the excited mode, and $\rho = O[\exp(-2i\nu g)]$), which contains a segment of the real axis of the sheet $\text{Re } \nu_1 > 0$ and in which the function $F_\nu(k_z)$ is analytic. These considerations are consistent with the obvious fact that resonance excitation is admissible only for modes whose fields decay with increasing distance from the waveguide in the buffer layer and whose propagation constants satisfy the equation $F_\nu(h) = 0$.

The analyticity properties of the function $F_\nu(k_z)$ in the vicinity of the roots can be assessed from Figs. 3a and 3b. The solid curves represent the function $\text{Im } k_z(\text{Re } k_z)$ [equivalent to $\text{Im } h(\text{Re } h)$] for the roots of the equation $F_\nu(k_z) = 0$. The dashed lines indicate the cuts for the function $\nu_1(k_z)$ as defined by the conditions $\text{Im } k_z = k_0^2 \text{Im } \varepsilon_s / (2 \text{Re } k_z)$ and $k_0^2 \text{Re } \varepsilon_s - (\text{Re } k_z)^2 + (\text{Im } k_z)^2 < 0$. The cuts pass below the real axes $\text{Im } k_z = 0$. Curves 0– through 4– correspond to their counterparts in Figs. 1a and 1b. It follows from Fig. 3a that only the segments of curves 1– and 3– to the left of the branch point of the function $\nu_1(k_z)$ can exist in the domain H . An analogous situation is met for the segments of curves 0–, 2–, and 4– below the cut. In this case the domain H belongs to a two-sheeted Riemann surface “glued” along the edges of the cut. Now, looking at Figs. 1a and 1b, we infer that the efficient excitation of waveguide modes is possible only for waveguide films whose thicknesses exceed critical values ($d > d_k$). On the other hand, resonance troughs corresponding to the excitation of leaky modes associated with curves 1–, 3– and their analogs 5–, 7–, ... can be observed for $d < d_k$. These conclusions are illustrated in

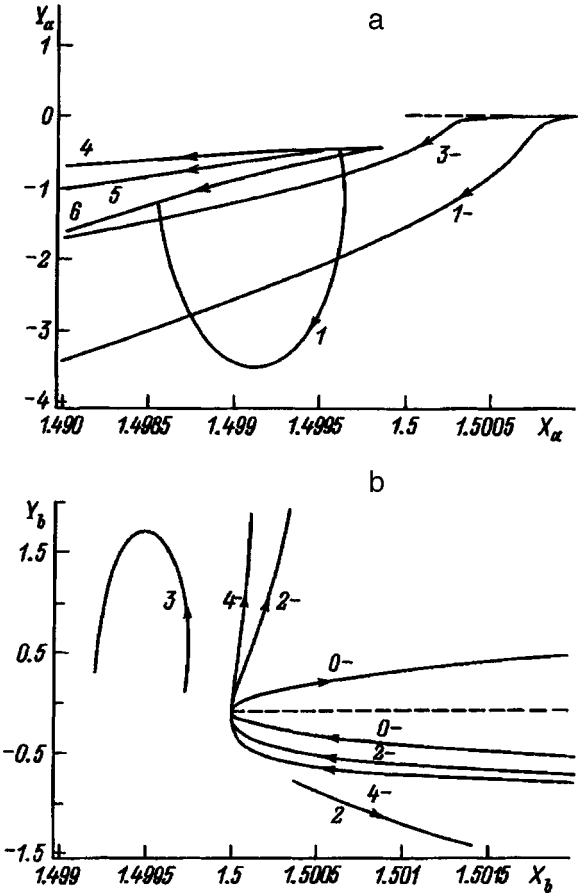


FIG. 3. Positions of the roots of the equation $F_\nu(k_z) = 0$ on the Riemann sheets $\text{Re } \nu_1 > 0$ (a) and $\text{Re } \nu_1 < 0$ (b). $X_{a,b} = A_{a,b} + B_{a,b} \text{Re } k_z/k_0$, $Y_{a,b} = C_{a,b} + D_{a,b} \text{Im } k_z/k_0$; for curves 0– to 4–: $A_{a,b} = 0$, $B_{a,b} = 1$, $C_{a,b} = 0$, $D_{a,b} = 10^3$, $D_b = 10^5$; 1) $A_a = 1.494$, $B_a = 5.45 \times 10^{-3}$, $C_a = -0.44$, $D_a = 30$; 2) $A_b = 1.498$, $B_b = 1.47 \times 10^{-3}$, $C_b = -0.72$, $D_b = 19.7$; 3) $A_b = 1.497$, $B_b = 2.65 \times 10^{-3}$, $C_b = -9.77 \times 10^{-2}$, $D_b = 14.8$; 4–6) $A_a = 4.35 \times 10^{-2}$, $B_a = 1$, $C_a = 0$, $D_a = 4 \times 10^4$. The arrows indicate directions of decreasing d .

