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Calculation of Complex Propagating Modes in Arbitrary,
Plane-Layered, Complex Dielectric Structures.
I. Analytic Formulation. II. Fortran Program MODEIG.

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Abstract

A method is presented for calculating complex eigenmodes of propagation in plane-layered structures composed of homogeneous, isotropic materials having arbitrary complex dielectric properties. The formulation is completely general, permitting any number of guiding and non-guiding layers, with loss or gain each layer. All modes having complex propagation constants and field distributions can be calculated with equal ease. These include modes having gain or attenuation in the direction of propagation, and having bounded or unbounded, leaky, or radiative properties in the transverse direction. A 2x2 vector-matrix representation for the differential equations, field solutions, and boundary conditions is used, which permits a simple constructive definition for the characteristic equation regardless of the complexity of any particular structure. A general complex root-searching algorithm is used to calculate the mode eigenvalues, and several novel features greatly improve the efficiency of the search. Field distributions and power density across the structure may be efficiently calculated using the same 2x2 matrix multiplications. A FORTRAN program has been written to implement the calculations, and a listing is included. The program has proved to be highly efficient and accurate.

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1. INTRODUCTION

1.1 Summary

This report describes an analytic formulation and computer program for the calculation of complex modes of electromagnetic wave propagation in plane-layered dielectric structures. Emphasis throughout is on complete generality: structures of any number of layers, any complex material parameters, and any types of proper or improper modes of the discrete or continuous spectrum are allowed. An effort was also made to achieve efficient and accurate numerical calculations.

The structures of interest are composed of any number of plane layers, having piecewise constant, homogeneous, but isotropic, dielectric material properties. The dielectric permittivities in the different layers may be arbitrarily complex, with positive or negative imaginary part representing absorption loss or active gain. The real part may also be negative, representing metal or isotropic plasma layers. In directions parallel to the planes the structures are assumed to be uniform in all parameters. Such systems of layers are generally viewed as open waveguiding structures. There are two open semi-infinite outer dielectric layers, so that radiation can occur in the transverse direction, normal to the planes. Usually some of the inner layers will have the highest permittivity (index of refraction), and a finite number of truly bound and guided modes will exist. But the method is not limited to such cases. And it is not necessary to make any a priori assumptions about which layers are guiding layers, or which layers have large or small, real or complex permittivity. The special case of constant surface-impedance boundaries, including metals, in place of the outer semi-infinite layers is easily included.

Modes of propagation parallel to the planes are characterized by a normalized propagation coefficient, β , which is common to all layers, and is allowed to be arbitrarily complex. The imaginary part, positive or negative, represents the rate of attenuation or gain of the mode in the direction of propagation. Such complex modes may arise whenever any of the material parameters are complex-valued or when there is radiation loss into the semi-infinite layers.

Emphasis is on discrete modes of propagation, which are solutions of a homogeneous, two-point, eigenvalue problem in the transverse dimension. These arise when restrictive homogeneous boundary conditions are imposed at the outer boundaries of the structure. The discrete complex values of β for these modes are roots of a transcendental eigenvalue (characteristic) equation. A central part of the problem is the formulation of the characteristic function, and the numerical calculation of its roots.

The discrete modes include those which are proper, bound, modes having square integrable field distributions across the structure. This necessarily implies an outward exponential decay for the fields in the semi-infinite layers. Other discrete modes include the well known leaky modes, which are improper, or not square integrable across the guide. But for small imaginary part for β these modes may have some physical interpretation, and can provide excellent approximate solutions to some field problems. Other discrete modes also exist as mathematical roots of the same characteristic equation, but do not necessarily have a physical interpretation. All these modes are solutions of the same mathematical problem, and the improper modes are no more difficult to solve for than the proper modes.

The objective of this work was to obtain a method for calculating these discrete modes in very general structures with any number of layers. And it

was also the objective to be able to calculate leaky modes in particular, and the improper modes in general, in addition to the proper modes. The capability to include complex material parameters was not initially an objective, but it could be provided with little difficulty.

The primary motivation for the work arose in the context of integrated optics. There was a need to calculate the modes of propagation in planar optical guiding structures; but the structures of interest were composed of more than a few layers, including, for example, two dissimilar guiding layers separated by more than one intermediate layer. And there was a need to calculate leaky modes in such structures. There has also been an increasing recognition of the usefulness and importance of including leaky modes in the expansion of field distributions in general dielectric guides.

Motivation for including complex material parameters arises in guiding structures which include metal layers, or lossy dielectrics such as semiconductor materials where free carrier absorption can often be significant. Also, a complex permittivity with negative imaginary part can describe the recombination gain in the active layers of semiconductor lasers, and the popular double heterostructure (DH) GaAlAs lasers are inherently multilayer structures. For the design of such DH lasers it is highly desirable to have the capability to calculate complex propagating modes in the presence of both loss and gain in different layers.

Previous formulations and methods for calculating modes in layered structures are reviewed. For structures of only a few layers methods have frequently been published, but these cannot be extended to more layers. A few methods exist which are valid for many layers, such as the well known transverse resonance method. However, the characteristic functions for these methods are shown to have undesirable analytic properties, which can

make them very inefficient or unusable with numerical complex root searching routines. These characteristic functions have extraneous zeros or poles; and for the transverse resonance method an infinite number of movable poles are interspersed among the zeros. Most general methods do not describe an efficient method for calculating the field distributions once the mode propagation constants are known.

The field problem is here formulated directly in terms of the actual E and H field components throughout the structure, with emphasis on the tangential fields at the boundaries. Maxwell's curl equations reduce to coupled first-order differential equations in the two tangential field components. Solutions to these equations are easily stated in vector-matrix form, without the need for reference to a wave equation or any need for transverse wavelike solutions in the inner layers.

Normalized variables are used throughout to control the order of magnitude of the field quantities and other parameters to be programmed. All material parameters and modal propagation constants are normalized to those of free space. Field variables are normalized so that, by duality, the same variables serve for either TE or TM polarizations. When programmed, the one formulation may be used equally well for calculations of both polarization.

The field solutions for any value of β , for a discrete mode or not, are given in terms of a 2x2 vector-matrix representation. This representation is most commonly encountered in the analysis of optical multilayer filters, where propagation is normal to the layers. The formulation remains completely valid for propagation parallel to the layers, but all quantities must be allowed to become complex. The tangential fields at any two planes

in the structure are related by a matrix transformation. By chain matrix multiplication across the structure the field solutions are defined and easily calculated everywhere in the structure.

Boundary matching conditions at all the material boundaries are satisfied at the outset. This is possible because the tangential fields, which are required to be continuous at the boundaries, are in fact the primary dependent variables. In particular, a transformation matrix exists for each layer, depending only on the parameters of that layer. The satisfaction of the interior boundary matching conditions may be considered to be a part of the definition of the differential equation throughout the structure, or to be a part of the construction of the solutions. They need not be considered a part of the definition of the characteristic function, which arises only with the imposition of the outer boundary conditions.

The boundary conditions at the outer boundaries are distinct from the matching conditions at the material discontinuities; they resemble the radiation condition at infinity, but for the fully complex case and for improper modes they do not have the same physical interpretation. These boundary conditions, the definition of the transverse propagation constants κ_1 and κ_N in the semi-infinite layers, and the classification of the modes, are all intimately related.

Classification of modes following the conventions of surface waves is reviewed. But in the present case the classification must be made in the two semi-infinite layers simultaneously. The classification is described in terms of the regions of the complex κ_1 and κ_N planes. These necessarily have an additional branch point and branch cut not encountered when there is a single semi-infinite layer over a surface wave structure.

Principal branch specifications for κ_1 and κ_N , in their respective complex planes, are an important part of the statement of the outer boundary conditions, and of the eigenvalue problem in general. A non-conventional and completely arbitrary branch specification is used, which greatly improves the efficiency of root searching for the discrete modes. Proper and improper modes are not distinguished by their location on a principal or secondary branch for κ_1 and κ_N , or Riemann sheets for β . Rather, by choice of orientation of branch boundaries and cuts, both proper and improper modes can exist on the same sheet. As a result, the root search for improper modes is no more difficult than for proper modes. Also, there is little difficulty in calculating modes which are "near cut-off", having roots located near to branch cuts associated with the conventional branch specifications.

The phase integral, of the transverse propagation constant κ , across all the inner layers of the structure, is used in ordering the discrete modes and for assigning a mode index to each.

Several special cases of modes are easily included in the formulation. Field distributions for modes of the continuous spectrum can be calculated for specified values of β without the need for a root search. But it is emphasized that these are not solutions of the transverse eigenvalue problem for the discrete spectrum of modes. The boundary conditions are different. Allowance for complex material parameters requires some generalization of the description of the continuous spectrum beyond that usually given for the simple three-layer case and for lossless media. The spectrum of plane waves in the semi-infinite layer is also easily included; for lossy materials these are not the same as for the continuous spectrum.

Special attention is given to the definition and construction of the characteristic function. Emphasis is placed on its analytic properties for the benefit of efficient complex root searching. The characteristic equation is described from several viewpoints, including that of a mathematical two-point boundary value problem, in terms of reflection and transmission coefficients, and as a Wronskian determinant between two specially constructed field solutions.

It is shown that the characteristic function is a determinant of only a 2×2 matrix, regardless of the number of layers. By the sequence of 2×2 matrix transformations across the structure, a single matrix transformation between the tangential fields at the two outer boundaries is easily calculated. This matrix completely characterizes the interior structure, quite independently of the outer semi-infinite layers or boundary conditions. The characteristic function is then defined in terms of this matrix and a matrix representation of the boundary conditions. It is also advantageous to consider β^2 , rather than β , to be the eigenvalue parameter whose complex plane is to be searched for roots.

The characteristic function defined here has no poles or extraneous roots, and in the β^2 -plane it has only one pair of unavoidable branch points and cuts associated with the two outer boundary conditions. The relationship of this characteristic function to that of the transverse resonance method is discussed. Explicit expressions for the 2, 3, and 4-layer structures are listed for comparison with other versions.

A general purpose complex root searching algorithm is used for calculating the roots of the characteristic equation in the β^2 -plane. Usually called Muller's method, it is an iterative procedure based on a local

quadratic approximation to the characteristic function. Several important improvements are incorporated which greatly increase the rate of convergence in the early stages of the iterations. Initial guesses, at which to start the search for each of several roots, are calculated by interpolations based on the phase integral. Altogether, with the maximally analytic characteristic function, use of the β^2 -plane, improvements in the root searching method, and excellent initial guesses, rapid and efficient calculation of the discrete modes is realized. As few as 2 or 3 iterations are needed per root for simple guides where good guesses are possible, or when only small changes in parameters are made from a previously calculated case. More commonly, convergence to an accuracy of 10^{-10} is obtained in 3 to 7 iterations. Where convergence is not obtained in 10 to 15 iterations, the root search in nearly every case has been found to be entangled in a branch cut.

Field distributions across the structure, for any value of β , of the discrete or continuous spectrum, are easily calculated. The values of the tangential fields at all the boundaries are calculated by the sequence of matrix multiplications, and constitute a set of values sufficient to completely characterize a field solution. The same 2×2 matrix method is then used in an incremental manner to efficiently calculate the fields at closely spaced points across the structure. These may be used for plotting purposes or possibly for numerical integrations.

The transverse and propagating Poynting power density for any mode is easily calculated from the calculated field values with little additional effort.

Part II describes a FORTRAN computer program which implements the formulation described for actual calculations. Part I of the report is intended to serve as documentation for the program.

A rather large program results, intended for complete case by case solutions for any arbitrary structure. The program is made possible by, and depends on, the complex variable capability of FORTRAN, including the library functions for complex elementary functions. Complete flexibility of program usage is available through a large number of input variables. Large amounts of output are available under users option to provide detailed information for each case.

The program has proved to be quite efficient and capable of high accuracy. On a CDC-6400 computer of 14 digit floating point resolution a convergence criteria of 10^{-12} has been routinely realized for modes in structures up to 7 layers. Using a non-optimizing compiler, sets of 7 modes at a time are calculated (to a convergence criteria of 10^{-10}) for a seven layer structure in about 2 to 3 seconds of a cost of 25 cents. Detailed field values across the structure for all seven modes take a comparable amount of time.

The original objectives of this work have been fully realized. With the present formulation and program it is now feasible to obtain quantitative results for any complex modes in arbitrary structures. This is a capability which has not previously existed.

1.2 Objectives and Motivating Problems

The work reported here was carried out in the context of integrated optics, and of wave propagation along multilayered dielectric guiding structures. This background is assumed of the reader, and is represented by the book by Marcuse [1], and the one edited by Tamir [2]. A vast literature in this area now exists, and further reference to it is made only as specifically needed. Wave propagation in dielectric guides at microwave frequencies, is, of course, quite equivalent, and this earlier interest is well represented in the books of Collin [3] and Shevchenko [4]. An even more general background on fields and waves, and wave propagation including layered media, is found in Felsen and Marcuvitz [5]. These references may be consulted for citations to earlier literature.

The overall objective of the present work was to develop a formulation for direct calculation of complex modes in very general arbitrary structures. Here, complex modes refer to discrete eigenmodes of propagation parallel to the planes, and having complex-valued propagation coefficients. Such complex modes arise whenever, a) any of the dielectric materials have losses (or gain), representable by a complex permittivity, or b) modes are unbounded or improper, where the imaginary part can sometimes be interpreted as attenuation due to radiation loss from the propagating energy. The calculation of bound modes in simple lossless guides (of 3 or 4 layers) appears repeatedly in the literature. Provision for material losses is uncommon except for simple cases (say 2 or 3 layers), and is often treated by approximate methods. Similarly, the well known "leaky" improper modes are often treated by approximate methods, and rarely for structures of more than 4 layers.

For more complicated structures the only recourse is to direct numerical methods. For more than a few layers, and especially for complex material parameters, analytical methods become intractable. A few formulations of the field problem for modes in layered structures have appeared which have the potential for describing a completely arbitrary case. But these formulations have been found to be unsuitable or inefficient for numerical purposes, as described later.

Therefore, one objective was to arrive at a formulation more suitable for being programmed for calculation. Thus, the formulation should be as simple as possible, not depending on the number of layers, and also be numerically accurate and efficient. It was anticipated that a 2x2 matrix method similar to that used for multilayer optical filter analysis would serve the purpose, and remain valid for complex parameters. The objective for complex propagation constants is reasonable because of the capability for complex calculations in the FORTRAN language. When the propagation constant is allowed to be complex, most field parameters must also become complex, and there is little difficulty in including the capability for fully complex material parameters. Hence a capability for a completely arbitrary complex structure was reasonable.

Once numerical methods are resorted to there is the potential for very accurate results. So another objective was to use the best possible numerical techniques. For example, by choice of variables and expressions, singular and indeterminate situations, where considerable loss of significant digits could result, were to be avoided. A relatively efficient method for complex root searching was known to be available. So there was hope that results could be obtained which were limited only by the unavoid-

able accumulation of roundoff error in whatever computer was used.

Initial motivation for this work arose in connection with periodic coupling between two dissimilar guides in a dielectric structure. Such a coupler is in contrast to the well known grating couplers between a guide and an incident or radiated beam. Specifically, there is interest in periodic coupling between a low index glass fiber transmission line and a surface guide on a high index substrate. All active integrated optical devices are fabricated on a relatively high index substrate, such as LiNbO_3 with $n \approx 2.2$ [2, p. 175], or GaAs with $n \approx 3.5$ [2, p. 243]. On the other hand, the glass fiber has an index and mode propagation constant of approximately $n = 1.5$. With this large index mismatch, one of the few hopes for distributed couplers is to use periodic coupling, introduced in the layer separating the two guides. Such periodic coupling has been suggested several times [6-9], but little progress has been made in analyzing such a structure or demonstrating its feasibility.

The structure of interest is shown in Fig. 1.1, where initially a planar geometry is assumed for simplicity. It is a five-layer structure with an externally mounted glass guide [6], layer 2, separated from the substrate guide, layer 4, by the isolation layer 3. The latter would incorporate the periodic variation, of a variety of possible types, with a period Λ . The permittivity indicated for layer 3 would be the average over the periodic variations. Depending on the type of periodic structure used, it may be necessary to subdivide layer 3 into more layers, say 2 or 3. The condition for efficient net coupling between the glass guide mode of β_1 , and the substrate guide of β_2 is simply that $K \equiv 2\pi/\Lambda = |\beta_1 - \beta_2|$. But

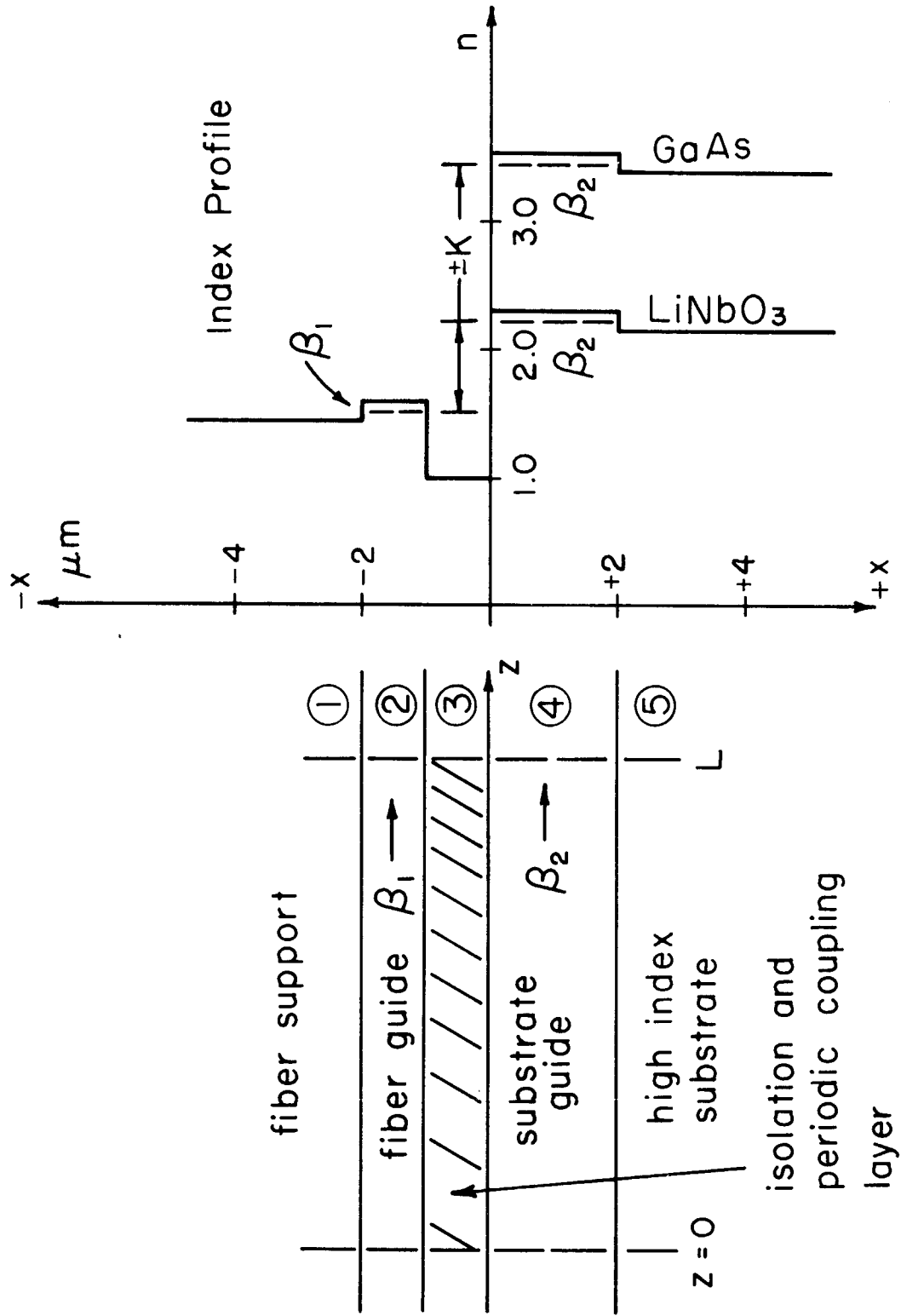


Figure 1.1 Planar, externally mounted, fiber-guide to high index substrate-guide coupling configuration.

there are other competing coupling and scattering processes which are also present and make the coupler difficult to analyze. Clearly, the periodic layer also serves as a grating coupler between either guide and radiated beams in both outer layers. These arise as both negative and positive higher order diffraction processes, associated with terms $\pm nK$. Further, any modes in the glass guide, because of the high index substrate, must be leaky modes, as for a prism coupler. This structure is unlike the prism coupler, however, because of the presence of the substrate guide.

The feasibility of this coupler concept depends on whether, by choice of structure parameters, and perhaps by blazing effects [2, p. 118; 10-11] or resonance effects (below), the coupling to radiated beams can be minimized, while permitting a useful amount of power to be coupled between guides.

It is not the purpose of this report to describe any analysis of this structure. It is mentioned as an example of how quickly practical structures can become very difficult to analyze. It provides several examples of types of modes which cannot be described by the familiar methods for three and four layer structures, and more general methods must be considered.

When the phase mismatch between two guides is small, and only bound modes are considered, then familiar coupled mode theory may be used. For coupling between two rather arbitrary asymmetric guides (a 5-layer structure) the work of Watts [12] and Wilson and Reinhart [13] may be mentioned. Except for the leaky mode properties of guide 1, this approach could be used for approximate analysis of the structure of Fig. 1.1.

Because the periodic structure introduced in layer 3 is considered to be weak, the waveguiding properties of the structure are dominated by the modes, both proper and improper, of the overall 5-layer structure. The periodic perturbation then serves as a coupling mechanism between the modes. It is not appropriate to consider this as a problem of wave propagation in a periodic structure, using representations in terms of Bloch waves. Therefore, it has been a primary motivation to be able to solve for propagating modes in the basic 5-layer structure of Fig. 1.1, and this necessarily includes leaky modes.

An important recent development in the theory of grating couplers has been the recognition that, even for some simple structures, the traditional first order approximations for calculating the coupling efficiency fails completely. This was first pointed out by Kiselev [14], and some quantitative calculations and experimental demonstrations were provided in a companion paper by Zlenko and Kiselev, et al. [15]. Later, Rigrod and Marcuse [16] presented a confirming analysis for similar cases, and indicated that equivalent results could be obtained from coupled mode theory. These results showed that for some configurations (the grating layer placed between a surface guide and a high index substrate) the coupling efficiency could be very dependent on the grating period and guide thickness. For some combinations of these parameters the coupling efficiency could be large; but most dramatically, for other slightly changed values, the efficiency could become essentially zero. The effects were described as interference effects between two different diffracted orders, which both contribute to the radiated beam. First order perturbation analysis (repre-

senting most previous work on grating couplers) considers only one diffracted order at a time, and it assumes that the field distributions due to the incident modes are not altered by the presence of scattered fields. The newly recognized interference effects can also be described as transverse resonance effects. For some guide thicknesses, and grating diffraction angles, strong standing wave fields can be excited in the guide. Then, for even weak diffraction, large diffracted fields can exist in the guide. This is contrary to the assumptions of the first order perturbation method.

We point out here that these results can also be described as periodic coupling between the guided mode and other leaky modes of the same guide. Thus, if β_1 is the propagation constant for the bound mode, and β_2 is the real part of the propagation constant for a leaky mode, then strong coupling to the radiated beam (from the leaky mode) can be expected when the phase matching condition is satisfied, $K \equiv 2\pi/\Lambda = |\beta_1 - \beta_2|$. This qualitative description has been confirmed by using preliminary results of the present formulation. Leaky modes were calculated for the structure used by the above authors [15, Fig. 6; 16, Figs. 4 and 6]. For each of six points, where comparison was possible, the maximum radiation occurs when the phase match condition was satisfied. The sharp nulls, of apparently zero coupling efficiency, occur whenever $|\beta_1 - K|$ is midway between the values of β_2 for two adjacent leaky modes. Agreement was within the accuracy with which values for β could be read from the figures.

Recognition of these transverse resonance effects calls into doubt any analysis of the structure of Fig. 1.1 which is based on first order perturbation methods. It is likely that the concept of periodic coupling between

bound and leaky modes can be developed to provide quantitative results for the efficiency of coupling between radiated beams and modes in more arbitrary structures. This approach is directly applicable to that of Fig. 1.1, and provides additional motivation toward a capability for calculating leaky modes in general.

There has also been an increasing interest recently in the use of leaky waves for describing field solutions in open guiding structures. Traditionally, leaky waves have been considered nonphysical, and not usable for the representation of real field solutions; although the usefulness of a single leaky mode to describe radiation from leaky wave antennas and prism couplers is well known. Shevchenko [17], Shatrov [18] and others [19-20] have shown, however, that it is possible to include leaky modes in a general field expansion. The expansion over the continuous part of the spectrum can be replaced by a summation over the set of discrete improper modes. Within the guide, and in its vicinity, the inclusion of a few of these improper leaky modes can lead to rapidly convergent representations for the fields. Golichev and Krasnushkin [21] have presented an elegant description of the alternatives of representations by integrals over continuous spectra or by summations over sets of discrete modes. For optical fiber guides, Sammut and Snyder, et al. [22-24], have shown that weakly leaky modes play an important and practical role in excitation and attenuation measurements.

In order to make greater use of leaky modes in describing excitation and propagation in layered structures it is first necessary to be able to make quantitative calculations of the propagation constants and field distributions. Methods for such calculations in general structures are rarely considered in the literature. Usually, only the bound proper modes are of

interest; and where improper modes are mentioned, quantitative calculations of the mode parameters are rarely carried out.

Hence, one of the motives for the present work was to obtain a method for numerically calculating leaky and improper modes in very general layered structures. It was believed that, in using numerical methods, and if the mathematical problem were properly formulated, then improper modes should be no more difficult to calculate than the proper modes.

Another area where complex modes are important is in propagation in layered structures which include dissipative losses. In most analysis of dielectric structures such losses are usually ignored, except perhaps in the simplest (say, 3-layer) cases. A very important active area at present is that of semiconductor double heterostructure (DH) lasers, which are inherently complicated multilayer structures [2, p. 271; 25-27]. In many actual structures the free carrier absorption losses can be significant, affecting the lasing threshold. It is very desirable to be able to calculate mode parameters, especially mode attenuation or gain, and field distributions, in layered structures with losses permitted in any layer. Even more important is the inclusion of gain (due to the active recombination region) in some layers. From the viewpoint of a complex permittivity, the difference between loss and gain is only in the sign of the imaginary part. In semiconductor lasers leaky modes can also be important because of limitations on the choice of material permittivity. In fact, leaky mode concepts have been proposed to help control the selection of lasing modes [28]. As an example of structure complexity Suematsu, et al. [29-30], have demonstrated a 7-layer twin-guide laser with gain in one guide, which is coupled to an output guide with feedback structure. There can be losses in all layers

and leaky radiation into the outer layers, though these were not included in any of their approximate analysis.

If a method were capable of directly solving for modes in general structures, with material loss or gain, then analysis of semiconductor heterojunction laser would be an area of immediate practical benefit. This provided additional motivation to keep the formulation completely general, with arbitrarily complex material parameters allowed throughout. Two examples of DH lasers are used later to demonstrate the capabilities of the present formulation and program.

Even in a simple case, of bound modes in a system of two coupled similar guides, there is some motivation for direct calculation of the exact modes of the overall structure. Coupled mode theory is nearly always used to describe such a structure. The resulting representation of the fields, in terms of approximate normal modes, can be excellent in the case of weakly coupled guides; but it is not valid for close, strongly coupled, guides. If a general method for solving multilayer structures were available, such coupled guide problems could be solved directly. If sufficient accuracy were possible, then the effective coupling coefficient between guides (a parameter of the coupled mode theory) could be obtained by calculating differences between propagation constants of the isolated guides and of the system of coupled guides. Since an exact calculation gives the exact normal modes for the complete structure, it is even possible to suggest that the fields for modes in the individual guides could be written approximately as linear combinations of the normal modes. This is the converse of the viewpoint of coupled mode theory, and would be useful in the case of strongly coupled guides.

A last example is that of hollow waveguides [1, p. 43], which have a role in gas laser resonators and for guiding long-wavelength infrared radiation. The guiding layer is of lower index than the walls, and all modes are necessarily leaky modes, though the rate of loss for the lowest order modes can be very small.

In most practical structures the magnitudes of coupling coefficients and the rates of power loss for leaky modes are relatively small. These may be on the order of 10^{-3} to 10^{-8} , say, relative to the magnitude of the real part of the propagation coefficient. For direct calculations of these quantities the propagation coefficients must then be calculated to better than this in relative accuracy. For example, if an 8 digit floating point computer is used, and there is a minimum of round-off error in calculating β , then a value of coupling coefficient or leakage rate of 10^{-5} could be obtained with 2 to 3 digit accuracy.

These considerations provide some motivation for obtaining maximum possible numerical accuracy from any implementation of the formulation. It is worth investing some attention to questions of efficient and accurate numerical methods. Because of the many layers, complex parameters, and the need for finding roots by iterative procedures, numerically efficient procedures and minimization of round-off error can make the difference whether or not it is feasible to calculate modes in some structures.

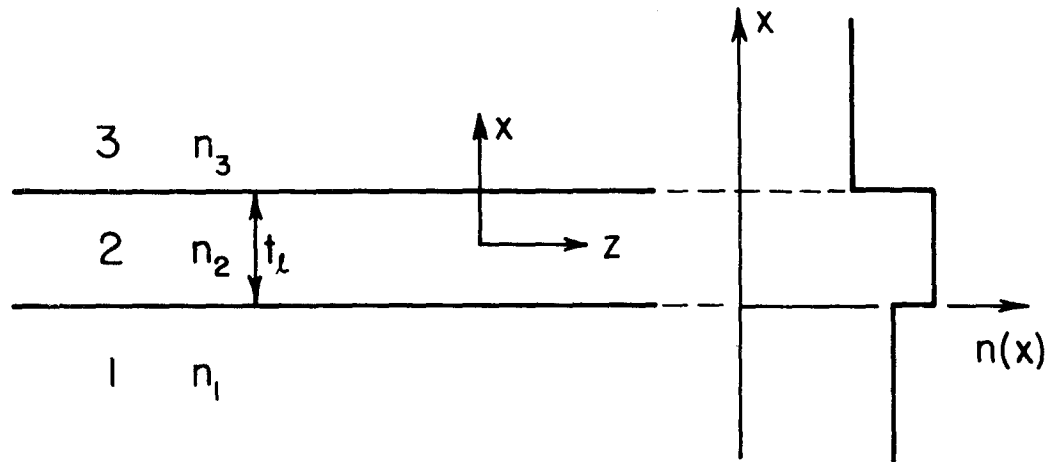
1.3 Previous Methods

The three-layer asymmetric dielectric structure, and its characteristic equation for bound guided modes, is ubiquitous in the literature of integrated optics [1, Sect. 1.3; 2, Sect. 2.3]. This is shown in Fig. 1.2 for the TE modes. This structure is the prototype for all planar dielectric guides, and is also used to obtain approximate solutions for modes in rectangular guides [1, Sect. 1.7]. The reader is assumed to be familiar with the formulation for the fields in the three layer problem, the traditional characteristic equation, and with the properties of the bound guided modes.

In this report we are interested in the calculation of more general structures: of arbitrary numbers of layers, and for dielectric properties which may be lossy, or active (lasers, with gain), or even having a negative permittivity (metals and plasmas). We are also interested in arbitrarily complex modes which may have attenuation or gain the direction of propagation, due to either the material properties, or due to radiation loss (leaky, unbounded modes) in the transverse direction.

With some care, the formulation for the three-layer structure can be used when the material parameters are complex, and also used for leaky unbound modes beyond cut-off. For the single symmetric guide, Burke [31] has presented extensive results for the general case of lossy materials, and included improper modes. His method does not generalize to the asymmetric guide.

Several attempts have been made to extend the formulation for the three layer case, particularly the form of the characteristic equation, to describe modes in four-layer structures. These are of interest for beam



Propagation factor $\exp i(k_z z - \omega t)$:

$$k_z^2 + k_x^2 \equiv k_0^2 n^2, \quad k_0 \equiv 2\pi/\lambda \equiv \omega/c$$

$$\beta \equiv k_z/k_0, \quad \kappa \equiv +i\gamma \equiv k_x/k_0$$

$$\kappa_l^2 \equiv -\gamma_l^2 \equiv n_l^2 - \beta^2, \quad l = 1, 2, 3$$

Characteristic Equation for TE_m mode:

$$f(\beta) \equiv k_0 \kappa_2 t_2 - \phi_1 - \phi_3 - m\pi = 0$$

$$\phi_1 \equiv \tan^{-1} \gamma_1/\kappa_2; \quad \phi_3 \equiv \tan^{-1} \gamma_3/\kappa_2$$

$$n_1, n_3 \leq \beta \leq n_2; \quad 0 \leq \phi_1, \phi_2 \leq \pi$$

Figure 1.2 Three-layer Dielectric Guide and Characteristic Equation.

coupling to guides (prism couplers) [32] and also for guides involving an additional layer of perturbing material [33, 34], often a metal [35-40]. In extending the formulation in this way, a priori assumptions are usually made about the additional layer being either a part of the guiding layer or not. The choice of notation and range of values for the parameters strongly reflects these assumptions. It is not unfair to say that it is impossible, by extension of the three-layer formulas, to obtain the characteristic equation for more than four layers; or to obtain a four-layer characteristic equation which is valid for all physically interesting values for the index of the two inner layers.

One relatively simple procedure for calculating propagation constants of modes in layered structures is the so-called transverse resonance method [2, p. 107; 5, p. 215; 41]. It is applicable to any number of layers, of complex dielectric materials, and can be adapted to complex modes. The method is based on the close analogy between the transverse propagation of the fields in the layered structure, and the more familiar voltage-current propagation on two-wire transmission lines. The layered structure can be modeled by cascaded sections of transmission lines, having appropriate characteristic impedances and (transverse) propagation constants, but which are functions of the mode propagation constant. By imposing conditions on the solutions in the semi-infinite layers (transmission lines), the wave impedance can be transformed from layer to layer, leading to the definition of a characteristic equation whose roots are the mode eigenvalues for the layered structure. The transverse resonance method has a close relation to the method described here, since many of the numerical quantities needed for the recursive calculation are the same.

The transverse resonance method has some undesirable numerical properties, however, which makes it unusable for complex root searching. And the method itself does not provide a procedure for calculating the field distributions once the eigenvalues are found. The relationship to the present method is pointed out later.

Harris has developed an extensive formulation for fields and modes in layered structures of arbitrary number of layers [41-47]. A representation in terms of vector potentials was chosen, assuming exponential solutions to the wave equation, with two undetermined amplitude coefficients, in each layer. The field continuity conditions, at each interface between layers, lead to a pair of simultaneous equations for the amplitudes in any two adjacent layers. For eigenmodes, a single exponential solution (an "out-going wave" only) is assumed in each semi-infinite layer. For $N+1$ material layers, there are a total of $2N$ simultaneous equations, homogeneous in as many unknown amplitude coefficients. The characteristic function for the modes is taken to be the determinant, D_{1N} , of the $2N$ by $2N$ matrix of coefficients, all being functions of the common modal propagation constant and of the layer parameters. The characteristic equation, in the propagation constant k_z say, is simply that $D_{1N}(k_z) = 0$; that is, the condition for the existence of nonzero solutions for the $2N$ amplitudes.

This method considers the eigen-condition to be the simultaneous satisfaction of all boundary conditions. Because of the use of D_{1N} , it might be called the grand-determinant approach to the characteristic equation. The determinant is of order $2N$, and for all but the smallest N it becomes impracticable to calculate directly. Harris showed that D_{1N} may be calculated recursively; starting with a single boundary, the effect of each additional

layer is incorporated by use of a two-term recurrence relation [43, Eq. A8; 46, p. 334]. This is possible only because the coefficient matrix is sparse, being pentadiagonal, and Harris' recursive method appears to be a special case of a more general recurrence relation for determinants of such matrices [43]. One unfortunate aspect of D_{1N} , as defined, is that it also has roots which are not eigenmodes. It becomes zero whenever the transverse propagation constant, $k_x = (k_\ell^2 - k_z^2)^{1/2}$, $k_\ell^2 \equiv \omega^2 \mu \epsilon$, becomes zero in any interior layer indexed by ℓ . That is, in addition to the eigenvalue roots, k_z , $D_{1N}(k_z)$ has additional zeros, branch points, and associated branch cuts, for every $k_z = k_\ell$ of the inner layers. This has serious, though somewhat correctable, consequences for numerical root searching methods.

Harris used his formulation in the analysis of prism and periodic beam couplers [43, 45, 46], and several others have used it for periodic couplers [49] and metal-clad wave guides [50]. Interestingly, and in spite of its potential generality, the method does not appear to have been used for structures of more than five layers. And, with one exception [51], the formulation does not appear to have been used for direct calculation of leaky modes in prism couplers or for modes beyond cut off in normal guides. Rather, the formulation has been used as a basis for first order approximations for leakage rates of tunneling modes [43], for losses in metal clad guides [50], and for coupling between two guides [47]. Had a general root searching procedure been used with the formulation, some exact numerical results could have been obtained for these problems.

For any modal propagation coefficient, k_z , the field solutions in Harris' formulation (the set of amplitude coefficients in all layers) were stated in terms of Cramer's rule, requiring $2N$ additional determinant

evaluations. These can also be carried out recursively. However, the current state of the art of computational linear algebra considers Cramer's rule and use of determinants as numerically very inefficient and of poor accuracy.

Canosa and de Oliviera [52], and Ixaru [53], have also used a grand determinant method for calculating the energy eigenvalues for a one-dimensional Schroedinger equation. The potential is approximated by a set of stepwise constant intervals (layers), and continuity conditions are applied to the scalar function and its derivative at all the boundaries. By a sequence of elementary matrix operations, on the coefficient matrix for the resulting set of equations, they showed that the grand determinant for the characteristic equation could be evaluated as a determinant of a 2×2 reduced matrix. The latter is obtained as a $2N$ -fold product of 2×2 submatrices, and inverses of some submatrices, of the $2N \times 2N$ coefficient matrix. Their interest was limited to real potentials and real eigenvalues, but otherwise it is very similar to Harris' method. Because of the 2×2 matrix operations it is closer to the method presented here. In [52] a root searching method similar to the one used here was used to locate the eigenvalues, but it was not used for finding complex roots.

C. A. Ward, et al. [54], have obtained a general expression for the dispersion (characteristic) equation for TM modes in structures of N layers of complex dielectrics. Their applications were primarily to surface plasma waves (polaritons, plasmons) along metal-dielectric boundaries, where TE modes are unimportant. By examining their characteristic equations for 2, 3, 4 and 5 layers they were able, by induction, to deduce a general expression. This is a sum over $2^{(N-2)}$ terms, each term being a product of $N-1$

factors. It was implied that their general expression was easily programmed for calculation, and that it offered some advantages over recursively calculated expressions. This does not agree with the common understanding, in computational mathematics, that recursively defined functions, and calculations based on a recursive procedure, offer the highest efficiency (minimum number of operations) and minimum programming complexity. An expression similar to Ward's was previously obtained, but not emphasized, by Harris for the characteristic equation in his formulation [42, Eq. 5; 47].

Ward's characteristic equations have a property even more serious than Harris'. Namely, for all layers, the same points $k_z = k_\ell$ in the k_z plane, for which the transverse propagation constants, k_x , become zero, are now branch poles of the characteristic function. The function behaves as $1/k_x$ in the neighborhood of each of these points; and there is a branch cut connecting each to the point $k_z = \infty$, which is an additional N-fold multiple zero of the characteristic function. This situation is evident from the equation in Fig. 2 of Ref. 54, where, for all layers, the individual k_x as used here (their $\alpha_m \equiv k_{mz}$) appear in the denominators throughout. An approximation to first order in k_x , for any layer as $k_x \rightarrow 0$, shows the function to behave as $1/k_x$. These branch poles probably make this characteristic function unusable for general root searching methods. Certainly it would be nearly impossible to calculate mode propagation constants, k_z , which happened to lie close to the poles at k_ℓ for any of the layers. Approximate pole-zero cancellation could make the zero invisible to the root searching routine. Further, it is possible for the root searching procedure to wander off to $k_z \rightarrow \infty$, seeking the additional roots there.

The extraneous zeros or poles in these characteristic functions can be numerically removed. This is done by dividing Harris' function by the product of k_x over all the inner layers, or by multiplying Ward's function by the same product. If this is done numerically, after calculation of the function as originally defined, then an indeterminate form of $0/0$ or ∞/∞ can result, with considerable risk of round off error. It is best to define the characteristic functions to have a well behaved form in the first place.

It may be argued that characteristic functions should have a property of maximum analyticity. That is, in the eigenvalue parameter, the characteristic function should have only those zeros which are true eigenvalues of the problem; and elsewhere the function should have no singularities, except those which are unavoidable and fundamental to the problem. Characteristic functions are not unique. For, multiplication by any analytic function will leave the eigenvalues unchanged, but it may introduce additional zeros which are not eigenvalues. Multiplication by a nonanalytic function will ordinarily leave the eigenvalues unchanged, but will introduce additional singularities. Such a situation exists with Ward's characteristic function, and as seen later, is also true of the transverse resonance method. Other transformations of the characteristic function are sometimes made which can introduce additional singularities. For example, if $D(\lambda)$ is a characteristic function, having zeros in the complex λ -plane, then $f(\lambda) = \tan D(\lambda)$, or $f(\lambda) = A \tan D(\lambda)$, will have the same zeros; but $f(\lambda)$ then can also have additional zeros, infinities, or branch points. This is the case for the traditional characteristic function for the three layer case. The method presented here has attempted to avoid unnecessary roots and singularities.

By choice of variables, and sequences of operations, all quantities are well behaved and finite throughout the calculations leading to the characteristic equation.