Fig. 2, curve 1, which is calculated on the basis of Eqs. (9)–(12) and (15) for $d/\lambda_0 = 3$ and $g/\lambda_0 = 0.16$. Its right minimum corresponds to a waveguide (0–) mode, and its left minimum corresponds to a leaky (1–) mode.

We now discuss the prismatic mode excitation of thin films having a lower real part of the permittivity than the surrounding media. Curves 1–3 in Fig. 3a and 3b represent solutions of the equation $F_\nu(k_z) = 0$ for optical-range TM modes guided by a silver film ($\varepsilon_2 = -18 - i0.47$) surrounded by dielectric media ($\varepsilon_g = 1$, $\varepsilon_s = 2.25 - i3 \times 10^{-6}$). On curve 1 we have $\text{Re } \nu_1 > 0$ and $\text{Im } \nu_1 > 0$, i.e., it refers to waves leaking into the domain $y < -d$. The start of the curve ($d \rightarrow \infty$) corresponds to a plasmon mode of the interface $y = 0$, and the end ($d \rightarrow 0$) corresponds to a surface-wave mode of the interface between two dielectrics. Curve 2, along which $\text{Re } \nu_1 < 0$ and $\text{Im } \nu_1 < 0$, begins at the point corresponding to a plasmon mode of the interface $y = -d$ and goes to infinity [$\text{Re}(k_z/k_0) \rightarrow \infty$, $\text{Im}(k_z/k_0) \rightarrow -\infty$] as $d \rightarrow 0$. On curve 1 we have $\text{Re } \nu_1 < 0$ and $\text{Im } \nu_1 > 0$. It refers to waves entering the waveguide from the domain $y < -d$, their fields growing as $y \rightarrow -\infty$ and $z \rightarrow \infty$. According to the preceding discussion, modes corresponding to curves 1 and 2 admit

resonance excitation. An additional restriction for such excitation is given by condition (16), which, in particular, rules out the possibility of the excitation of a dielectric-dielectric interface (surface-wave) mode. Curves 4–6 in Fig. 3a represent solutions of the equation $F_\nu(k_z)=0$ for the three lowest optical-range TE modes guided by a silicon dioxide film ($\varepsilon_2=2.121975-i2.9134\times 10^{-6}$) terminated in air ($\varepsilon_g=1$) and in a silicon substrate ($\varepsilon_s=15.21-i0.39$). For all these curves we have $\text{Re } \nu_1>0$ and $\text{Im } \nu_1>0$, i.e., they refer to modes leaking into the substrate. Curves 4–6 begin at the point $k_z/k_0=\sqrt{\varepsilon_2}$ ($d\rightarrow 0$), which is far from the cut of the function $\nu_1(k_z)$ (outside the field of view of the figure). Accordingly, all the investigated modes admit resonance excitation. We have confirmed these conclusions by calculations of the $R_2(k_z)$ curves, which are characterized by resonance troughs (similar to those in Fig. 2) corresponding to excitation of the indicated modes.

3. INVERSE PROBLEMS OF RECONSTRUCTING COMPLEX MODE PROPAGATION CONSTANTS AND THE PARAMETERS OF WAVEGUIDE FILMS

The measurement of the complex mode propagation constants h plays an important role in the investigation of the properties of waveguides and surface layers. An approach based on experimental recording of the resonance troughs of the $R_2(k_z)$ curves^{13–16} is widely used at the present time to determine h . In this approach, however, rather limited information about the indicated curves is taken into account; only the coordinates of the minima of the functions $R_2(k_z)$ are measured, and they are identified with the real parts of the propagation constants $\text{Re } h$. The imaginary parts $\text{Im } h$ are determined in additional measurements, where attenuation of the modes is observed along the direction of their propagation.¹⁴ This procedure for the determination of h is time-consuming in the experimental realm and has a fundamental shortcoming in that the perturbing influence of the prism on the investigated structure is ignored.

One of the important applications of waveguide methods is to reconstruct the parameters of waveguide films. In this case the values of h for two modes of known order can be used to write a system of two dispersion relations containing inverse trigonometric functions; the numerical solution of these equations gives the quantities ε_2 and d (Refs. 13 and 14). However, difficulties are encountered in connection with the rigorous solution of the system, owing to the presence of branch points and cuts for the inverse trigonometric functions. This problem is particularly significant when modes existing under near-critical conditions are used.