A extensive background literature in wave propagation in plane-layered media exists since before the advent of interest in optical waveguiding [55-58]. This work can be considered for various alternatives in formulating the general problem, but it has remained largely uncited in the literature of integrated optics. The reasons are probably that some problems are best approached by different formulations, and previous methods have not been the most convenient for guided wave optics.

Radio propagation in the earth-ionosphere region [56, 58] is dominated by an interest in point observers, and real electric and magnetic point sources. In most cases both points are located within the one guiding region, which often has continuously varying parameters. Thus, there is emphasis on representations in terms of vector potentials, Green's functions, and approximations methods. Budden [56, 57] formulated the characteristic equation almost exclusively in terms of a round trip phase integral across the guiding region, including reflection coefficients and phase shifts at the outer boundaries. This method is poorly suited to a problem with multiple separated guiding layers.

Radio propagation over plane layered models of the earth has similar emphasis [58], but source and observer are often taken to be outside the layered region. Propagation along the plane surface of a structure then may emphasize reflection coefficients as seen from the outside. Propagating modes, as seen from the outside, form the context for most literature on surface wave properties of complex modes.

A very different emphasis exists in the analysis of optical multilayer filters [59, 61], where there are no point sources or point observers. Interest is primarily in wave propagation transversely to the layers, due to plane waves incident from the outside. The formulation is usually in terms of the actual field variables, angles of incidence and reflection, and reflection and transmission coefficients. A well developed matrix method exists for analysis and design of different types of filters. There is no interest in wave propagating or guiding properties along the planes. Losses are rarely included.

On the other hand, for optical guiding structures there is little interest in transverse propagation properties, but propagation along the plane is of paramount interest. The mode concept is used, and there is little use for reflection or transmission coefficients. No point sources are used, and interest in incident beams is primarily in the degree to which specific modes are excited, rather than how the beams are reflected and transmitted.

The present formulation was chosen to be as simple as possible, with the fewest possible field quantities, and directly related to the quantities of interest. (There was no need for vector potentials or Green's functions.) The components of E and H are sufficient, without the need even to define the wave equation or oppositely traveling wave amplitudes. The field components across the structure are simply related by the matrix transformations as used in optical multilayer filter analysis. However, all quantities must now be allowed to become complex. Formally, the 2×2 matrix method remains completely valid even in the fully complex case. But there is little reason to retain the notion of angles of propagation in each layer,

since as often as not these angles become imaginary or complex. It is simpler to use the geometric components, k_x and k_z , of a complex propagation vector; but it becomes necessary to keep in mind some specifications of branches in defining these quantities, since they involve square root relationships.

The choice of the 2x2 matrix representation was also influenced by the fact that it leads to a very direct and useful definition for the characteristic equation. Because of the problems of analyticity of the characteristic function for other methods, some care was used in its definition. Considerable help is available from the mathematical literature on two-point boundary-value problems involving vector-matrix differential equations.

The phase integral concept is adopted for the purpose of indexing the modes, and for calculating some initial guesses at which to start the complex root search.

For the benefit of the reader several additional papers may be cited, which include one aspect or another of the formulation used here. Hansen [62] includes the case of material absorption, and also a matrix representation for the N-layer case. But he did not consider propagating modes. Berreman [63] gives an extensive description of a 4x4 matrix formulation, as is essential for anisotropic material. But he also was interested in

true guided modes in multilayers of anisotropic materials. His formulation is the closest to that used here; the fourth order system and lack of separation into simple TE and TM polarizations make his case necessarily a more complicated problem. He recognized that the characteristic function was a determinant of fourth order, but no root searching method was proposed for actually calculating the modes in a general case. Complex modes were not considered. Finally, Heitman and van den Berg [66] present a contrasting formulation for the fields in a multilayer for a very different purpose. Their representation was entirely in terms of propagating wave amplitudes in all layers, with amplitudes all related by wave transformation matrices. These papers may be consulted for additional details and alternatives in formulating the field problem in layered media.

In the literature on modal propagation there is essentially no discussion of the problem of calculating the roots of the characteristic equation once it is formulated. For the simple three layer case and real variables, the graphic method is often described. And for a slightly more complicated case, of four layers or for complex permittivity, a numerical method is sometimes mentioned but not described. In the literature and texts on numerical methods, and on optimization methods, the calculation of roots is extensively discussed. A very limited portion of these methods are directly applicable to calculating roots of complex functions. For calculation of modes in the most general case here, an efficient complex root search method is essential. An existing method has been chosen for use; and, with several important improvements, appears to be ideally suited to the problem. This is described in Chapter 5.

2. FORMULATION OF THE FIELD PROBLEM

2.1 The Layered Structure. Geometry and Variables.

The geometry chosen for the layered structure is shown in Fig. 2.1, together with the field variables and other quantities defined later.

The $+z$ direction is chosen as the direction of mode propagation, with k_z denoting the propagation coefficient. Thus, a propagation factor $\exp i(k_z z - \omega t)$ is being assumed, but not shown, for all field components in all layers 1 through N. Note the sign in the time factor $\exp(-i\omega t)$, and that k_z is the same in all layers. With this propagation factor the differentials in Maxwell's equations have the following implications:

$$\partial/\partial z \rightarrow +ik_z, \quad \text{and} \quad \partial/\partial t \rightarrow -i\omega.$$

That k_z is common to all layers is a statement of the concept of propagating modes. Attention is restricted to field solutions for which it is true, and for which further requirements of physical admissibility are satisfied. These modes may also be described as solutions of the eigenvalue equation in the operator $(-i\partial/\partial z)$; that is $(-i\partial/\partial z)F = k_z F$, with k_z being the eigenvalue. The latter may be considered a continuous spectral transform variable, in terms of which the general fields might be expressed by integral representations; or k_z may be considered at fixed values for which solutions are sought and which also satisfy the further conditions.

In this report central interest is on k_z (or rather k_z^2 in a normalized form as described later) as the eigenvalue parameter of a transverse eigenvalue problem (in x rather than in z). The discrete values of k_z are sought for which the fields solutions satisfy additional boundary conditions in the outer layers, 1 and N.

In the transverse direction, y , the structure is taken to be uniform and infinite. So for all material properties and field variables it is being assumed that

$$\partial/\partial y \rightarrow 0.$$

The stratification is taken to be in the x direction, in which the material layers are to be piecewise homogeneous and isotropic. There are a total of N layers and $N-1$ boundaries, located at x_ℓ . The choice of origin is arbitrary. Two semi-infinite layers are separated by $N-2$ layers of finite thickness. The layers and boundaries are indexed from 1 to N in the direction of increasing x . Note that each material layer and its upper boundary have corresponding indices. A layer ℓ has $x_{\ell-1}$ and x_ℓ as its lower and upper boundaries respectively, and x_ℓ separates layers ℓ and $\ell+1$. Boundaries x_0 and x_N are taken to be reference planes for exponential solutions in the semi-infinite layers, and do not imply a material discontinuity. They are used to simplify the discussion of the boundary conditions imposed on solutions in the outer layers, as distinct from the boundary matching conditions at all the material discontinuities at x_1 to x_{N-1} . When this distinction is made, and for actual calculations, x_0 and x_N may be taken to coincide with x_1 and x_{N-1} , respectively. Only if these are different is it necessary to define the distances t_1 and t_N ; otherwise the finite material layers are indexed only from $\ell = 2$ to $N-1$ (i.e., t_2 to t_{N-1}).

In this formulation the complex valued μ and ϵ are considered to be the fundamental constitutive parameters for the materials. These are taken to have given numerical values, and no model for any material dispersion is included. This specifically applies to the imaginary part of ϵ , which usually varies with frequency but depends on the particular model assumed.

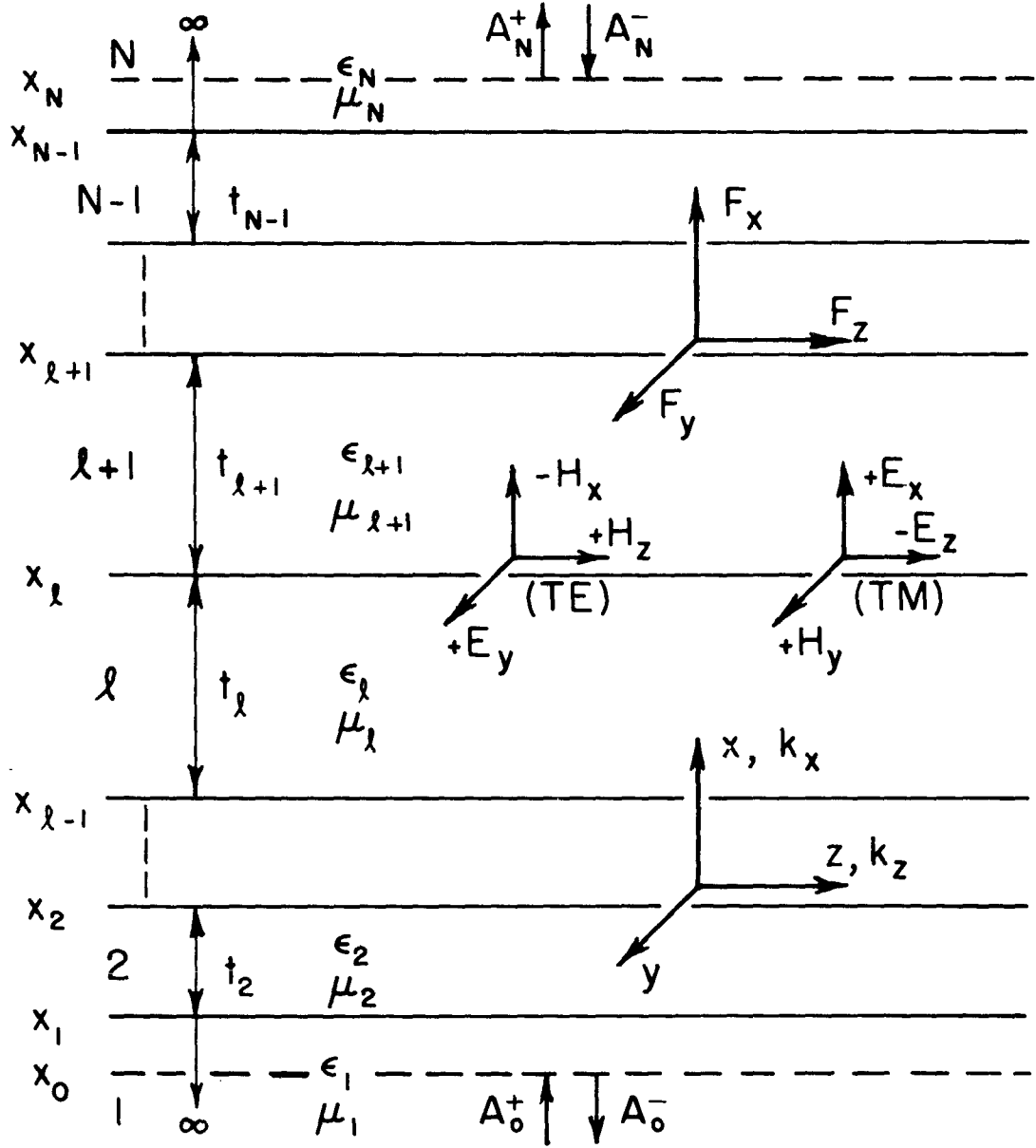


Figure 2.1 Geometry and field variables for layered structure. There are N different material layers, and $N-1$ boundaries located at x_l . Two semi-infinite layers, 1 and N , are separated by $N-2$ layers of finite thickness, t_l . The structure is uniform in z , the direction of mode propagation; it is also uniform in the transverse direction, y . x_0 and x_N are reference planes in the semi-infinite layers, at which complex amplitudes A_0^\pm and A_N^\pm are defined for exponential solutions. F_x , F_y , and F_z are normalized field variables corresponding to the E- and H-fields shown for the two polarizations.

If dispersion curves of k_z vs. frequency are of interest then the values of $\text{Im } \epsilon$ must be supplied, or the formulation must be extended by assuming some particular model (say for a metal, plasma, or recombination gain in semiconductor). The index of refraction, n , is often more convenient (when $\mu = \mu_0$) for numerical values and for discussion purposes, but it is not as fundamental a physical parameter as ϵ . For example, when a material varies rapidly compared to a wavelength (say in periodic structures or finely stratified media) it is the average of ϵ rather than the average of n which determines the wave propagation properties [10, 11; 55, p. 84].

In this report many quantities should be indexed according to the material layer or boundary; such as ϵ and μ , the field solutions in each layer, and the tangential fields at the boundaries. However, to simplify the notation such indexing will be avoided as much as possible. Most quantities should be understood to be defined and different in each layer, and so indexed; only if reference to a specific layer or boundary is needed will be index, l , be used.

In the coordinate system shown, and with the assumed propagation factor, Maxwell's curl equations reduce to the following six components:

$$k_z E_y = -\omega \mu H_x, \quad k_z H_y = +\omega \epsilon E_x \quad (2.1x)$$

$$\frac{\partial H_z}{\partial x} - ik_z H_x = +i\omega \epsilon E_y, \quad \frac{\partial E_z}{\partial x} - ik_z E_x = -i\omega \mu H_y \quad (2.1y)$$

$$\frac{\partial E_y}{\partial x} = +i\omega \mu H_z, \quad \frac{\partial H_y}{\partial x} = -i\omega \epsilon E_z \quad (2.1z)$$

Equations (2.1x) simply establish a proportionality between x and y field components, while the other four equations are coupled first-order differ-

ential equations among the field components.

Maxwell's divergence equations will be satisfied everywhere if the boundary conditions at all the internal material boundaries, x_ℓ , are satisfied. These are field-continuity conditions, and are most easily stated in terms of the tangential field components. That is, E_y , H_z , H_y , and E_z are each to be continuous at every x_ℓ . Therefore, the field solutions for Eqs. (2.1) in adjacent layers, as functions of x , must reduce to the same values for the tangential fields at their common boundary. If $F_\ell(x)$, $x_{\ell-1} \leq x \leq x_\ell$, represents any one of the tangential fields within layer ℓ , then the boundary conditions may be stated as

$$F_\ell(x_\ell) \equiv F_{\ell+1}(x_\ell) \quad \ell = 1, N-1 \quad (2.2)$$

for all components.

It is, of course, equivalent to state the boundary conditions in terms of the continuity of the normal components of D and B at the interfaces. But this is not as useful and direct as the above form.

The field components in Eqs. (2.1) separate naturally into two independent sets, corresponding to the two polarizations designated as TE and TM. For example, if $E_y = 0$, then H_z and H_x are necessarily zero; and similarly, if $H_y = 0$, then E_z and E_x are also zero. Therefore, the two sets (E_y, H_z, H_x) for the TE case and (H_y, E_z, E_x) for the TM case may separately be zero or non-zero, and solutions for the two cases may be considered separately. It is only because the structure has been assumed to be uniform in the y and z directions, and because the material parameters are isotropic, that this is possible. Otherwise all six field components will be non-zero and must be considered together.

The non-zero E_y or H_y components are the namesakes for the designation as

TE or TM polarization. They are transverse both to the z -direction of propagation and to the x -direction normal to planar layers, and are tangential to the planes. The non-zero H_z or E_z are the two other tangential components, and lie in the direction of propagation. (These are the namesakes for the alternative polarization designation as H- or E-modes, respectively.) The normal components, H_x and E_x , are also transverse to the direction of propagation and, together with E_y and H_z , determine the propagating Poynting power density; e.g., $S_z = (1/2)E_y H_x^*$ for the TE case. The tangential components, E_y and H_z for the TE case say, determine the transverse Poynting power flow across the layers or boundaries, $S_x = (1/2)E_y H_z^*$. This power is usually zero and ignored for guided modes, but it is very useful in giving the rate of power loss for a leaky mode. In semiconductor lasers it also can give directly the rate of power flow from an active guide to a parallel passive guide.

Most formulations for propagation in layered structures consider a reduced second-order wave equation; obtained by differentiation of one of Eqs. (2.1y) or (2.1z), and elimination of two field components, to obtain an equation in a single component, usually E_y or H_y . The other two components may then be expressed (by means of Eqs. (2.1)) in terms of the solutions obtained for the second-order equation.

Here we choose to emphasize Eqs. (2.1) as being a set of coupled first-order equations in all the field variables simultaneously. By using (2.1x) to eliminate one variable, the system reduces to two coupled first-order equations, (2.1y) and (2.1z). For the TM case, for example, the two coupled equations in H_y and E_z are

$$\frac{\partial H_y}{\partial x} = -i\omega\epsilon E_z, \quad \frac{\partial E_z}{\partial x} = (i/\omega\epsilon)(k_z^2 - \omega^2\mu\epsilon)H_y.$$

These coupled first-order equations lead directly to a vector-matrix form for the differential equation, and also directly to the matrix representation for the solutions, and to the chain-matrix representations for layered structures as used in thin-film optics.

It is possible to take the viewpoint that because Maxwell's equations are in fact coupled first-order equations, then such equations are more basic or fundamental than the second-order wave equation; that the reduction to the second-order equation involves a loss of information (an integration factor); and that, if solutions to the first-order equations are directly obtainable, then it is unnecessary to consider the second-order wave equation. The latter situation exists in the case of numerical solution of differential equations, for which highly accurate and reliable programs have been developed in recent years. In every such program higher n-th order differential equations are solved numerically by first transforming them to an equivalent set of n coupled first-order equations. The same situation exists in the present case; since solutions to the first-order equation are easily stated, there is no need to consider the wave equation.

To simplify the notation, and to permit simultaneous treatment of both TE and TM polarizations, we first introduce some normalized variables.

2.2 Normalization and Duality

For numerical and programming purposes, it is advantageous to use normalized variables, which for typical problems have values not too many orders of magnitude different from unity. This should be true in a general

sense, and also in the sense of not choosing variables which accidentally may become infinite at certain points in the solution or in some limiting case of the parameter values. For example, in standard units the permittivity, ϵ , the permeability, μ , and the velocity of light, all differ from unity by about eight orders of magnitude. Further, in the optical regime, the wavelength and frequency differ from unity by six to fourteen orders of magnitude. Therefore, it is essential to use some form of normalized variables for the closely related parameters of the modal propagation constants, phase and group velocities, mode wavelengths, etc. An additional example is that of the E and H field values, which generally will differ in magnitude by a factor of 377, the impedance of free space. It is useful to normalize both E and H to comparable units having the dimensions of the square root of power or energy density. There is the added advantage of the normalized E and H then having comparable values for TE and TM cases.

When a formulation for numerical calculations is to be programmed for both TE and TM polarizations, a great savings of effort is realized by choosing variables so that, by duality, as much of the program as possible is identical for the two cases. Duality, as a transformation which leaves Maxwell's equations unchanged, is well-known [3, p. 29], and in some problems duality can be used to convert a known solution in one polarization into the solution for the other polarization. Here, duality is used to allow one set of variables to serve equally well for both polarizations. In the present case this can be done in a rather complete way, because no explicit electric or magnetic current sources are considered. Therefore, it is possible to choose field variables which represent both electric or magnetic fields, alternatively for the two polarizations. The ratio of these fields, the wave impedance or admittance, also requires a dual interpretation. After initial

definition of some quantities, which use either μ or ϵ depending on polarization, the formulation and programming serves for both polarizations.

The concept of wave impedance and wave admittance plays an important role in the present formulation. For reasons discussed below, the variables representing these quantities are chosen, by duality, to represent admittances (H/E) for the TE case and impedances (E/H) for the TM case.

All material parameter values are normalized to the characteristic values of free space. In each layer the permittivity, ϵ , and the permeability, μ , are always taken in the relative sense.

$$\mu_r \equiv \mu/\mu_0 \quad \text{and} \quad \epsilon_r = \epsilon/\epsilon_0 .$$

The characteristic impedance or admittance of each material, or the wave impedance/admittance for any solutions, E/H, are also normalized to the values in free space; that is, by the impedance

$$\eta_0 = (\mu_0/\epsilon_0)^{1/2} .$$

For quantities which depend additionally on frequency or wavelength, a convenient reference value, say ω_0 or λ_0 , or even k_0 , is chosen to be used in normalizing related quantities. Specifically, all frequencies and wavelengths are referred to ω_0 and λ_0 ,

$$\omega_r \equiv \omega/\omega_0 \quad \text{and} \quad \lambda_r = \lambda/\lambda_0 .$$

But, more importantly, all propagation constants are then normalized to k_0 , that of free space (at the reference frequency);

$$k_0 \equiv \omega_0 (\mu_0 \epsilon_0)^{1/2} \equiv \omega_0 / c \equiv 2\pi/\lambda_0 ,$$

where c is the free-space velocity of light.

The zero subscript has a double implication; it refers to both free-space values and to the reference value assumed, for say λ_0 . The latter may be the wavelength of interest for a specific problem, in which case $\omega_r = \lambda_r = 1$. Or λ_0 may be used to set the units in which the wavelengths are expressed; such as for optical use $\lambda_0 = 1\mu\text{m}$, and λ_r states the wavelength for particular problems in units of microns. Also, λ_0 may be used to specify a central value about which a range of wavelengths is considered, as for dispersion curves as λ_r is varied. If ω_r is not unity then the appearance of Maxwell's equation and other derived equations remains unchanged by the normalization; ω , μ , and ϵ are simply replaced by their relative values.

All propagation coefficients are normalized to k_0 and are therefore dimensionless. Thus, we define for the modal propagation constant

$$\beta \equiv k_z/k_0 .$$

In each material layer, for a common β or k_z , the different transverse propagation coefficients k_x are defined by

$$k_x^2 \equiv \omega^2 \mu \epsilon - k_z^2 = k^2 - k_z^2 ;$$

and in normalized form are denoted by κ ,

$$\begin{aligned} \kappa &\equiv k_x/k_0 , \\ \kappa^2 &\equiv \omega_r^2 \mu_r \epsilon_r - \beta^2 \equiv v^2 - \beta^2 . \end{aligned}$$

If $\omega_r = 1$, then v becomes the index of refraction, n , for the layer material. Since all quantities may be complex, a principal branch specification for the complex square root is needed in defining κ from κ^2 (above). This definition of $\kappa(\beta^2)$ must be considered with care, especially when needed in integral

representations where β is taken to be the independent variable [5, p. 459]. In the present problem there is particular interest in κ for the two semi-infinite layers, and is discussed in Sect. 3.3. Note that κ has a consistent definition in all layers. For real v and β , then κ is pure real or imaginary, respectively, as β is less or greater than v . Often in the literature the transverse constant is defined differently in different layers, depending on a priori assumptions about the magnitude of β relative to v in each layer. This is done to keep the constant real, but it results in a formulation which does not easily generalize to structures or modes not satisfying the initial assumptions. With some attention to branch specifications the present formulation is completely general.

For use with the normalized propagation constants, it is also useful to define normalized distances in the x direction. Let

$$\xi \equiv k_o x, \quad \text{and} \quad \tau_\ell \equiv k_o t_\ell ;$$

so ξ is a free-space radian distance and τ_ℓ the free-space radian thickness of each layer ℓ . In each material layer a phase, optical, or electrical distance, θ , will be

$$\theta \equiv \kappa \xi \equiv k_x x \equiv \kappa k_o x ,$$

and the corresponding thickness of each layer may be defined as θ_ℓ ,

$$\theta_\ell \equiv \kappa_\ell \tau_\ell \equiv \kappa_\ell (\xi_\ell - \xi_{\ell-1}) \equiv k_{x\ell} t_\ell .$$

If κ is real, and for $\beta^2 > v^2$ both real, then θ and θ_ℓ will be real and true radian phase distances. However, κ may also be imaginary, and in general complex, in which case θ also includes the total exponential growth or decay factor for the distance. Of course θ depends on β^2 through $\kappa(\beta^2)$.

Table 2.1 shows the field variables and quantities which have dual meanings for the TE and TM cases.

Parameters ρ and σ are alternatively proportional to μ and ϵ , and permit some simplification of expressions, but are infrequently used. Also $\rho\sigma \equiv v^2 \equiv \omega_r^2 \mu_r \epsilon_r$, where v has the nature of an index of refraction multiplied by ω_r . If $\omega_r = 1$ then $\rho\sigma = n^2 = \mu_r \epsilon_r$ and $v = n$ is the index of refraction in each material.

$Y_x(\beta^2)$ is, for given β^2 , defined and different in each layer. It is the characteristic transverse wave admittance (TE) or impedance (TM) for the layer, and plays an important role in the formulation. It is well to keep in mind that Y_x is always proportional to $\kappa(\beta^2)$ in each layer; it is generally complex, may be pure imaginary, and can become zero. Y_x is, of course, affected by choice of principal branch for $\kappa(\beta^2)$. It is because κ can become zero that Y_x is used, rather than the characteristic impedance, $Z_x \equiv 1/Y_x$, for a layer. Formally, the impedance can be used equally well in formulating the problem; and is perhaps more common, as for the transverse resonance method. However, then κ will appear in the denominator. So if the impedance (TE) or admittance (TM) are used, they can become infinite and unusable as a numerical parameter for calculations.

Y_z is the longitudinal wave admittance (TE) or impedance (TM) and relates F_x and F_y . Since Y_z is proportional to β it depends on the choice of sign for β . In this report β will always be taken to have positive real part, so all modes are assumed to have phase propagation in the positive z direction. For any such mode there will always exist a corresponding backward propagating mode with opposite sign for β and Y_z . The only difference in the field distribution for the two modes will be the opposite sign of F_x relative to F_y .

Neither Y_x or Y_z is the characteristic admittance (impedance) of the material of a layer, $Y = (\epsilon_r/\mu_r)^{1/2}$. Rather, Y_x and Y_z should be considered parameters of the field distribution in the layer, not of the material.

The E and H field components, in addition to being normalized by $\sqrt{\eta_0}$ to become the F-variables, are taken with different signs as required by duality. The resulting equations then have exactly the same form for either polarization. The sign differences are closely related to the directional sense for the Poynting vectors and wave admittances when defined in terms of the F-variables. Positive F_x , F_y , and F_z geometrically form a right handed triad.

F_y and F_z are the tangential fields of principal interest, being involved in the coupled first order equations and the boundary matching conditions at all x_ℓ (or ξ_ℓ). F_y may be emphasized somewhat because it is never zero in general, and the other two, F_z and F_x , may always be expressed in terms of F_y . F_z can vanish identically "at cut-off" in a layer when $\kappa = 0$ at $\beta^2 = v^2$, in which case the other fields cannot be expressed in terms of F_z . F_x is the field component normal to the planes; it is always strictly proportional to F_y (though the proportionality depends on β), and is needed only for calculating the z-directed Poynting power.

S_x and S_y are the complex, time-averaged, Poynting power densities in the respective directions. They have a directional sense, and when positive-real represent power flow in the positive x or z direction. As defined, the imaginary part represents alternatively, by duality, the net magnetic or electric reactive stored energy exchange.

The energy density due to the respective field components is denoted by W_y , W_z , and W_x . These represent real stored energy of the electric or magnetic type depending on the polarization. The imaginary part (only if μ or ϵ

VARIABLE	POLARIZATION	
	TE	TM
ρ	$\omega_r \mu_r$	$\omega_r \epsilon_r$
σ	$\omega_r \epsilon_r$	$\omega_r \mu_r$
$Y_x(\beta^2) \equiv \kappa/\rho$	$\kappa/\omega_r \mu_r$	$\kappa/\omega_r \epsilon_r$
$Y_z(\beta^2) \equiv \beta/\rho = F_x/F_y$	$\beta/\omega_r \mu_r$	$\beta/\omega_r \epsilon_r$
F_y	$+E_y/\sqrt{\eta_o}$	$+H_y\sqrt{\eta_o}$
F_z	$+H_z\sqrt{\eta_o}$	$-E_z/\sqrt{\eta_o}$
F_x	$-H_x\sqrt{\eta_o}$	$+E_x/\sqrt{\eta_o}$
$S_x \equiv \frac{1}{2} F_y F_z^*$	$\frac{1}{2} E_y H_z^*$	$-\frac{1}{2} E_z^* H_y$
$S_z \equiv \frac{1}{2} F_x^* F_y$	$-\frac{1}{2} E_y H_x^*$	$\frac{1}{2} E_x^* H_y$
$W_y \equiv \frac{\sigma}{4\omega_r} F_y ^2$	$(\epsilon/4) E_y ^2$	$(\mu/4) H_y ^2$
$W_z \equiv \frac{\rho}{4\omega_r} F_z ^2$	$(\mu/4) H_z ^2$	$(\epsilon/4) E_z ^2$
$W_x \equiv \frac{\rho}{4\omega_r} F_x ^2$	$(\mu/4) H_x ^2$	$(\epsilon/4) E_x ^2$

Table 2.1 Normalized variables having dual meanings for TE and TM polarizations. All values are defined separately in each layer; and depend on μ_r , ϵ_r , ω_r , values relative to free-space at a reference frequency.
 $\eta_o^2 \equiv \mu_o/\epsilon_o$, $\kappa^2(\beta^2) \equiv v^2 - \beta^2 \equiv \rho\sigma - \beta^2$. For $\omega_r = 1$ then $v^2 = n^2 = \mu_r \epsilon_r$, with n the index of refraction.

are complex) represents the density of energy absorption or gain at a point. Identification of components of the energy density as due to the transverse (W_x, W_y) or to the longitudinal (W_z) fields is useful in power-energy relationships. Sums and differences in these components are directly related to the phase and group velocity for bound modes (see Sect. 6.3).

Duality extends completely to all quantities, always implying the interchange of electric and magnetic quantities between the two polarization cases. As an example of this completeness note that the imaginary part of the Poynting power changes meaning also. A positive imaginary part, over a closed volume, represents for the TE case an excess of electric energy over magnetic energy density; whereas for the TM case the opposite is true. This may be seen in the definition of the Poynting components S_z and S_x , where F_x and F_z are conjugated but not F_y . So in the TE case H is conjugated as usual, but for the TM case it is E that is conjugated. A similar situation exists with regard to the various terms of the energy density, the transverse and longitudinal fields contributing to the type of energy depending on the polarization.

In the remainder of this report, and for programming purposes, the normalized variables will be used (although for discussion purposes it is often simpler to still refer to x rather than ξ). Further reference to μ and ϵ should be understood to mean the relative values without using the subscript, r . The frequency and wavelength for the problem will be taken to be the reference values ω_0 and λ_0 so that the relative frequency $\omega_r \equiv 1$, and ω_r will not appear. Only for programming purposes is it useful to retain the capability of an operating frequency other than the reference frequency. (So that propagation constants can be normalized to a fixed reference value, rather than to a value that varies from case to case as the

frequency (k_o) is varied.)

For $\omega_r \equiv 1$ all propagation constants are normalized to the free space value of k_o at the frequency of interest, and have the form of indices of refraction, n . Thus we will write in each layer

$$v^2 = n^2 \equiv \mu\epsilon, \quad \kappa^2 = n^2 - \beta^2,$$

and numerical values of κ and β can always be compared to the index of refraction of the material in each layer. n , as defined from n^2 , will always be taken to have positive real part. So the sign of the imaginary part of n will be the same as that of n^2 , positive for dissipative material and negative for media with gain.

In this report β^2 (rather than β) is considered to be the primary mode parameter. This is possible because β always enters into the problem as β^2 ; no parameters of the problem depend on the sign of β . For any eigenvalue found for β^2 there are two modes with opposite signs for β , and so propagating in opposite directions. (It may be mentioned that the use of β^2 corresponds to the use of the energy as the eigenvalue parameter in quantum mechanics. Further, β^2 corresponds to the parameter $-\lambda$ used by Felsen and Marcuvitz [5, Sect. 3.3] in the description of characteristic Green's functions for waveguides. The integral representations may be carried out in the $\beta^2 = -\lambda$ plane, rather than in the β -plane.)

For the numerical eigenvalue search it is much more efficient to use the characteristic function in β^2 . As seen later, the characteristic function then has better analytical properties than it would have if β were used as the independent variable.

2.3 Transverse Differential Equation

In terms of the normalized variables, Maxwell's equations are listed in Table 2.2 along with their equivalents for the two polarizations.

The last two equations in the table constitute the transverse differential equations for the tangential field components. These may be written in vector-matrix form as

$$\frac{d}{d\xi} \begin{bmatrix} F_y \\ F_z \end{bmatrix} = (+i\kappa) \begin{bmatrix} 0 & 1/Y_x \\ Y_x & 0 \end{bmatrix} \cdot \begin{bmatrix} F_y \\ F_z \end{bmatrix} \quad (2.5a)$$

or as

$$\frac{dF(\xi)}{d\xi} = K(\beta^2) \cdot F(\xi) ; \quad (2.5b)$$

where $F(\xi) \equiv \text{col}[F_y, F_z]$ is a vector, and $K(\beta^2)$ is the coefficient matrix on the right, including the factor $(+i\kappa)$.

Equation 2.5 is defined in each layer, with parameters κ and Y_x different in each, but always dependent on the value of β^2 common to all layers. Within each layer the differential equation has a constant coefficient and relatively simple solutions. The system is second order (in the sense of the dependent variable being a two-component vector), so within each layer there always exist two linearly independent vector solutions. It is useful to allow $F(\xi)$ to also represent a matrix solution composed of two independent column vectors.

Differential equations in adjacent layers are related by having the same values of $F(\xi)$ at their common boundaries (the boundary matching conditions). That is, proceeding in either the positive or negative ξ (the x) direction, the final value of F in each layer is the initial value of F for

the differential equation in the next layer. In this sense Eq. (2.5) is a differential equation defined for the whole structure, and it has unique solutions $F(\xi)$ defined everywhere on the structure.

Two properties of the coefficient matrix $K(\beta^2)$ are noteworthy. First, $\det K = \kappa^2$, and the matrix eigenvalues of K are $+ik$ and $-ik$. Thus, if a linear transformation were chosen to diagonalize K and transform F , the solutions would be $\exp(+ik\xi)$, and $\exp(-ik\xi)$, and any other F -solutions are expressible as linear combinations of these two. κ is the transverse propagation constant in each layer. Further, unless $\kappa^2 = 0$, $K(\beta^2)$ is nonsingular with distinct eigenvalues, which assures the linear independence of the solutions throughout the layer. At $\kappa^2 = 0$ the eigenvalues are repeated (zero) and $\exp(\pm 0) \equiv 1$ are not independent solutions; but two independent solutions still do exist, as shown later.

Secondly, the trace of K is zero, $\text{Tr}K = 0$, with the consequence that the Wronskian determinant for any matrix solution, $F(\xi)$, is a constant [67, p. 75; 68, p. 302]; $\text{Det } F(\xi) = \text{const.}$ for all ξ , and has the same value in all layers. This property corresponds to the fact that the second order differential (wave) equation for any one field component contains no term in the first derivative; and, more physically, it corresponds to the reciprocity property [3, p. 39].

In addition, because Y_x is proportional to κ , K is an even function of κ in all layers; and consequently K does not depend on the choice of sign or principal branch specification for $\kappa(\beta^2)$. K is analytic everywhere in the complex β^2 -plane, and it is also an analytic function of the parameters μ and ϵ . In consequence, solutions will always be continuous functions of the parameters of the structure [69, p. 40]. Any general solutions to the differential equation are being referred to here, not necessarily eigenmode

Normalized Equation	Unnormalized Equation and Equivalent Form	
<u>x-equation</u>	TE	TM
$F_x = Y_z F_y$	$k_z E_y = -\omega \mu H_x$	$k_z H_y = +\omega \epsilon E_x$
$(Y_z = \beta/\rho)$	$\beta F_y = +\omega_r \mu_r F_x$	$\beta F_y = +\omega_r \epsilon_r F_x$
	$(Y_z \equiv \beta/\omega_r \mu_r)$	$(Y_z \equiv \beta/\omega_r \epsilon_r)$
<u>y-equation</u>		
$\frac{dF_z}{d\xi} = i(\sigma F_y - \beta F_x)$	$\frac{dH_z}{dx} - ik_z H_x = +i\omega E_y$	$\frac{dE_z}{dx} - ik_z E_x = -i\omega \mu H_y$
	$\frac{dF_z}{d\xi} = i\omega_r \epsilon_r F_y - i\beta F_x$	$\frac{dF_z}{d\xi} = i\omega_r \mu_r F_y - i\beta F_x$
<u>z-equation</u>		
$\frac{dF_y}{d\xi} = +i\rho F_z$	$\frac{dE_y}{dx} = +i\omega \mu H_z$	$\frac{dH_y}{dx} = -i\omega \epsilon E_z$
$= +i(\kappa/Y_x) F_z$	$\frac{dF_y}{d\xi} = i\omega_r \mu_r F_z$	$\frac{dF_y}{d\xi} = +i\omega_r \epsilon_r F_z$
$(Y_x = \kappa/\rho)$	$(Y_x \equiv \kappa/\omega_r \mu_r)$	$(Y_x \equiv \kappa/\omega_r \epsilon_r)$
<u>yx-equation</u>		
$\frac{dF_z}{d\xi} = +i(\kappa Y_x) F_y$	$\frac{dF_z}{d\xi} = \frac{i\kappa^2}{\omega_r \mu_r} F_y$	$\frac{dF_z}{d\xi} = \frac{i\kappa^2}{\omega_r \epsilon_r} F_y$

Table 2.2 Maxwell's curl equations in normalized variables, and equivalent expressions. The yx-equation results from the y- and x-equations by elimination of F_x , and leads to the definition for $\kappa \equiv (\omega_r^2 \mu_r \epsilon_r - \beta^2)^{1/2}$. For other variables see Table 1.1.

solutions, which arise only with the imposition of additional outer boundary condition.

2.4 Field Solutions and Transformation Matrices for Layers

Within any layer the general solution of Eq. (2.5) is

$$\begin{bmatrix} F_y(\xi_b) \\ F_z(\xi_b) \end{bmatrix} = \begin{bmatrix} \cos\theta & +(i/Y_x)\sin\theta \\ +(iY_x)\sin\theta & \cos\theta \end{bmatrix} \cdot \begin{bmatrix} F_y(\xi_a) \\ F_z(\xi_a) \end{bmatrix} \quad (2.6a)$$

or in matrix notation

$$F(\xi_b) = C(\xi_b, \xi_a) \cdot F(\xi_a) , \quad (2.6b)$$

where $\theta \equiv \kappa(\xi_b - \xi_a)$, and ξ_a and ξ_b are any two points within the layer ℓ , $\xi_{\ell-1} \leq \xi_a, \xi_b \leq \xi_\ell$. There is no implication about which of ξ_a or ξ_b is larger or smaller. All other quantities may be complex, and an additional layer index, ℓ , is understood, especially for κ and Y_x .

This solution is easily obtained using the techniques for systems of differential equations having constant coefficients. These methods are well known [67-69], and in engineering applications are most frequently encountered in state-variable methods for analysis of linear systems [70]. Here (2.6) is simply stated as the solution, as is easily shown by direct substitution into (2.5). Specific solutions obtain if, at either ξ_a or ξ_b , F is specified as an initial condition, and the solution is taken as a function of the other ξ .

Equation (2.6b) also represents the general solution if $F(\xi)$ is taken to be a matrix; $C(\xi_b, \xi_a)$ is unchanged. If ξ_a is a useful initial point, and $F(\xi_a) = I$, is the unit matrix, then the matrix solution at any ξ

$$F(\xi) \equiv C(\xi, \xi_a)$$

is referred to as a fundamental matrix, in terms of which any vector solutions may be expressed [68, Sect. 7.9; 69, p. 44]. The matrix $C(\xi, \xi_a)$ itself satisfies the differential equation (2.5), its two columns being independent vector solutions.

The inverse transformation from ξ_b to ξ_a , for expressing $F(\xi_a)$ in terms of $F(\xi_b)$, is simply obtained by the inverse matrix relation. And the inverse of $C(\xi_b, \xi_a)$ can be written by inspection: either by interchanging ξ_b and ξ_a , reversing the sign of θ , or reversing the sign of the off diagonal elements. That is,

$$F(\xi_a) = C^{-1}(\xi_b, \xi_a) \cdot F(\xi_b) ;$$

with

$$C^{-1}(\xi_b, \xi_a) \equiv C(\xi_a, \xi_b) \equiv \begin{bmatrix} \cos\theta & -(i/Y_x)\sin\theta \\ -(iY_x)\sin\theta & \cos\theta \end{bmatrix} ,$$

and θ is defined as before.

If ξ_a and ξ_b in (2.6) are taken to be the boundaries of any finite layer, say $\xi_b = \xi_\ell$ and $\xi_a = \xi_{\ell-1}$, then (2.6) becomes the general relation (a linear transformation) between the tangential fields at successive boundaries:

$$F_\ell = C_\ell \cdot F_{\ell-1} ;$$

where

$$F_\ell \equiv \begin{bmatrix} F_y(\xi_\ell) \\ F_z(\xi_\ell) \end{bmatrix}$$

and

$$C_{\ell} \equiv C(\xi_{\ell}, \xi_{\ell-1}) \equiv \begin{bmatrix} \cos\theta_{\ell} & +(i/Y_x)\sin\theta_{\ell} \\ +(iY_x)\sin\theta_{\ell} & \cos\theta_{\ell} \end{bmatrix} \quad (2.7)$$

with $\theta_{\ell} \equiv \kappa_{\ell}(\xi_{\ell} - \xi_{\ell-1}) \equiv \kappa_{\ell}\tau_{\ell}$ being the complex (phase) thickness of the layer.

The matrix C_{ℓ} for a layer (sometimes called the characteristic matrix) is the quantity of central interest in the matrix methods for the analysis of multilayer optical filters [59; 60, p. 19; 61, Sect. 2.6]. It is also analogous to the ABCD matrix relating voltages and currents between cascaded two-ports or sections of transmission lines [3, p. 87]. The inverse matrix for a complete layer is easily written, just as for any two points in the layer.