More efficient approaches to the solution of the indicated inverse problems are described below. The real and imaginary parts of a mode propagation constant of a planar waveguide structure (inhomogeneous in the general case) are determined simultaneously with allowance for the perturbing influence of the prism by integrating the function $R_2(k_z)$ in the vicinity of the resonance troughs. The quantities ε_2 and d are determined by the system of equations (13) for two values of h . The solution of the system reduces to the determi-

nation of the roots of entire functions by the method discussed above.

Expanding the function $F_\nu(k_z)$ in a Taylor series in the domain H , we obtain the following approximation for the function $R(k_z)$ in the vicinity of resonances⁷:

$$R = \frac{1-\delta}{1+\delta} - \frac{4\delta}{1-\delta^2} \frac{\Delta h}{k_z - \bar{h}} + O(|\Delta h|). \quad (18)$$

Here δ is calculated for $k_z = \text{Re } h$, \bar{h} is the mode propagation constant of the waveguide–prism system, and $\Delta h = \bar{h} - h$. Equation (18) is defined in the case of the excitation of an arbitrary plane-layered waveguide structure, for which

$$\Delta h = - \frac{i\nu(1-\delta)\exp(-2i\nu g)}{(\varepsilon_g)^T(1+\delta)I \text{Re } h}, \quad (19)$$

$$I = \int_{-d}^{\infty} \frac{\psi^2(y)}{[\varepsilon(y)]^T} dy + \frac{\psi^2(-d)}{2i\nu_1(\varepsilon_s)^T}, \quad (20)$$

where the function $\psi(y)$ with the normalization $\psi(0)=1$ describes the distribution of the field of the excited mode, and

$$\nu_1 = \sqrt{k_0^2 \varepsilon_s - h^2}, \quad \nu = -i\sqrt{(\text{Re } h)^2 - k_0^2 \varepsilon_g}.$$

To solve the inverse problem for h , it is convenient to introduce the parameters¹⁷

$$p_1 = \frac{\text{Im } \bar{h}}{k_0}, \quad (21)$$

$$p_2 = - \frac{2\delta\nu\exp(-2i\nu g)}{(\varepsilon_g)^T(1-\delta)Ik_0 \text{Re } h}, \quad (22)$$

$$p_4 = \frac{\text{Re } \bar{h} - k_z}{k_0}, \quad (23)$$

which characterize the mode attenuation of the external prismatic structure, the coupling of the prism with the waveguide, and the deviation of the z -component of the exciting wave vector from the resonance value of $\text{Re } \bar{h}$. The parameter p_2 is complex-valued in general, i.e., $p_2 = |p_2|\exp(i\sigma)$. However, in the case of primary practical interest—weakly damped modes—the inequalities $|\text{Re } I| \gg |\text{Im } I|$ and $\sigma \ll 1$ hold. They permit small quantities $O(\sigma^2)$ to be omitted in the subsequent calculations. Taking Eqs. (18)–(23) into account, we obtain

$$R_2 = |R|^2 = 1 + [4|p_2|(p_1 + |p_2| - p_4\sigma)]/(p_1^2 + p_4^2). \quad (24)$$

It follows from Eq. (24) that the presence of mode attenuation ($\sigma \neq 0$) parts asymmetry to the function $R_2(p_4)$, the degree of asymmetry increasing as the losses increase (Fig. 2). We now determine the coordinate of the minimum of $R_2(p_4)$, denoting it by $p_4^{(0)}$. Differentiating Eq. (24), we obtain

$$p_4^{(0)} = - \frac{p_1^2 \sigma}{2(|p_2| + p_1)}, \quad (25)$$

TABLE I.

| Mode order | Polarization | h/k_0 (exact) | g/λ_0 | h/k_0 (reconstructed) | Mode order | ε_2 (reconstructed) | d/λ_0 |
|---|-----------------|------------------------------------|---------------|------------------------------------|------------|------------------------------------|---------------|
| Waveguide film, $\varepsilon_2 = 2.295225 - i3.03 \times 10^{-5}$, $d/\lambda_0 = 5$ | | | | | | | |
| 1 | TE _w | $1.512636 - i9.819 \times 10^{-6}$ | 0.28 | $1.512636 - i9.819 \times 10^{-6}$ | 1-2 | $2.295225 - i3.030 \times 10^{-5}$ | 4.99998 |
| 2 | TE _w | $1.505806 - i8.999 \times 10^{-6}$ | - | $1.505805 - i8.999 \times 10^{-6}$ | 1-3 | $2.295222 - i3.030 \times 10^{-5}$ | 5.00089 |
| 3 | TM _w | $1.512560 - i9.805 \times 10^{-6}$ | - | $1.512560 - i9.806 \times 10^{-6}$ | 2-3 | $2.295225 - i3.030 \times 10^{-5}$ | 4.99999 |
| Waveguide film, $\varepsilon_2 = 2.295225 - i3.03 \times 10^{-5}$, $d/\lambda_0 = 3$ | | | | | | | |
| 1 | TE _w | $1.509681 - i9.295 \times 10^{-6}$ | 0.16 | $1.509674 - i9.296 \times 10^{-6}$ | 1-2 | $2.295251 - i3.031 \times 10^{-5}$ | 2.9943 |
| 2 | TE _L | $1.498070 - i3.363 \times 10^{-3}$ | - | $1.498177 - i3.585 \times 10^{-3}$ | 1-3 | $2.295090 - i3.029 \times 10^{-5}$ | 3.0131 |
| 3 | TM _w | $1.509436 - i9.223 \times 10^{-6}$ | - | $1.509432 - i9.222 \times 10^{-6}$ | 2-3 | $2.295269 - i3.031 \times 10^{-5}$ | 2.9937 |
| Silver film, $\varepsilon_2 = -18 - i0.47$, $d/\lambda_0 = 0.06$ | | | | | | | |
| 1 | TM _L | $1.031124 - i4.595 \times 10^{-3}$ | 1.6 | $1.031198 - i4.668 \times 10^{-3}$ | 1-2 | $-18.0039 - i0.4694$ | 0.06014 |
| 2 | TM _w | $1.625144 - i4.617 \times 10^{-3}$ | 0.16 | $1.624916 - i4.595 \times 10^{-3}$ | | | |
| Silicon dioxide, $\varepsilon_2 = 2.121875 - i2.913 \times 10^{-5}$, $d/\lambda_0 = 3$ | | | | | | | |
| 1 | TE _L | $1.448039 - i2.524 \times 10^{-4}$ | 0.32 | $1.448039 - i2.526 \times 10^{-4}$ | 1-2 | $2.121977 - i2.966 \times 10^{-5}$ | 2.99981 |
| 2 | TE _L | $1.421781 - i9.937 \times 10^{-4}$ | - | $1.421779 - i9.960 \times 10^{-4}$ | 1-3 | $2.121977 - i2.967 \times 10^{-5}$ | 2.99983 |
| 3 | TE _L | $1.377055 - i2.279 \times 10^{-3}$ | - | $1.377052 - i2.290 \times 10^{-3}$ | 2-3 | $2.121981 - i3.517 \times 10^{-5}$ | 2.99984 |

$$R_2^{(0)} = 1 + \frac{4|p_2|(p_1 + |p_2|)}{p_1^2}, \quad (26)$$

where $R_2^{(0)} = R_2(p_4^{(0)})$.

It follows from Eq. (26) that

$$|p_2| = 0.5p_1[\operatorname{sgn}(g/g_0 - 1)\sqrt{R_2^{(0)}} - 1]. \quad (27)$$

Here g_0 is the thickness of the buffer layer, for which $R_2^{(0)} = 0$. To find the parameters p_1 and σ , we isolate the interval $(p_4^{(0)} - \Delta k_z/k_0, p_4^{(0)} + \Delta k_z/k_0)$ of variation of p_4 and form the integrals

$$I_1 = \int_{-\Delta k_z/k_0}^0 R_2(p_4^{(0)} + x) dx,$$

$$I_2 = \int_0^{\Delta k_z/k_0} R_2(p_4^{(0)} + x) dx,$$

where $R_2(p_4)$ is a function of the form (24).

Calculating the quantities $(I_1 + I_2)/2$ and $(I_1 - I_2)/2$, we obtain

$$\left[1 - \frac{1}{2\Delta k_z} \int_{-\Delta k_z}^{\Delta k_z} R_2(k_z^{(0)} + x) dx\right] [1 - R_2^{(0)}]^{-1} = \frac{p_1 k_0}{\Delta k_z} \arctan\left(\frac{\Delta k_z}{p_1 k_0}\right), \quad (28)$$

$$\sigma = \left[\int_{-\Delta k_z}^0 R_2(k_z^{(0)} + x) dx - \int_0^{\Delta k_z} R_2(k_z^{(0)} + x) dx \right] \{4k_0|p_2|[(1 + (k_0 p_1/\Delta k_z)^2)^{-1} - \ln(1 + (\Delta k_z/(k_0 p_1))^2)]\}^{-1}, \quad (29)$$

where $R_2(k_z)$ is the experimentally recorded function on the interval $(k_z^{(0)} - \Delta k_z, k_z^{(0)} + \Delta k_z)$, and $k_z^{(0)}$ is the coordinate of the minimum of this function.