Fields at any two boundaries separated by more than one layer are also related by a matrix transformation. The matrix is easily obtained as the product of all matrices for the intervening layers. By induction,

$$F_{(\ell+1)} = C_{(\ell+1)} \cdot F_{\ell} = C_{(\ell+1)} \cdot C_{\ell} \cdot F_{(\ell-1)} ;$$

and in general,

$$F_p = C_{p,q} \cdot F_q$$

$$C_{p,q} \equiv \prod_{\ell=q+1}^p C_{\ell} , \quad p > q .$$

The pre- and post-subscripts for the matrix are useful in designating the two boundary indices (and their order) between which the matrix is defined. In-

verse matrices are easily designated by reversed order of the subscripts.

The properties and use of the subscripts may be summarized:

$$\begin{aligned} {}_{\ell}C_{(\ell-1)} &\equiv C_{\ell}, & (\ell-1)C_{\ell} &\equiv C_{\ell}^{-1} \\ {}_{\ell}C_{\ell} &\equiv I & {}_qC_p &\equiv {}_pC_q^{-1} \\ {}_pC_q &\equiv {}_pC_{\ell} \cdot {}_{\ell}C_q & &\text{for any } \ell. \end{aligned}$$

The last relation indicates that the matrix for any part of the structure may be factored as a product of the two matrices for any partition of the structure. (Mathematically, ℓ need not lie between p and q .)

A matrix transformation also exists between any two points which lie within different layers. The necessary matrix will have two factors for the transformations from each interior point to a reference boundary for each layer, and a factor for the transformation between boundaries. Thus, one may write for ξ_b in layer p , and ξ_a in layer q :

$$F(\xi_b) = [C(\xi_b, \xi_p) \cdot {}_pC_q \cdot C(\xi_q, \xi_a)] \cdot F(\xi_a)$$

Therefore, $C(\xi_b, \xi_a)$ is defined for any two points ξ in the structure, provided the factor ${}_pC_q$ is understood whenever the two points are not within the same layer.

A matrix for a single layer, ℓ , will always be referred to, by the single post-subscript, as C_{ℓ} . It is emphasized that $C_{\ell}(\beta^2)$ depends only on the parameters μ, ϵ , and the thickness for the one layer. Changes in parameters of adjacent layers or elsewhere in the structure have no effect on C_{ℓ} . Similarly, any changes in ℓ , say ϵ or its thickness, are fully characterized by the changes in C_{ℓ} ; and the effects on the overall structure are isolated to the single factor C_{ℓ} in any overall matrix product.

The matrix $C(\beta^2) \equiv {}_N C_0$ for the overall structure between the two outer boundaries ξ_0 and ξ_N , completely characterizes the finite part of the structure. Once $C(\beta^2)$ is known for some value of β^2 , then the transformation between the fields at the outer boundaries is determined; no other information about the interior structure or the field distributions is needed. Neither the semi-infinite layers in which the finite layers are embedded, nor the outer boundary conditions, have any effect on the function $C(\beta^2)$. This is the great advantage of the present formulation over a grand-determinant method.

The eigenvalue problem can be completely stated in terms of the matrix function $C(\beta^2)$ and the outer boundary conditions. By the definition of C , the interior boundary-matching conditions are always satisfied, so these may be considered to not be a part of the eigenconditions leading to discrete modes.

For the overall matrix, and its inverse, another notation, C^+ and C^- , is useful. We let

$$C^+ \equiv {}_N C_0, \quad \text{and} \quad C^- \equiv {}_0 C_N = (C^+)^{-1},$$

so then

$$F_N = C^+ \cdot F_0, \quad F_0 = C^- \cdot F_N,$$

at the outer boundaries.

The matrix transformations here are defined with a sense of direction. Multiplication from the left always implies transformation of the fields to increasing values of the index l or increasing x . Often in the literature the opposite sense of direction is used. For cascaded two-ports, matrix multiplication on the left always represents transformations from the output

back toward the input, from higher to lower index values. The matrices of Eq. (2.6) and (2.7), or their analogs in other applications, often appear with negative signs for the off-diagonal elements. This is due either to the opposite choice for the sense of direction for the transformation, or to the opposite choice for the sign of the exponential time factor, say as $\exp(-j\omega t)$. The present choice is logically more useful for programming purposes. (e.g., for do-loop indexing.)

The following properties are held by a C-matrix for any layer, the whole structure, or between any two points in the structure.

The determinant is unity, $\det C \equiv 1$. This may be shown directly from the defining form in (2.6) and (2.7); and for the whole structure it follows from the fact that the determinant of products of matrices is the product of the individual determinants. Physically this corresponds to the reciprocity relation for the tangential field components. Had non-reciprocal materials been assumed the determinant would no longer be constant, and generally a 2x2 matrix formulation would not be adequate. (In Ref. 59 this property is mistakenly attributed to energy conservation.)

In layers of purely lossless material, and for real β , the diagonal elements are pure real and the off-diagonal elements pure imaginary. This remains true for the product of any number of similar matrices. For complex β , for leaky modes, or for a structure with any layer having a complex ϵ , or μ (any loss or gain), it can no longer be true.

Within any homogeneous layer the two diagonal elements of the matrix will be equal, but for more than a single layer it will generally not be true. The only exception is for a symmetric structure, which can be shown to have a C-matrix of the same form as (2.6) [61, p. 248]. That is, for an overall symmetric structure there will be an equivalent θ and Y_x , but these will be a

complicated function of β^2 and of the parameters of all the intervening layers. A general non-symmetric structure matrix can be shown to be representable as the product of two matrices having the form of (2.6) [61, p. 247]. These properties are useful in the design of multiple-layer thin film filters.

The C-matrix for any number of layers is an even function of $\kappa_\ell(\beta^2)$ for all the included layers. This follows because $\cos\theta$, $Y_x \sin\theta$, and $(1/Y_x) \sin\theta$ for all even functions of the respective κ_ℓ . (Recall that θ_ℓ and $Y_{x\ell}$ are proportional to κ_ℓ .) Since $\cos\theta$ and $\sin\theta$ are analytic functions of κ , then, and in spite of the square root in defining $\kappa(\beta^2) \equiv (n^2 - \beta^2)^{1/2}$, the matrix C for any number of layers is an analytic and single-valued function of β^2 everywhere. $C(\beta^2)$ has no singularities in the finite plane; the potential branch points at $\kappa_\ell = 0$ for $\beta^2 = n_\ell^2$ do not occur because of the even functions involved. Consequently, the formulation and calculations are never affected by the choice of principal branch specification for κ_ℓ in the inner layers. This fact is of fundamental importance to the analyticity of the characteristic equation and to the complex root search for eigenmodes.

The special case of a layer "at cut-off", with $\beta^2 = n_\ell^2$, $\kappa_\ell = 0$, is of some concern. Physically this corresponds to plane-wave components propagating parallel to the layer, with no component of transverse phase propagation or exponential change in the field components across the layer. Although the coefficient matrix $K(\beta^2)$ in (2.5) is then singular, with $\kappa = 0$ a repeated eigenvalue, the solution within the layer and the matrix C_ℓ are well behaved with only a slight numerical problem. For $\kappa \rightarrow 0$, C_ℓ becomes

$$C_\ell \approx \begin{bmatrix} 1 + i\rho_\ell \tau_\ell & \\ 0 & 1 \end{bmatrix}, \quad (2.8)$$

Recall that $\rho = 1/\omega_r \mu_r$ (TE), $= 1/\omega_r \epsilon_r$ (TM); and that $Y_x = \kappa/\rho$, so that $Y_x \sin\theta \rightarrow \kappa^2 \tau/\rho$ and $(1/Y_x) \sin\theta \rightarrow \rho \tau$. That is, to first order in small κ , C is independent of κ . For numerical purposes $(1/Y_x) \sin\theta$ becomes indeterminate in the form $0/0$; however, it is easy to use a power series expansion for $(\sin\theta)/\theta \equiv \text{sinc}\theta$ for accurate evaluation of this term. This series would be $(1/Y_x \sin\theta \approx \rho \tau(1 - \theta^2/3! + \theta^4/5! - \theta^6/7! + \dots))$. The other elements of C_ℓ do not require any special consideration. Across a layer at cut-off, F_y is constant and F_z is zero (the first column of C above), or F_y changes linearly with x and F_z is constant (the second column of C).

For calculating detailed field values, incrementally as a function of x , the matrix representation provides a rapid and efficient method. This is described in Sect. 6.2.

2.5 Exponential Solutions and Outer Layers

It is, of course, possible to express the fields in any layer as linear combinations of positive and negative exponentials (e.g., as "waves" propagating transversely in the layer if κ is real, or as real exponentials if κ is imaginary). This form of solution is important in the two semi-infinite layers, because they are directly related to the boundary conditions imposed at the outer boundaries for the eigenmode problem.

Exponential solutions, denoted by $A^+(\xi)$ and $A^-(\xi)$, may be considered to be solutions of the second order wave equation, or as vector solutions of the diagonalized form of the matrix equation (2.5). Either way, the field

variables in any layer, ℓ , may be written as

$$\begin{bmatrix} F_y(\xi) \\ F_z(\xi) \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ Y_x & -Y_x \end{bmatrix} \cdot \begin{bmatrix} A^+(\xi) \\ A^-(\xi) \end{bmatrix}, \quad (2.9)$$

with

$$\begin{bmatrix} A^+(\xi) \\ A^-(\xi) \end{bmatrix} = \begin{bmatrix} \exp(+i\theta) & 0 \\ 0 & \exp(-i\theta) \end{bmatrix} \cdot \begin{bmatrix} A_\ell^+ \\ A_\ell^- \end{bmatrix} \quad (2.10)$$

where $\theta(\xi) = \kappa_\ell(\xi - \xi_\ell)$ as before, and A_ℓ^+ , A_ℓ^- are complex amplitude coefficients with ξ_ℓ as a reference plane. That is, $A_\ell \equiv A(\xi_\ell)$. Equation (2.9) is, in fact, the transformation which diagonalizes the coefficient matrix K in (2.5), and $A(\xi) \equiv \text{col}[A^+(\xi), A^-(\xi)]$ is a vector solution of the diagonalized equation $dA/d\xi = \text{diag}[+i\kappa, -i\kappa] \cdot A$. The two columns of the transformation matrix in (2.9), $\text{col}[1, Y_x]$ and $\text{col}[1, -Y_x]$, are matrix eigenvectors of K .

Duality extends to the interpretation of the A_ℓ^\pm coefficients, which may be viewed as wave amplitudes of the same type as F_y , electric for the TE case, and magnetic for the TM case. F_z , a field of the complementary type, is obtained from $A(\xi)$ by multiplication by Y_x , the wave admittance/impedance. This contrasts with the usual representation, of incident and reflected waves say, always in terms of the E-field amplitude regardless of polarization.

At the outer boundaries (with the understanding that $\xi_0 \equiv \xi_1$ and $\xi_{N-1} \equiv \xi_N$) the solutions of (2.9) are matched to the field solutions in the inner layers via the tangential boundary fields F_1 , and F_N :

$$\begin{bmatrix} F_y \\ F_z \end{bmatrix}_1 = \begin{bmatrix} 1 & 1 \\ Y_1 & -Y_1 \end{bmatrix} \cdot \begin{bmatrix} A_1^+ \\ A_1^- \end{bmatrix}, \quad \begin{bmatrix} F_y \\ F_z \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ Y_N & -Y_N \end{bmatrix} \cdot \begin{bmatrix} A_N^+ \\ A_N^- \end{bmatrix} \quad (2.11)$$

where $Y_1 \equiv Y_{x1}(\beta^2)$ and $Y_N = Y_{xN}(\beta^2)$ are the admittances in the semi-infinite layers.

The field solutions in the semi-infinite layers are assumed to be of the form of Eqs. (2.9), (2.10) with A_ℓ^+ and A_ℓ^- determined by the outer boundary conditions. These conditions nearly always imply that only one of the two is nonzero, that only a single exponential solution exists. This is discussed in the next chapter. Of course, even in this case, the F-solution in layers 1 and N can still be expressed in form of Eq. (2.5) also, and may be more convenient for calculations.

The physical interpretation of $A^+(\xi)$ and $A^-(\xi)$ is determined by the real and imaginary parts of κ in the layer, and therefore is very dependent on the principal branch specification for κ . For a half space above a surface-wave structure the conventional specification is that $\text{Im } \kappa \geq 0$; in which case A^+ represents solutions having exponential decay in the positive x direction, and A^- solutions having exponential growth. The real part of κ may have either sign, so A^+ or A^- may imply either (but opposite) direction for the phase propagation. If primary interest is in real waves propagating across a structure (not eigenmodes), then the branch specification for κ might be $\text{Re } \kappa \geq 0$; in which case the superscript of A^\pm implies the direction (in x) of the phase propagation, and the real exponential behavior may be in either direction. If the branch specification is arbitrary (see Sect. 3.3), then no fixed physical interpretation can be made of the $A(\xi)$ solutions. So it is

emphasized that the superscripts of A^+ and A^- refer only to the sign of the associated exponent in (2.10), $\exp(\pm i\kappa\xi)$, regardless of how κ is defined. (As an extreme example, it is possible to specify $\text{Re } \kappa \leq 0$, in which case the direction of phase propagation would be opposite to that implied by the superscript.) However κ may be specified, the physical interpretation of any exponential solution can always be made on the basis of the actual signs found for the real and imaginary parts of κ for any mode.

To allow physical intuition in discussing modes it is still useful to refer to exponentials as positive or negative solutions, assuming that in general $\text{Re } \kappa$ and/or $\text{Im } \kappa$ are positive. Then positive and negative refers to the direction of phase propagation or exponential decay, although in any specific solution (e.g., a leaky mode) one or the other may have the opposite sense. Even more useful in the semi-infinite layers is to be able to refer to the direction of the solution as being outward or inward. In layer N this corresponds, respectively, to the positive and negative direction; but in layer 1 the sense is reversed. Thus, in layer N , A_N^+ may be referred to as the amplitude of the outward solution, and A_1^- the amplitude of the inward solution. But in layer 1, A_1^- is the amplitude of the outward (negative) solution, and A_1^+ is the amplitude of the inward (positive) solution. These implied directions are shown in Fig. 2.1. Generally, the boundary conditions allow only one or the other in each region. (A common description, as outgoing or incoming "waves", is being avoided because it does not apply to solutions dominated by a real exponential factor; as for bound modes and weakly leaky modes.)

Exponential solutions are not as useful for the inner layers although it is possible to develop a matrix approach based on a transition matrix relating the amplitudes of exponential solutions in any two layers [60, p. 29].

The boundary matching conditions necessarily require equating the tangential fields in the two layers, at their common boundary, in terms of the $A(\xi)$ solutions according to (2.10) and (2.11). The resulting transformation at a boundary, between the $A^\pm(\xi)$ in the two layers, corresponds to reflection-transmission at an impedance discontinuity. When this is followed by an additional phase propagation matrix for the transition from ξ_ℓ to $\xi_{\ell+1}$, a transition matrix T results, relating the coefficients $A_\ell \equiv \text{col}[A_\ell^+, A_\ell^-]$ in successive layers

$$A_{\ell+1} = ({}_{\ell+1})^T_\ell \cdot A .$$

For real κ , the T -matrices correspond to wave transition matrices for cascaded sections of transmission lines [3, p. 29].

The matrices $({}_{\ell+1})^T_\ell$ for all the layers may be chain multiplied together (as for the C -matrices) to give an overall transition matrix for the structure

$$A_N = N^T_1 \cdot A_1 ;$$

that is, relating the amplitudes of the exponential solutions in the two semi-infinite layers. As for the C -matrices, the T -matrix for any part of the structure may be factored at any boundary index to write,

$${}^T_{p\ q} \equiv {}^T_{p\ \ell} \cdot {}^T_{\ell\ q} \quad \text{for any } \ell .$$

The formulation used by Harris was dependent on a so-called general partition relation for the recursive calculation of the characteristic determinant. That partition relation can be shown to be equivalent to one of the four elements of the above equation for the wave transition matrices.

Conversely, it can be shown that the algebra of Harris' determinants and recursive relations can conveniently be written in the form of 2x2 matrix operations, though this was not noted by him.

This representation is not as convenient as that in terms of the fields and C-matrices, basically because the dependent variables, $A^+(\xi)$ and $A^-(\xi)$, are not those required to match at the boundaries. The boundary matching equations are more complicated, and the T-matrices for each layer depend on the material parameters in two adjacent layers (depending on κ , μ , ϵ , and Y_x for both ℓ and $\ell+1$). A T-matrix is about twice as complicated as the corresponding C-matrix to compute. Further, the matrix ${}_{\ell}T_m$ is singular for $\beta^2 = n_{\ell}^2$ as $Y_{\ell} \rightarrow 0$, and corresponds to the non-existence of the inverse transformation of (2.9), at boundary ℓ , from F_{ℓ} back to A_{ℓ} . For example, the limiting form of $C_{\ell}(\kappa_{\ell} \rightarrow 0)$ in Eq. (2.8) cannot be written in terms of exponentials in κ unless A_{ℓ}^- is first allowed to be proportioned to $1/\kappa_{\ell}$ and the limiting form as $\kappa_{\ell} \rightarrow 0$ is used. That is, A_{ℓ}^- becomes infinite. This is not acceptable numerically, even though the probability of occurrence in an actual calculation may be small. For these reasons, and because there appear to be no compensating advantages, the representation in terms of exponential solutions and T-matrices is not considered suitable for numerical purposes.

Because of the importance of the exponential solutions in the semi-infinite layers it is, nevertheless, useful to define the overall T-matrix for the structure, but this is most conveniently done in terms of the C-matrix. If the fields F_1 and F_N expressed as in Eq. (2.11) are related by the C^+ matrix as $F_N = C^+ \cdot F_1$, then the vectors A_1 and A_N are related by the following two reciprocal relations

$$A_N = {}_N T_1 \cdot A_1, \quad A_1 = {}_1 T_N \cdot A_N$$

with

$${}_N T_1 \equiv {}_1 T_N^{-1} = \begin{bmatrix} 1 & 1 \\ Y_N & -Y_N \end{bmatrix}^{-1} \cdot C^+ \cdot \begin{bmatrix} 1 & 1 \\ Y_1 & -Y_1 \end{bmatrix}.$$

A similar definition could be written in terms of C^- , or also written for ${}_1 T_N$. Note that $\det {}_N T_1 = Y_1/Y_N$ and $\det {}_1 T_N = Y_N/Y_1$.

The overall T-matrix permits some physical interpretation in terms of transmission and reflection coefficients for the structure, particularly for real $\beta^2 < n_1^2, n_N^2$, when A^+ and A^- represent real waves having some component of propagation in the transverse direction. Thus, A_1^+ and A_N^- may represent the amplitudes of incoming waves; while A_1^- represents a reflected or transmitted outgoing wave in layer 1, and A_N^+ an outgoing wave in layer N. The ratios of these components may be taken to be the reflection and transmission coefficients for the structure. However, for eigenmodes the A^\pm amplitudes do not generally represent propagating waves, especially since the branch specifications for κ_1 and κ_N may be arbitrary, and a positive exponential solution does not necessarily represent a positive going wave. Here, therefore, reflection and transmission coefficients must be understood only in a generalized sense as the ratios of the amplitudes of the exponential solutions at x_0 and x_N .

For an inward solution in layer 1 only ($A_N^- = 0, A_1^+ \neq 0$), let r^- be the reflection coefficient at x_1 , and t^+ the transmission coefficient into layer N. Similarly, for an inward solution in layer N only ($A_1^+ = 0, A_N^- \neq 0$), let r^+ be the reflection coefficient at x_N and t^- the transmission coefficient into layer 1. Note that the superscript $-/+$ refers, respectively, to both

the direction (negative or positive) as well as the layer (1 or N) of the reflected or transmitted component. In terms of the elements of T_1 these coefficients can be written as

$$t^+ = A_N^+ / A_1^+ = Y_1 / (Y_N T_{22}) \quad (A_1^- \equiv 0)$$

$$r^- = A_1^- / A_1^+ = -T_{21} / T_{22} \quad (A_1^- \equiv 0)$$

$$t^- = A_1^- / A_N^- = 1 / T_{22} \quad (A_1^+ \equiv 0)$$

$$r^+ = A_N^+ / A_N^- = T_{12} / T_{22} \quad (A_1^+ \equiv 0)$$

Note that all reflection and transmission coefficients depend on $1/T_{22}$.

In the present problem there is some interest in the T-matrix and the transmission/reflection coefficients for the insight they can give to the characteristic equation or eigenmode condition. Namely, that eigenmodes imply the existence of outward solutions in the absence of any inward, exciting, fields; that is, at poles of the reflection and transmission coefficients, or zeros of T_{22} above. This leads to one representation of the characteristic equation, and is discussed further in Sect. 4.4.