Consequently, identifying $R_2^{(0)}$ with the minimum value of the function $R_2(k_z)$, we can determine the values of the parameters p_1 , p_2 , and $p_4^{(0)}$. We first solve Eq. (29) for p_1 ; this equation has a single root by virtue of the monotonicity of the function $f(x) = x \arctan(x^{-1})$ in the domain $x \leq 0$. The quantities p_2 and $p_4^{(0)}$ are then determined from Eqs. (25), (27), and (29) by direct calculation. According to Eqs. (21)–(23), the required mode propagation constant is

$$h = k_z^{(0)} + p_4^{(0)} + i[p_1 - p_2(1 - \delta)^2(2\delta)^{-1}]. \quad (30)$$

We note that the quantity δ in (30) depends on $\operatorname{Re} h$. However, since $|p_4^{(0)}|$, $|p_1|$, and $|p_2|$ are small, it can be evaluated for $h = k_z^{(0)}$ and, if necessary, refined by an iterative procedure. We also note that the integration operations in Eqs. (28) and (29) ensure stability of the reconstructed value of h against noise of the function $R_2(k_z)$.

We now address the problem of reconstructing the parameters of a waveguide film ε_2 and d . We assume that values of h have been found for two modes, the values of ε_g and ε_s are given, ε_2 is situated in the domain G of the complex plane, and d lies in the interval (d_1, d_2) . We fix a certain d in this interval and substitute the first value of h into Eq. (13). We see at once that $F_\nu(\varepsilon_2)$ is an entire function, so that its roots in the domain G can be found by the scheme of Sec. I. We note that, in general, there can be several roots of this kind [if G is interpreted as the entire complex plane, the number of such roots can be unbounded by virtue of the exponential asymptotic behavior of $F_\nu(\varepsilon_2)$ in the limit $|\varepsilon_2| \rightarrow \infty$; Ref. 9]. We denote the roots so obtained by $\varepsilon_{2j}^{(1)}$ ($j = 1, 2, \dots$). Solving Eq. (13) analogously, for the second value of h we have a different set of roots $\varepsilon_{2k}^{(2)}$ ($k = 1, 2, \dots$). The quantity $\Delta = \min_{j,k}(\Delta_{jk})$ can be found by direct sequential inspection of the differences $\Delta_{jk} = |\varepsilon_{2j}^{(1)} - \varepsilon_{2k}^{(2)}|$. Now, plotting the function $\Delta(d)$, $d \in (d_1, d_2)$, and

determining its minimum, we arrive at the required values of ε_2 and d .

Table I gives examples of how the above-described computational scheme can be implemented for the thin-film waveguide structures discussed in the article. The data have been obtained with the rigorously calculated $R_2(k_z)$ curves (the one in Fig. 2 and others similar to it) used as “experimental” curves. The quantity Δk_z is chosen on the basis of the condition $R_2(k_z^{(0)} + \Delta k_z) = (1 + R_2^{(0)})/2$. The first column of the table lists the conditional mode orders. The polarization of the modes is denoted by the symbols TE_p and TM_p , where $p=W$ for waveguide modes and $p=L$ for leaky modes. We note that the quantity $|\Delta h|$ increases as $|\text{Im } h|$ increases, lowering the accuracy of approximation of Eq. (18). The growth of $|\Delta h|$ follows from Eqs. (19)–(22) with allowance for the fact that high-contrast resonance troughs of the $R_2(k_z)$ curve can be obtained if $|p_2| \sim |\text{Im } h|/k_0$. The latter estimate is readily obtained by comparing relations (19), (22), and (26) and taking the inequality $\sigma \ll 1$ into account. On the other hand, all the data in the table have been obtained for values of g such that $R_2^{(0)} < 0.75$. This remark accounts for the noticeable increase in the error of solution of the inverse problems as the losses of the selected modes increase. We also call attention to the possibility of reconstructing the parameters of single-mode (for a fixed polarization) waveguide films from the values of h for waveguide and leaky modes (rows 4–6 in Table I). The accuracy of reconstruction in this case is higher than when h is used for orthogonally polarized waveguide modes, because the sys-

tem of dispersion relations is poorly conditioned in the latter case.

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