2.6 Application to Continuously Varying Material Parameters

An advantage of the present formulation of the complex mode problem is that for numerical purposes it remains applicable to structures containing plane stratified but nonhomogeneous layers. Whenever the material parameters vary continuously with x (rather than being stepwise constant) it is still possible to numerically integrate the coupled first-order equation (2.5) between any two points in ξ . An accurate solution can be obtained which

corresponds to (2.6) for the constant coefficient case. Subroutines for such numerical integration of systems of first order differential equations have recently reached an advanced state of the art and are readily available [71-74].

It is emphasized that characteristic matrices, $C(\xi_b, \xi_a)$, also exist for nonhomogeneous layers. That is, the transformation for the tangential fields between any two points is still linear and described by a single matrix, although it cannot be written in terms of elementary functions, resembling (2.7). Though these characteristic matrices must be calculated numerically, they have all the properties listed in Sect. 2.3, just as for a homogeneous layer. Therefore, an inhomogeneous layer can be embedded between any other homogeneous layers of a structure, or the whole structure itself may be inhomogeneous. The characteristic matrix for any inhomogeneous layer may be chain multiplied together with other matrices, to obtain the overall matrix for the structure between the outer boundaries. In particular, the role of the overall characteristic matrix in defining the eigenvalue problem (Sect. 4.1) in no way depends on whether it is for a structure which is piecewise homogeneous or continuously varying. When an inhomogeneous layer is encountered a call to a numerical integration subroutine would replace the evaluation of Eq. (2.7).

Frequently an inhomogeneous structure is approximated by a number of piecewise homogeneous steps [52]. Accurate results can be obtained by using a sufficiently large number of small steps, but it is very difficult to state the degree of accuracy obtained or to determine the number of steps needed. Recent advances in numerical integration have emphasized provision for objective error control, and automatic changing of step size [73, 74]. The user can specify in advance the accuracy desired, and the program repeatedly

changes the step size as necessary. Where the coefficients or the solution change rapidly small steps are used, and where the changes are slow the step size is made large. When low accuracy is acceptable the numerical integration can be rapid, the step size being no smaller than necessary for the stated accuracy.

For wave-guiding structures the variation of the material parameters, $n^2(x)$, is usually simple and quite slow (compared to the wavelength). To integrate (2.5) it is only necessary to provide a formula for n^2 at any x requested by the program. The numerical integration can then be quite efficient for low order modes having few oscillations across the structure; integration could become costly only for higher order modes having a large total number of oscillations, because these must be calculated in detail using a large number of steps. It may also be mentioned that there is no difficulty in numerically integrating through any point where κ becomes zero, as $n^2(x)$ passes through the value β^2 . These are the so-called turning points at which WKB approximate solutions become singular and invalid; Eq. (2.5) is well behaved there. Lastly, the advantages of using first order differential equations over the second order wave equation are significant. In the former, the material parameters μ or ϵ always enter as simple linear coefficients; but in the latter non-constant μ and ϵ lead to additional first order derivative terms in the wave equation, requiring evaluation of the derivatives of μ or ϵ as well [5, p. 1].

It is unlikely that any user-developed piecewise approximation method or finite difference solution can compete with presently available numerical integration subroutines in terms of accuracy and efficiency.

2.7 The Field Admittance/Impedance

The ratio of tangential fields F_z and F_y for any solution is of some interest as a field quantity, primarily because of its use in the transverse resonance method. This may be written as an admittance (TE) or an impedance (TM) as [3, p. 78]

$$Y(x) = F_z(x)/F_y(x)$$

Since $Y(x)$ depends on the field solution, and varies with x , it is not a characteristic parameter of a material or a layer (as is Y_x). Rather, $Y(x)$ is a property of the solution.

From the solution, as in Eq. (2.6), $Y(\xi)$ may be written as

$$Y(\xi_b) = \frac{(iY_x) \sin \theta + Y(\xi_a) \cos \theta}{\cos \theta + Y(\xi_a)(i/Y_x) \sin \theta};$$

where $\theta = \kappa(\xi_b - \xi_a)$, and a layer index is implied. If numerator and denominator of this expression are multiplied by $Y_x/\cos \theta$ the more familiar form using $\tan \theta$ is obtained [2, p. 109], as for the transformation of a wave impedance from one point on a transmission line to another. For numerical purposes the above form is more desirable because it avoids the possibility of indeterminate forms (∞/∞) arising from the $\tan \theta$ coefficients. In any form though, $Y(\xi)$ can become infinite since the denominator may go to zero; that is at a node for F_y . As elsewhere, there is a preference for $Y(\xi)$ rather than its reciprocal $Z(\xi) = F_y/F_z$, because the latter can become nearly infinite all across a layer which is near cut off.

Because F_y and F_z are continuous at all boundaries then $Y(\xi)$ is also continuous everywhere. Hence the well known property that $Y(\xi)$ can be

transformed between any two points in ξ by a sequence of transformations. In particular, using θ_{ℓ} for each layer, $Y(\xi)$ can be transformed from boundary to boundary all across a structure.

The transverse resonance method makes use of $Y(\xi)$ defined for two special field solutions. Namely, the solution for which there is only an outgoing wave in layer N leads to the concept of the admittance $\vec{Y}(\xi)$ "seen" at a point ξ "looking" in the positive direction. Similary $\hat{Y}(\xi)$, seen when looking in the negative direction, corresponds to the solution for which there is only an outgoing wave in layer 1. The characteristic equation for the transverse resonance method is that [2, p. 108; 6, p. 217, p. 279]

$$\vec{Y}(\xi) + \hat{Y}(\xi) = 0;$$

where the left side is a function of β^2 as a parameter. It is important to mention that the same equation is obtained regardless of the choice for the point ξ . However, since each term can become infinite, there is the risk of obtaining the indeterminate form $(\infty - \infty)$ for some choices of ξ .

There is a direct relation between the chain matrix multiplication of the previous sections and the successive transformations of the field admittance/impedance. It is well known that the transformation of Y from ξ_a to ξ_b above is a bilinear or Möbius (conformal) transformation in a complex plane of Y [3, p. 374]. Such a transformation may be written in an elegant form using matrices [75, p. 299; 76]. And if, for purposes of illustration, the impedance $Z(\xi) \equiv 1/Y(\xi) = F_z/F_y$ is used rather than Y , then the matrices involved are in fact the C -matrices.

A general Möbius transformation from a complex variable z to $w(z)$ is $w(z) = (az + b)/(cz + d)$; with a, b, c, d being the parameters of the transformation, and $ad - bc \neq 0$. The inverse transformation exists,

$z(w) = (dw - b)/(-cw + a)$. If the parameters are displayed as a matrix M , then the Möbius transformation may be written in an operator notation M : as

$$w(z) = M:z = \frac{az + b}{cz + d}, \quad \text{with } M = \begin{bmatrix} a & b \\ c & d \end{bmatrix}.$$

That is, M is a matrix, and M : denotes the operator whose action on z is defined by the equation. The inverse transformation is easily written as $z(w) = M^{-1}$, where M^{-1} is just the matrix inverse of M . That $\det M \neq 0$ is important, and it may usually be chosen to be unity. The great advantage of this operator form is that the composition of successive transformations and the inverse transformations all follow the rules of matrix algebra and inversion.

If $Z(\ell)$ denotes the field impedance $Z(\xi_\ell)$ at the boundaries, then by using the matrix C_ℓ the transformation from $Z(\ell-1)$ may be written in operator form using C_ℓ : as

$$Z(\ell) = C_\ell:Z(\ell-1) \equiv \frac{Z_{\ell-1} \cos \theta_\ell + (i/Y_\ell) \sin \theta_\ell}{Z_{\ell-1} (iY_\ell) \sin \theta_\ell + \cos \theta_\ell}.$$

Similarly, $Z(q) = {}_q C_p:Z(p-1)$ for any two boundaries p and q . This notation is compact; the matrices involved in the successive transformations may be multiplied together before writing out the impedance transformation. Thus, the transverse resonance relation may be written as

$$\vec{Z}(p) = {}_p C_N:Z_N \equiv {}_N C_p^{-1}:Z_N$$

$$-\vec{Z}(p) = {}_p C_1:Z_1$$

where Z_1 and Z_N are the impedances of the two semi-infinite layers. (For the outward-only waves in these layers these are the same as the field impedances.) Therefore, the algebra of the chain matrix representation and that of the admittance/impedance transformations is essentially equivalent.

For continuously varying material stratification $Y(\xi)$ is a continuous function of ξ (except at possible points where $Y(\xi)$ is infinite). $Y(\xi)$ and $Z(\xi)$ then satisfy Riccati (non-linear) differential equations [77]. Using Eq. (2.5) these can be found to be

$$dY/d\xi - (i\kappa Y_x) + (i\kappa/Y_x) Y^2 = 0$$

$$dZ/d\xi - (i\kappa/Y_x) + (i\kappa Y_x) Z^2 = 0$$

Given the reciprocal relation between Y and Z , these are entirely equivalent equations. The expression for $Y(\xi_b)$ above is simply the solution of the first equation with constant coefficients in a uniform layer, with ξ_a being some initial point. The continuous $Y(\xi)$, and the Riccati equations, form the basis for the so called invariant embedding method [77]. Therefore it can be said that the use of the field admittance/impedance, and the transverse resonance method, correspond to the formulation of the invariant embedding method when applied to the case of piecewise constant coefficients (layers).

It may be argued that, because $Y(\xi)$ is only a single field variable, to be solved for or transformed across a structure, the invariant embedding and the transverse resonance methods are simpler than dealing with two components F_y and F_z and the matrix operations as done here. In any particular case this is not necessarily true. For example, the matrix transformation of F across one layer requires four complex multiplications; whereas the transformation of Y requires the same four multiplications plus a complex division

as well. In the inhomogeneous case, as either $Y(\xi)$ or $Z(\xi)$ passes through zero, it is necessary to repeatedly switch from one Riccati equation to the other. Also, use of $Y(\xi)$ as the ratio between field variables, sacrifices all knowledge about the magnitudes of the fields in the different regions of the structure. As discussed in Sect. 4.6, structures exist in which the fields can become exponentially very large or very small, and subject to considerable round off error. In these, nearly indeterminate cases, the use of $Y(\xi)$ above would give no hint that it may be very inaccurate.

2.8 The Phase Integral

Integration of κ across the structure for any value of β^2 gives a useful characteristic quantity, namely the phase integral:

$$\Phi(\beta^2) = \int_{\xi_0}^{\xi_N} \kappa d\xi .$$

The integral across any one layer, ξ_ℓ , is just the phase thickness, θ_ℓ , used before. Across the complete layered structure the phase integral reduces to the summation of the θ_ℓ ,

$$\Phi(\beta^2) = \sum_{\ell=1}^N \theta_\ell ,$$

where $\theta_\ell \equiv \kappa_\ell(\beta^2)\xi_\ell$. If, as usual, ξ_0 and ξ_N coincide with the outer material boundaries then the summation is over the finite layers, $\ell = 2$ to $N-1$. For the piecewise homogeneous structure, there is some ambiguity in the definition of Φ because it depends on the branch specification (the sign) of κ . For complex modes Φ is, of course, complex. The real part gives a measure of the total radian thickness of the structure of any mode

and is useful for ordering and indexing the modes. The imaginary part of Φ gives a measure of the maximum possible exponential growth or decay of the field distribution across the guide.

The phase integral plays a central role in WKB methods, for approximate solutions in guides of continuously varying index profiles [6, p. 337]. Budden [56, Chapt. 9; 57, Chapt. 7-8] used it for calculating modes in ionospheric waveguides. For a single guiding layer, the characteristic equation for the modes can be stated in terms of the transverse round-trip phase integral plus complex phase shifts at the boundaries (turning points). For successively higher bound modes in a guide the phase integral increases by about π for each higher mode index. Thus, it is possible to propose a mode indexing scheme by assigning an index m to any discrete mode β_m^2 as

$$m = \text{integer}[\Phi(\beta_m^2)/\pi] .$$

For single graded index guides, with quadratic variation of $n^2(\xi)$ for all ξ , the WKB solutions are exact [2, p. 54]. Then,

$$\Phi_m = \pi(m + 1/2), \quad \beta_m^2 = n_o^2 - (m + 1/2)n_o/k_o t$$

where n_o^2 is the peak value of n^2 , and t is the point (a full width) at which $n^2 = 0$. So Φ increases as integer numbers of π , and β_m^2 decreases from n_o^2 linearly with m .

For a slab guide, with uniform index n_o^2 and total thickness t , then

$$\Phi_m = \kappa_m k_o t = m\pi + \phi ;$$

where ϕ is the sum of the two phase shifts at the boundaries, as in Fig. 1.2. When n_o^2 is large, and for modes far from cutoff, $\phi \approx \pi$; and for modes near

cutoff, $\phi \approx 0$. (In the quadratic case above $\phi = \pi/2$.) The eigenvalues are

$$\beta_m^2 = n_o^2 - (m\pi + \phi)^2 / (k_o t)^2.$$

As before ϕ_m increases as $m\pi$; but now β_m^2 decreases linearly with m^2 , not with m .

When an arbitrary structure contains a single guiding region (though made up of several layers) the phase integral can be expected to increase linearly about as $m\pi$ for successive modes. The decrease of β_m^2 with m will be somewhere between quadratic and linear, or perhaps slower. For true bound modes, with small losses, the above proposed indexing method corresponds to that based on counting nodes across the structure. The simple variation expected of β_m^2 vs m (or vs the phase integral) also provides an excellent method for generating initial guesses for β^2 ; at which to start the complex root search, as described later in Sect. 5.5.

In the fully complex case of arbitrary structures the above model is not as dependable. If, for example, there are several separated guiding regions (say three weakly coupled guides) then ϕ for the lowest order mode will not be on the order of π (but perhaps 3π). And ϕ_m may be spaced only approximately at intervals of π . Near and beyond cutoff, where with increasing m all β_m^2 have large imaginary parts, the mode spacing with the real part of ϕ may be very poor. In fact it is not possible then to uniquely order and index the modes [57, p. 137]. Nevertheless, the integer part of $\phi(\beta^2)/\pi$ is a useful characteristic to calculate for each mode that is found.

Because of the ambiguity in defining ϕ for the fully complex case, it has been found useful to accumulate instead two sums, ϕ_R and ϕ_I , separately taking real and imaginary parts of θ_λ always positive. That is

$$\phi_R = \sum_{\ell=1}^N |\operatorname{Re}\theta_{\ell}| \qquad \phi_I = \sum_{\ell=1}^N |\operatorname{Im}\theta_{\ell}|$$

The first, in units of π , provides a measure of the mode index. The latter quantity provides an estimate for the maximum possible exponential change (in factors of e), of the field solutions across the structure. If ϕ_I is too large, such as for very weakly coupled guides, then there is risk of numerical error. This is discussed in Sect. 4.6.

3. BOUNDARY CONDITIONS, MODE CLASSIFICATION, AND BRANCH SPECIFICATIONS

Previous sections describe the transverse differential equation and its general solutions for arbitrary initial conditions anywhere in x . Additional boundary conditions must be imposed at the outer boundaries x_0 and x_N to restrict the domain of solutions to those which are physically allowed or mathematically useful. These conditions are distinct from the boundary-matching conditions at the outermost material discontinuities at x_1 and x_{N-1} . Rather, the boundary conditions at x_0 and x_N , because of the uniformity of the semi-infinite layer, correspond to conditions imposed at infinity. They resemble the so-called radiation condition requirement on fields at large distances from sources in finite regions.

In order to calculate complex modes, including both bound and unbound leaky modes, it is necessary to consider the relationship between the boundary conditions and the principal branch specification for κ_1 and κ_N in the semi-infinite layers. These specifications restrict the solutions to certain regions of the complex planes; and, similarly, different sectors of these planes imply different physical characteristics for the modes. These characteristics are useful in classifying the different possible modes. Two simple special cases are also described. When only one boundary condition is imposed, the continuous spectrum of (non-eigen) modes results. And in some cases a fixed value of surface impedance can approximate one or both boundary conditions; the resulting problem is greatly simplified, being independent of branch specifications.

3.1 Boundary Conditions

Conceptually the simplest statement of the boundary condition at either x_0 or x_N is that the field solutions are restricted to a single,

either inward or outward, exponential solution in the semi-infinite layers. From Eq. (2.9), assuming that A_1^+ and A_N^- are zero, for outward-only solutions, this condition may be written in a normalization independent manner as

$$\text{at } x_0 \quad Y_1 F_y + F_z = 0 \quad (3.1a)$$

$$\text{at } x_N \quad Y_N F_y - F_z = 0 \quad (3.1b)$$

(If inward-only solutions are instead specified at a boundary then the respective sign appearing before the Y would be reversed.) These conditions may be described as impedance-type boundary conditions, in that the ratio between the two components of the solution is being specified. The equations are homogeneous in the field components-- there are no source terms on the right. Sometimes these are described as mixed boundary conditions.

With the imposition of two boundary conditions, at opposite sides of the structure, the field problem has become a two-point boundary value problem. Because both the differential equation and the boundary conditions are homogeneous in the field variables (no sources) it is an eigenvalue problem; only for discrete values of the eigenvalue parameter, β^2 , do solutions for F_y and F_z exist. These values of β^2 are roots of a characteristic equation $D(\beta^2) = 0$, whose construction is described in Chapter 4.

It is of fundamental importance that the coefficients Y_1 and Y_N in the boundary conditions (3.1) depend on the eigenvalue parameter (through their proportionality to $\kappa(\beta^2)$). This dependence distinguishes the open waveguide problem from that of the closed waveguide, and distinguishes this problem from nearly all text-book discussions of two-point eigenvalue problems. It is necessary then to consider the principal branch specifications for the κ ; these specifications become an important part of the statement of the

boundary conditions. As a consequence, the associated branch points and cuts in the β^2 plane become unavoidable singularities of the characteristic function $D(\beta^2)$.

For any value of β^2 a solution always exists which will satisfy just one or the other of the boundary conditions. If only one boundary condition is imposed, then apart from normalization, it may be used as an initial condition and a solution is well defined everywhere. A solution exists for each of the two boundary conditions imposed separately, and for nearly all values of β^2 these two solutions are linearly independent. These play a useful role on several occasions in the following discussion.

3.2 Classification of Modes

An extensive literature exists on the properties of surface waves, and their classification according to the complex transverse propagation constant in a semi-infinite layer [78-82]. Thus, in addition to the longitudinal propagation characteristic implied by β , the signs of the positive and imaginary parts of κ in the semi-infinite layer determine the direction of exponential decay or growth and direction of transverse propagation. The reader is assumed to be somewhat familiar with the resulting concepts of proper or bound modes, improper or unbound, leaky, and forward or backward modes. This classification is fully applicable to the complex modes of the present structure, but with two differences.

Firstly, there are two semi-infinite layers in the present problem, whereas nearly all literature on surface waves concerns a single semi-infinite layer adjacent to the surface of a guiding structure. Hence the classification of a mode here must now include the characteristics of the mode in both semi-infinite layers. These characteristics can be different in the two

layers. But κ_1 and κ_N are not independent because they are both functions of β^2 ; therefore, the mode characteristics in the two layers are closely tied together. A minor matter of viewpoint is that modes in the present case are not surface waves in the usual sense. This is because the two surfaces may be widely separated, with the guiding structure arbitrarily thick in terms of wavelength. The guiding region of energy confinement may lie deep within the structure, and the outer boundary surfaces may have a negligible role in determining the propagation properties. Nevertheless, though very little of the energy may propagate in the semi-infinite layer, the mode characteristics in these layers determine whether it is a bound proper or an improper mode.

Secondly, nearly all literature on surface waves deals only with passive systems, but here the possibility of gain in any layer is included. This requires some broadening of the concepts of the types of possible modes; but to types which cannot be distinguished on the basis of the behavior in the semi-infinite layer. In a passive system, for example, exponential growth in the direction of phase propagation ($\text{Re } \beta$ and $\text{Im } \beta$ with opposite signs) always implies that the group velocity and power flow are then in the opposite direction [80-81]. In the present case such a mode may be indistinguishable from a forward mode with gain, where phase and group velocity are in fact in the same direction as power flow, but with exponential growth in the same direction being due to gain somewhere in the structure. At a fixed frequency, knowledge of β and of κ in a semi-infinite layer can only distinguish modes on the basis of the directions of phase propagation and exponential growth or attenuation.

For this reason we take phase propagation to be the positive z direction, in common for all modes, $\text{Re } \beta \geq 0$. Modes are then further classified

by the direction of exponential decay or growth, by the sign of $\text{Im } \beta$. Whether this is due to loss or gain, or forward or backward power flow, cannot be determined on the basis of β or κ only. (This contrasts with the usual comparison of modes, taken to have positive power flow and group velocity in common ($\text{Im } \beta \geq 0$), and further distinguished by forward or backward phase propagation (sign of $\text{Re } \beta$).) Here, modes will sometimes be described as attenuating or having gain, referring to the positive z direction. But this should be understood to be equivalent, in the passive case, to forward or backward power flow and group velocity.

A transformation commonly used, from the β - and κ -planes to a complex angle variable w , is [5, p. 462; 79]

$$\beta = n \sin w, \quad \kappa = n \cos w,$$

where n is the complex refractive index in the semi-infinite layer. When w is real it corresponds to the angle of propagation (measured from the outward normal) of a plane wave in the layer. This transformation is very useful and important in manipulating integral representations and paths of contour integrals. In much of the literature the properties of discrete modes is based on their location in the different regions of the w -plane. For numerical purposes, with emphasis on locating the discrete mode eigenvalues, the above transformation offers no advantage; and it is definitely detrimental to the complex root searching. For, the inverse transformation $w(\beta)$ or $w(\kappa)$ is multi-valued, and if the root search is carried out in the w -plane there is an infinite multiplicity of roots for each mode. Further, in the present case with two semi-infinite layers, it is necessary to single out one or the other layer as special, in which to make the above transformation. For these reasons this transformation was not considered for the present

formulation, but it must be understood if the discussion of mode classification here is to be compared with some in the literature.

The question of the conditions under which the modes of different types exist is not considered here. Neither the types of guiding structures required to support the different modes, nor the excitations necessary to excite them are examined. If and when calculated modes are found to lie in different regions, then the classifications serve to summarize their properties. Similarly, for any given structure, a root search may be started in any desired region to provide information as to whether modes of that type are supported by the structure.

Some regions or modes are described below as strictly nonphysical. This is meant in the sense that no physical interpretation for them has been proposed, nor any method of exciting them. These have rapid exponential growth in the x or z directions.

The distinguishable regions of the β^2 - and β -planes, and of the κ -plane for one semi-infinite layer, are shown in the next two figures. These are shown without regard yet to any branch specifications for κ , since the mode characteristics associated with each region do not depend on how these may be assigned to different branches or sheets. The figures differ from many in that a complex n^2 is now allowed for the outer layer. A lossy material is assumed, and with the positive imaginary part for $\epsilon = n^2$ exaggerated for clarity. Also, the β - and κ -planes are further divided into octants, to distinguish regions in which the real and imaginary parts are large or small relative to each other.

The β^2 -plane is shown in Fig. 3.1 with the different regions numbered. To the left of the imaginary axis, in regions 7 to 9 and indicated by E, the imaginary part of β is larger than the real part; in the z direction the mode

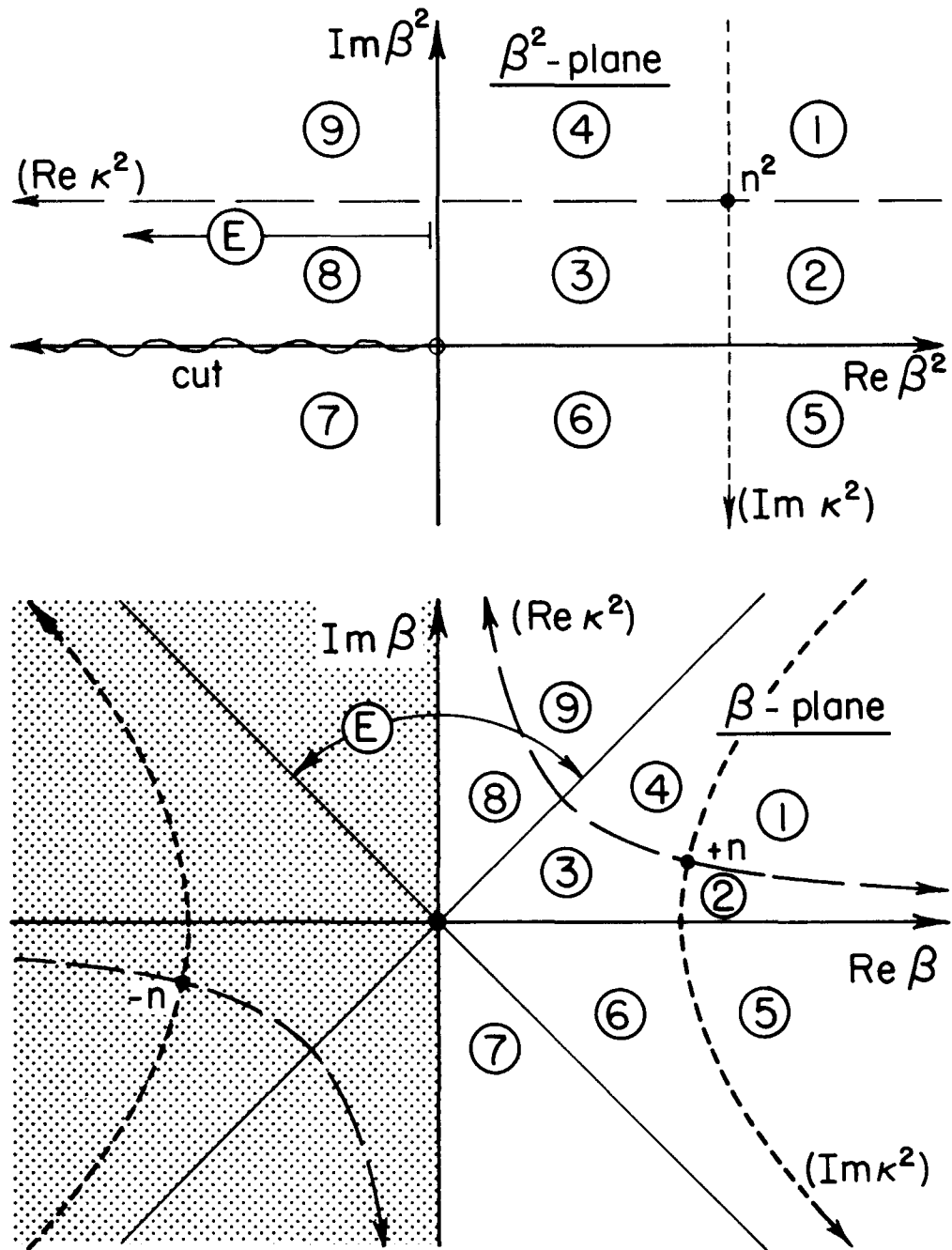


Figure 3.1 Regions of the complex planes of β^2 and β for $\kappa(\beta^2)$ in one semi-infinite layer. The imaginary part of n^2 for the layer is exaggerated for clarity. Numbered regions for different types of modes correspond to those of the κ -plane in Fig. 3.2.

behavior is dominated by the exponential decay (or growth). These modes are evanescent in the z direction of propagation and are not usually important.

The corresponding regions in the β plane are shown also, assuming $\text{Re } \beta \geq 0$ for the principal branch of β . The shaded second branch for β corresponds to equivalent modes, but having the opposite sense of propagation. The region for modes which are evanescent in the z direction is again denoted by E on either side of the imaginary axis. In the corresponding region on either side of the negative imaginary axis modes have a rapid exponential growth and may be considered as strictly nonphysical.

In Fig. 3.1 a branch cut is shown along the negative imaginary axis of β^2 , corresponding to the principal branch specification for β . Since the β^2 -plane is considered to be the primary domain of the eigenvalue parameter, and β is not specifically needed in what follows, the β -plane and the cut in the β^2 -plane is not further considered. However, if any mode of interest is found to lie near to or cross this branch cut in β^2 , then the question of branches in β and a possible transition to backward modes should be carefully reconsidered. Backward waves are most commonly associated with structures periodic in the direction of mode propagation. But they may also exist in uniform structures when some layer is an isotropic plasma or a metal, for which ϵ^2 has a negative real part [83, 84].

Modes are also described as fast or slow waves depending on $\text{Re } \beta$ being less or greater than $\text{Re } n$. For low losses in the layer these regions correspond to $\text{Re } \beta^2$ being less or greater than $\text{Re } n^2$, so slow waves are found in regions 1, 2, and 5, and fast waves in regions 3, 4, and 6. Slow and fast refer to the velocity of phase propagation of the mode relative to that in the one semi-infinite layer. A mode may be slow or fast with respect to each semi-infinite layer separately, depending on the relative values of n^2 in the

two.

Modes which propagate a significant distance in z (relative to the exponential behavior) lie in the right half of the β^2 -plane. In the first quadrant, regions 1 to 4, modes decay in the direction of propagation (passive forward modes, or backward modes with gain). In the fourth quadrant, regions 5 and 6, modes grow exponentially (passive backward modes, or forward modes with gain). The first quadrant may be further subdivided according to whether the real and imaginary parts of β^2 are greater or less than those of n^2 . In the β^2 -plane alone it is not possible to further distinguish modes. It is necessary to examine the κ -plane, or more specifically for any β^2 , to consider the two possible values of κ .

The complex plane for $\kappa(\beta^2)$ is shown in Fig. 3.2, with the different regions labeled corresponding to those in Fig. 3.1. The dashed and dotted lines are mappings of the real and imaginary axes of β^2 . Evanescent modes lie beyond the two hyperbolas to right and left, which depend only on $\text{Re } n^2$. And modes with gain, or otherwise having exponential growth in z , lie beyond the two hyperbolas in the first and third quadrants. These hyperbolas depend only on $\text{Im } n^2$, and in the lossless case they reduce to the real and imaginary axes of κ . The modes with gain then lie in the first and third quadrants, and attenuating modes lie in the second and fourth.

The directions of transverse phase propagation and exponential behavior are indicated, according to the signs of the real and imaginary parts of κ . Bound, proper modes (with respect to this layer) lie in the upper half plane, $\text{Im } \kappa > 0$. Field distributions for these modes are square integrable in x . Unbound, improper modes lie in the lower half plane, $\text{Im } \kappa < 0$. Outward phase propagation and power flow occurs in the right half plane, and in the left half plane the phase propagation and power flow is inward from

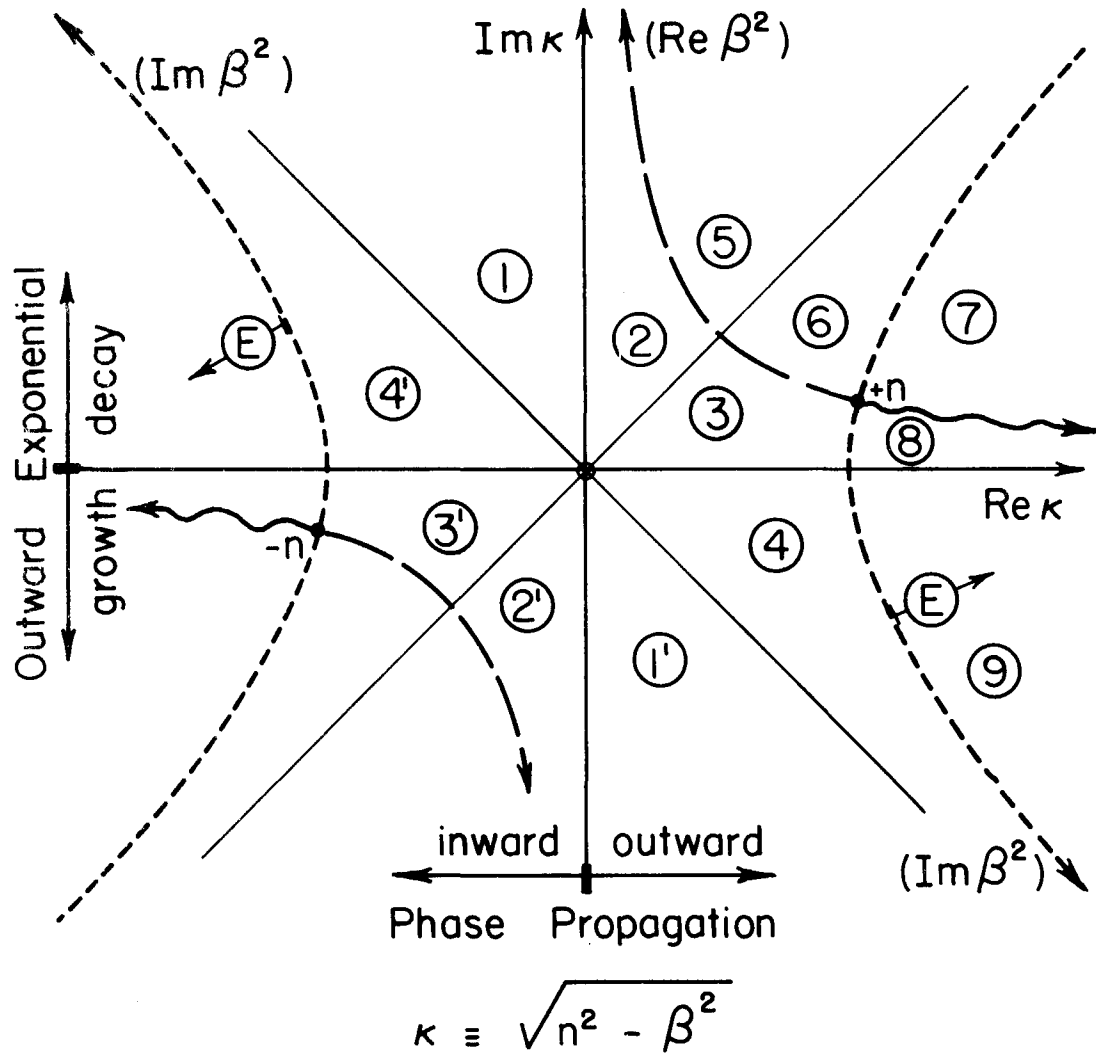


Figure 3.2 Regions of the complex plane of $\kappa(\beta^2)$ in one semi-infinite layer of index n . Numbered regions for different types of modes correspond to those of Fig. 3.1. The dashed and dotted lines are mappings of the real and imaginary axes for β^2 . Directions of transverse phase propagation and exponential behavior are indicated.

the semi-infinite layer into the structure.

Tightly bound, strongly guided modes are located in the octants on either side of the positive imaginary axis, regions 1, 2, and 5, where outward exponential decay dominates over phase propagation, $|\operatorname{Re} \kappa / \operatorname{Im} \kappa| < 1$. This is also the region for slow waves. Modes with strong outward exponential growth, in regions 1' and 2' and the negative imaginary axis are considered as strictly nonphysical.

Phase propagation dominates over the exponential behavior in the quadrants centered on the real axis, $|\operatorname{Im} \kappa / \operatorname{Re} \kappa| < 1$. Such modes have a significant component of transverse phase propagation and power flow in the semi-infinite layer near the structure. This is also the region for fast waves.

The characteristics of modes when located in the different regions are summarized below. Gain refers to modes having exponential growth in z , but this should also be understood to include the possibility of backward passive modes.

1. Tightly bound mode, weak inward phase propagation. Zenneck wave [3, p. 454; 57, p. 233]. Inward phase propagation and power flow. Power flow nearly parallel to surface with some small component flowing inward, as to make up for losses elsewhere in structure. For assumed value of n^2 , no modes with gain lie in this region.

Imaginary Axis. Purely bound mode, no transverse phase propagation or power flow. Pure exponential outward decay, power flow parallel to surface. Bound modes in lossless dielectric structure.

2. Tightly bound mode, weak outward phase propagation. Power flow is outward, but is absorbed in layer, not radiated. If layer is lossless, region 2 reduces to the positive imaginary axis.

With increasing gain somewhere in the structure (reducing the attenua-

tion rate in z), a bound mode with approximately constant $\text{Re } \beta > \text{Re } n$ will move from regions 1 to 2 to 5.

In regions 1, 2, and 5 $\text{Re } \beta^2 > \text{Re } n^2$, and for low losses in n^2 , then $\text{Re } \beta > \text{Re } n$; modes are slow waves with respect to the semi-infinite layer.

3. Weakly bound, attenuating in z , strong outward phase propagation. Includes spectrum of attenuating plane waves, propagating outward at an angle w measured from outward normal: $\kappa = n \cos w$, w real, along line between origin and $\kappa = n$. For a lossless layer region 3 reduces to a portion of real line $0 \leq \kappa \leq n$.

Real Axis. Part of the continuous spectrum. Pure outward phase propagation with constant amplitude. Not a plane wave if n^2 is lossy.

4. Passive leaky modes, unbound and improper, outward phase propagation. Power radiated into semi-infinite layer. This is the primary region of interest for beam coupling and radiation problems. For weakly leaky modes, then $\text{Re } \kappa \gg -\text{Im } \kappa$, near the real axis. Attenuation in z , which is necessarily associated with leaky modes, may be due to losses anywhere in structure. Loss need not be due only to that of leaky mode radiation.

In region 4, $\text{Re } \beta^2 < \text{Re } n^2$, and for small losses in n , then $\text{Re } \beta < \text{Re } n$; mode is a fast wave relative to the semi-infinite layer.

Note that a bound mode on the imaginary axis or in region 1 cannot become a leaky mode in region 4 unless: a) n^2 is lossy, and by passing through regions 2 and 3, or b) layer is lossless, and by passing through region 5 and 6 which extend up to the imaginary and real axes, namely a structure with gain. Therefore a bound mode in a lossless structure becomes, with decreasing frequency say, not a leaky mode, but an evanescent mode passing into region 4'.

5. Tightly bound, strongly guided, mode with gain. Passive backward bound mode. Outward phase propagation and power flow. Slow wave with respect to layer.

6. Weakly bound mode with gain, strong outward phase propagation and power flow. Backward leaky mode. A fast wave with gain.

A forward leaky mode, with increasing gain somewhere in structure, and with other parameters approximately constant ($\text{Im } \beta$ decreasing), will move from region 4 to 3 to 6.

7. Strong exponential growth in z , nonphysical. Backward evanescent mode.

8. Strong exponential decay in z , an evanescent mode. Bound in transverse direction.

9. As for 8, but unbound in transverse direction. Evanescent mode with gain.

Regions 1' to 4' correspond to an opposite choice of branch for κ , however the principal branch may be defined. In the β^2 -plane these regions are located on another Riemann sheet.

1'-2' Strong outward exponential growth, nonphysical.

3' Slow outward exponential growth unbound, inward phase propagation. Includes domain of single inward plane wave incident at a real angle. But with no outward, reflected, wave. Could be supported only by properly phased combination of plane waves incident on both sides of structure.

4' Weakly bound, inward phase propagation. Similar to region 1, but phase propagation dominant.

The regions complementary to 5 through 9, with opposite sign, could also be described, but these do not appear to have any physical significance or mathematical usefulness.

Modes may also be judged by the magnitude of κ relative to n . If κ is very small, and regardless of which quadrant it may be in, $|\kappa| \ll |n|$, then $\beta \approx n$. In the semi-infinite layer the wave propagation is nearly parallel to the surface and the mode is said to be near cut-off. In the transverse direction the solutions change slowly. It is well to keep in mind that the origin of each κ -plane corresponds to a branch point in the β^2 -plane for the characteristic equation. For modes with κ near the origin there is not much distinction between the inward and outward solutions, they are both nearly constant in x . The two possible modes may be nearly degenerate, and the proper one can be difficult to identify.

3.3 Branch Specifications for κ_1 and κ_N

Several points may be made concerning the role of principal branch specifications for κ_1 and κ_N . Firstly, it is a simple matter of mathematical necessity-- some branch must be specified. For calculations it is certainly necessary to let κ_1 and κ_N represent single-valued functions. The eigenvalue search must be carried out in a single-valued domain of β^2 . Any branch specification restricts each κ to a half-plane, and if the other half must be considered it must be done separately.

Secondly, the branch specifications for κ , and the consequent branch cuts in the β^2 or β planes, are largely arbitrary from the purely mathematical point of view. There is nothing in the statement of the differential equations, or the form of the equations for the boundary conditions, that requires a particular branch specification. Specific choices for principal branch are based on additional physical arguments or on convenience for calculations.

Conventionally the branch specifications have been used as a tool to restrict the solutions to those which are physically acceptable. For the fields to be bounded, have finite energy, or proper direction of propagation, the values of κ_1 , κ_N , and β must lie in certain regions of their complex planes. These regions can be equated to the respective principal branches and proper or principal Riemann sheets. On these, the eigenvalue problem is well defined and all roots which may exist will be physically acceptable modes.

However, for calculation of complex modes in general, and for efficiency in searching for complex roots as described later, a nonconventional and largely arbitrary branch specification has been found very useful. This allows proper and improper modes to appear on the same Riemann sheet in β^2 , simplifying their search. The classification of modes is then no longer described by the branch specifications. Whatever the branch specifications, regardless of how non-physical or unrealistic they may be, the resulting boundary conditions lead to a well defined and single valued characteristic function, with roots which can be found.

In a larger sense the characteristic function can be considered as defined and single valued on the set of four Riemann sheets of the β^2 -plane. No branch specifications are needed. Roots exist on all sheets. Any roots which are found can afterward be classified, and accepted or rejected, on the basis of their physical properties.

Because β^2 is common to all layers, then all the $\kappa_\ell(\beta^2)$ are implicitly functions of each other. To emphasize this fact for κ_1 and κ_N they may be written as

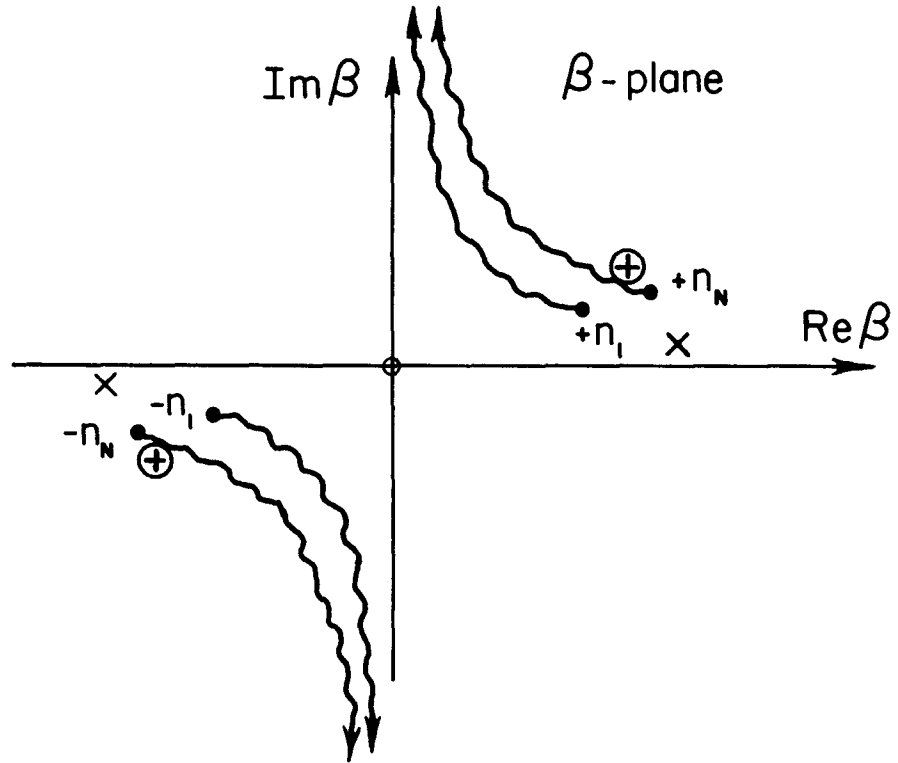
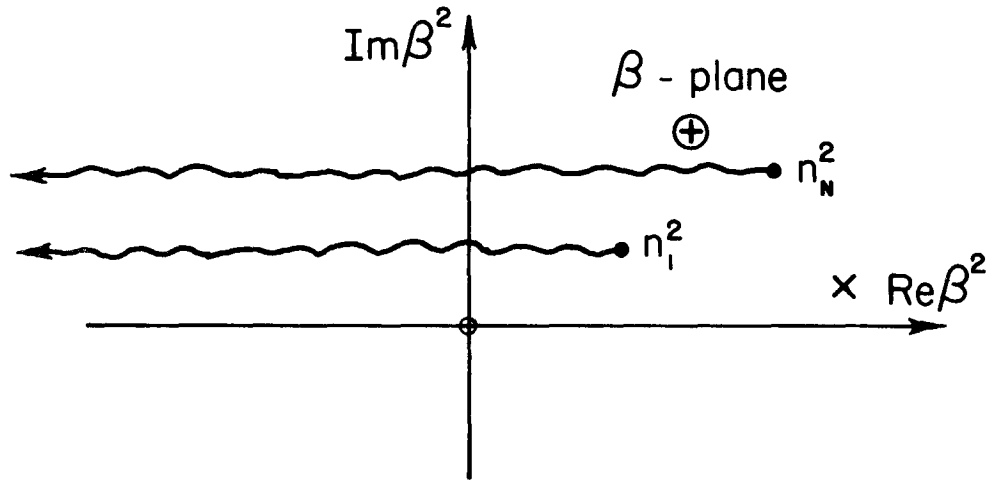
$$\kappa_1(\kappa_N^2) \equiv \sqrt{\kappa_N^2 - \Delta^2} \ , \qquad \kappa_N(\kappa_1^2) \equiv \sqrt{\kappa_1^2 + \Delta^2} \ ;$$

where $\Delta^2 \equiv n_N^2 - n_1^2 \equiv \kappa_N^2 - \kappa_1^2$ is independent of β^2 , and expresses the difference between the material parameters of the two semi-infinite layers. For functions which depend on both κ_1 and κ_N (say the characteristic equation), as well as for each κ as a function of the other, the κ -planes consist of two Riemann sheets and have branch points at $\pm \Delta$. Each κ -plane then also has a branch cut associated with the principal branch specification for the other κ . The boundary between the two half-planes (branches), in either κ -plane, maps to become the branch cut in the other κ -plane, and both of these map to become the branch cuts in the β^2 -plane.

Fig. 3.3 shows the complex planes of β^2 and β for functions which depend on both κ_1 and κ_N . The branch cuts correspond to the conventional specification of principal branch, $\text{Im } \kappa > 0$. The positive imaginary parts for both n_1^2 and n_N^2 are exaggerated for clarity. With two branches for each of κ_1 and κ_N there are then four Riemann sheets for the β^2 and β planes; the top sheet is taken as the principal sheet, associated with the principal branch for both κ_1 and κ_N . The locus for two possible modes is shown. The cross, on the top sheet, is for a proper mode attenuating in z and bounded, with exponential decay in both outer layers. The plus sign is for a mode which is bounded in layer 1, but leaky and unbounded in layer N . It is circled to indicate that it is located on a lower Riemann sheet.

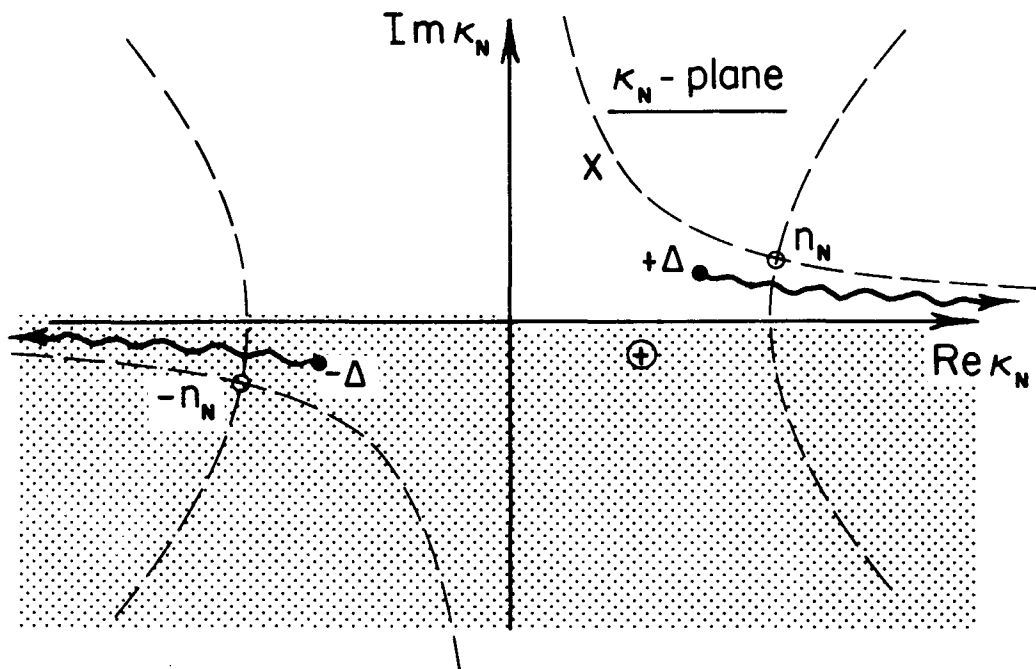
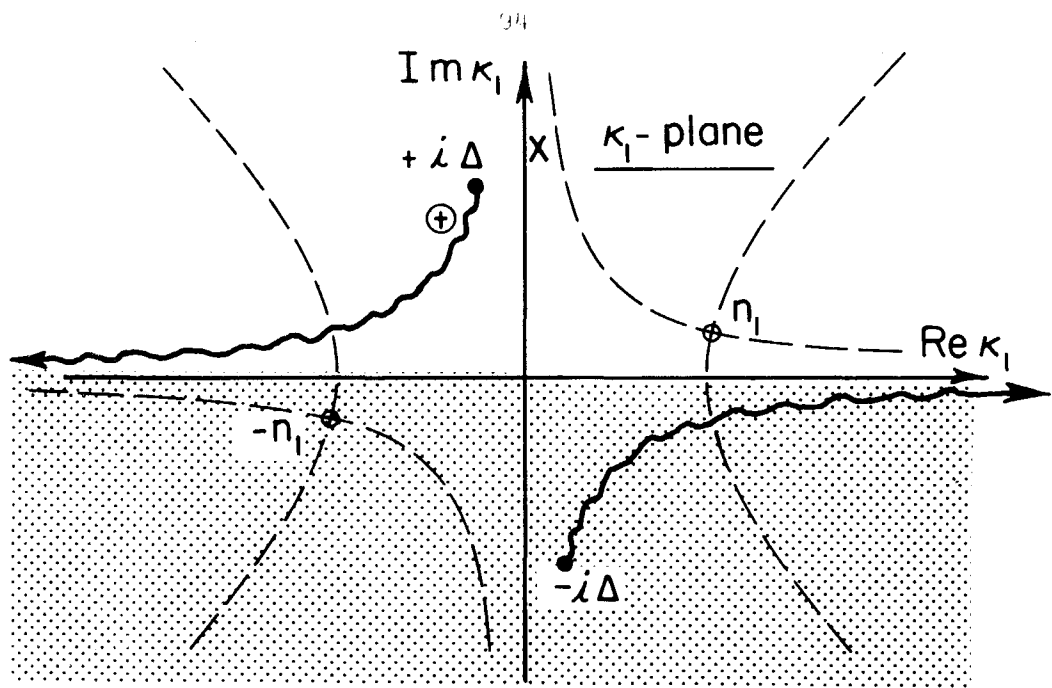
Fig. 3.4 shows the complex planes for κ_1 and κ_N , using the conventional branch specification for both. The principal branch is the upper half-plane, $\text{Im } \kappa > 0$, plus the positive real axis. The second branch is the lower half-plane and the negative real axis. The dashed hyperbolas, different in the two planes, are maps of the axes of the β^2 -plane, just as in Fig. 3.2.

The branch cuts in each κ -plane correspond to the real line (the boundary between the two branches) of the other κ -plane. That is, the real line



$$\kappa_1 = \sqrt{n_1^2 - \beta^2}, \quad \kappa_N = \sqrt{n_N^2 - \beta^2}, \quad \text{Im } \kappa \geq 0$$

Figure 3.3 Complex planes of β^2 and β , for functions of both κ_1 and κ_N . Branch cuts are shown for the principal branches, $\text{Im } \kappa \geq 0$, conventionally specified for bound surface waves. Each plane is composed of four Riemann sheets; the top principal sheet is the proper or physical sheet for both κ_1 and κ_N .



$$\Delta^2 \equiv n_N^2 - n_1^2$$

Figure 3.4 Complex planes of κ_1 and κ_N for conventional branch specifications. The principal branch for each κ is the upper half-plane, $\text{Im } \kappa > 0$, plus the positive real axis. The real axis of each plane maps to the branch cuts in the other κ plane, and both map to the cuts in Fig. 3.3. The dashed hyperbolas are maps of the axes of the β^2 -plane.

of each κ -plane maps to the branch cut appearing in the other κ -plane; and both map to the two cuts in the β^2 -plane of Fig. 3.3. Each κ -plane consists of two Riemann sheets, associated with the two half-planes of the other κ . The two sheets, for the two κ -planes, together correspond to the four sheets of the β^2 -plane.

The cross in Fig. 3.4, corresponding to that shown in the β^2 - and β -planes, shows the location of the possible bound mode. It is on the principle half of each κ -plane, and on the top sheet of each. The circled plus sign similarly shows the location of a mode which is bound in layer 1, but which is unbound and leaky into layer N. It is in the principal half-plane of κ_1 , but on its second Riemann sheet; this sheet corresponds to the second branch of κ_N , in which the mode is located, but on the top sheet there. Note that the bound mode in both κ_1 - and κ_N -planes is located in region 2 of Figs. 3.1 and 3.2. The mode which is leaky into layer N is located in region 1 for κ_1 , but in region 4 for κ_N .

Note that the locus of any mode, if it crosses the real line of either κ -plane then it necessarily crosses the branch cut of the other κ -plane, onto the other Riemann sheet.

The relationship between the two κ -planes, as described here for lossy materials, has been rarely noted in the literature. Nearly all the earlier literature on dielectric slab guides treats only a single semi-infinite layer, as for a dielectric layer on a metal plane, or else a symmetric slab where the two semi-infinite layers were the same, say air [31, 85]. For the symmetric guide a single κ represents the value in both semi-infinite layers. That is, κ is taken always on the same branch for both layers. That κ could be taken separately on different branches in the two layers does not appear to have been noted, and perhaps not recognized. Nearly all recent treatments

of asymmetric guides consider only bound modes, or modes which are leaky only to one side, say into a higher index substrate. Few have included losses in the outer layers, so a careful discussion of branch specifications has not been needed.

The behavior of modes, as they move along their loci in the complex planes of κ with changing parameters, has been discussed by Burke [31], Tamir [83] and Shevchenko [85, 86]. But these descriptions were for symmetrical slab guides, where the locus moved on a single plane for κ representing both outer layers.

The conventional branch specifications reject leaky modes as nonphysical; such improper modes, on other than the principal sheet for β^2 , are sometimes said to not exist. In order to calculate these, and other complex modes in general, there are three alternatives. The first two are algebraically equivalent.

a. The simplest viewpoint is that the other sheets of β^2 must be searched. That is, either κ_1 or κ_N , or both, are taken on their second branch. For any value of β^2 , the κ may be evaluated as on the principal branch; but their sign is explicitly reversed before being used in defining Y_1 , Y_N , the boundary conditions, and the characteristic equation.

b. Alternatively κ_1 and κ_N can always be taken on the principal branch, but the boundary conditions of Eq. 3.1 may be changed to specify inward-only solutions at either or both outer boundaries. Thus, with $\text{Im } \kappa > 0$, the signs before Y_1 or Y_N may be reversed to allow only solutions with outward exponential growth.

The only difference between a and b is the viewpoint of whether the sign change is associated internally with the quantity represented by κ , or whether

the external sign appearing before κ and Y is changed. For programming purposes these are not quite equal in convenience. It appears simplest to let κ_1 and κ_N always represent a fixed quantity on some principal branch (which may be arbitrarily specified). Then, as noted in Sect. 4.2, it is easy to calculate, as a matrix, the characteristic equations for all four possible choices of signs (inward and outward solutions) in Eq. 3.1. It is not easy to program the capability to allow κ_1 and κ_N to pass continuously onto their second branches.

c. The branch specification can be changed to reposition the branch cuts in the β^2 -plane away from the region of interest. Thus, by allowing an arbitrary specification of a principal branch for κ_1 and κ_N , these can be chosen so that the regions of interest in the κ_1 and κ_N planes are in fact on the principal branches and free of branch cuts. The principal branches no longer have physical significance.

The principal advantage of using an arbitrary branch specification, as in c, concerns the difficulty in calculating modes which lie near a branch cut. The complex root search depends on the characteristic equation being analytic in the neighborhood of a root. At a branch cut in β^2 the characteristic equation has a step discontinuity; it is not analytic, unless β^2 is allowed to pass onto another sheet in crossing the location of the cut. If β^2 is restricted to the principal branch then it becomes very difficult to calculate roots lying close to the cut. Also, a root at a considerable distance on the other side of the cut, on the continuation sheet, can cause the root search to repeatedly try to cross the cut. The direct solution to this problem is to reposition the branch cut out of the way; to place as much of the region of interest on one Riemann sheet, which can still be designated as the principal sheet. Simultaneously the branch boundary and half-planes

for κ_1 and κ_N are repositioned and redesignated.

A variety of nonconventional specifications can be considered, with curved or straight boundaries and cuts. The simplest choice is to use a straight line branch boundary in each κ -plane, necessarily through the origin, at some angle to real axis. The resulting cuts in β^2 are also straight lines, but the cuts in the β -plane and in the other κ -plane are along hyperbolas.

The locations of the branch points in any of the complex planes are unchanged by any choice of branches and cuts. Complex root searching will always be difficult in the neighborhood of these singularities.

Fig. 3.5 shows the branch cuts in the β -planes for a nonconventional branch specification for κ_1 and κ_N . The only difference from Fig. 3.3 is the location of the branch cuts. In the sectors between the positions of the cuts in the two figures there are changes in the assignments to the different Riemann sheets. What is now the top sheet in these sectors was previously on a lower sheet of Fig. 3.3. The plus sign for the mode which is unbound in layer N now appears on the top Riemann sheet. The locus of any eigenmode in the β^2 or β planes is unchanged, and the mappings between these and the κ -planes are unchanged by any repositioning of the branch cuts. Only the designations of the different Riemann sheets are affected.

The nonconventional branch specification for the κ_1 and κ_N planes are shown in Fig. 3.6. As before, the principal branch half-plane is shown unshaded. The branch boundary is a straight line, but now it is oriented at an arbitrary angle denoted by ϕ . The second branch is shown shaded. The right half of the branch boundary may also be assigned to the principal branch, and the left half assigned to the second branch. The only difference from Fig. 3.6 is the position of the branch boundaries and location of the cuts. The maps of the β^2 -axes and the locations of all mode eigenvalues in these

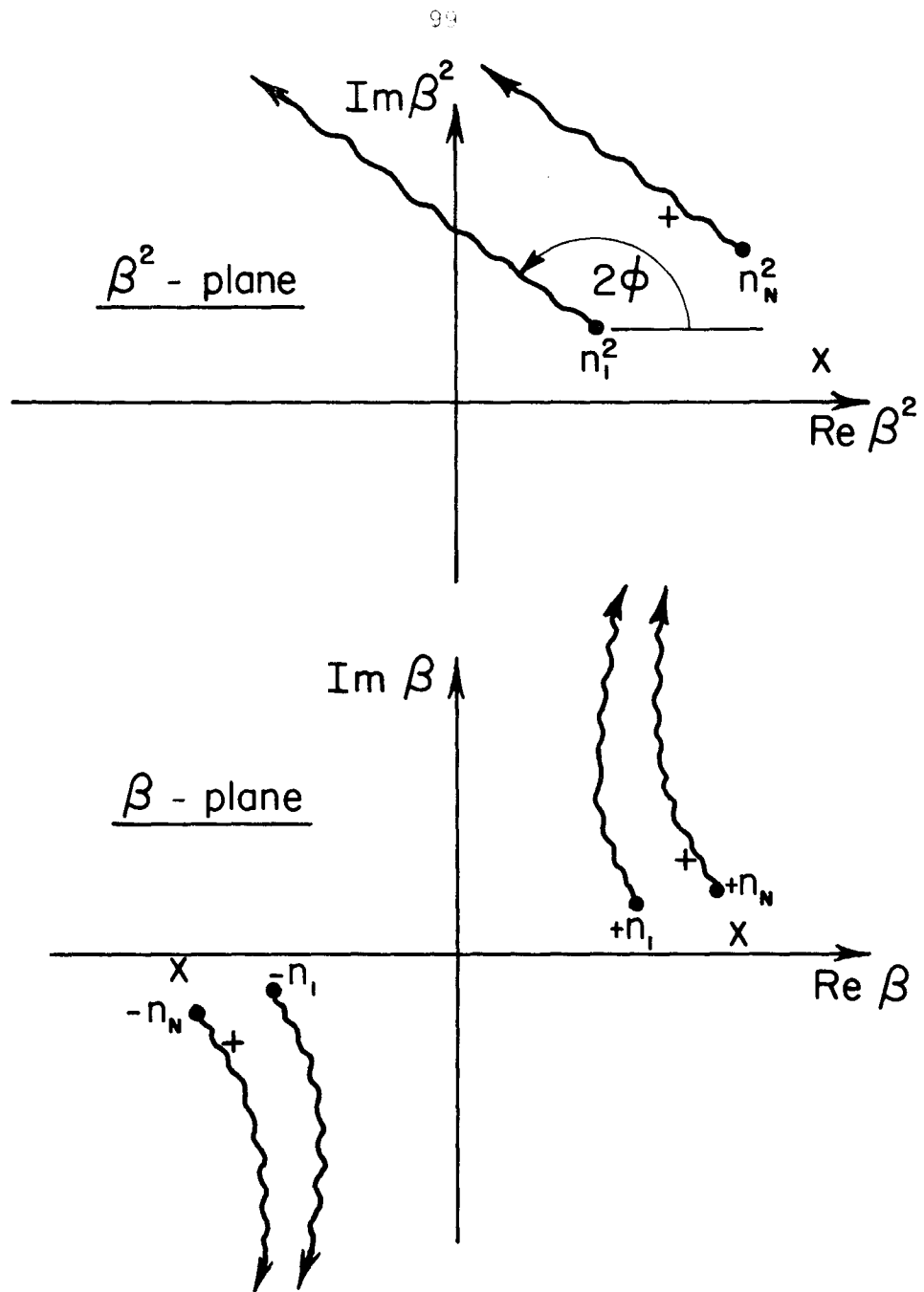


Figure 3.5 Complex β^2 and β planes for nonconventional branch specification for κ_1 and κ_N . Roots for bound mode, x , and leaky mode, $+$, can now appear on same Riemann sheet.

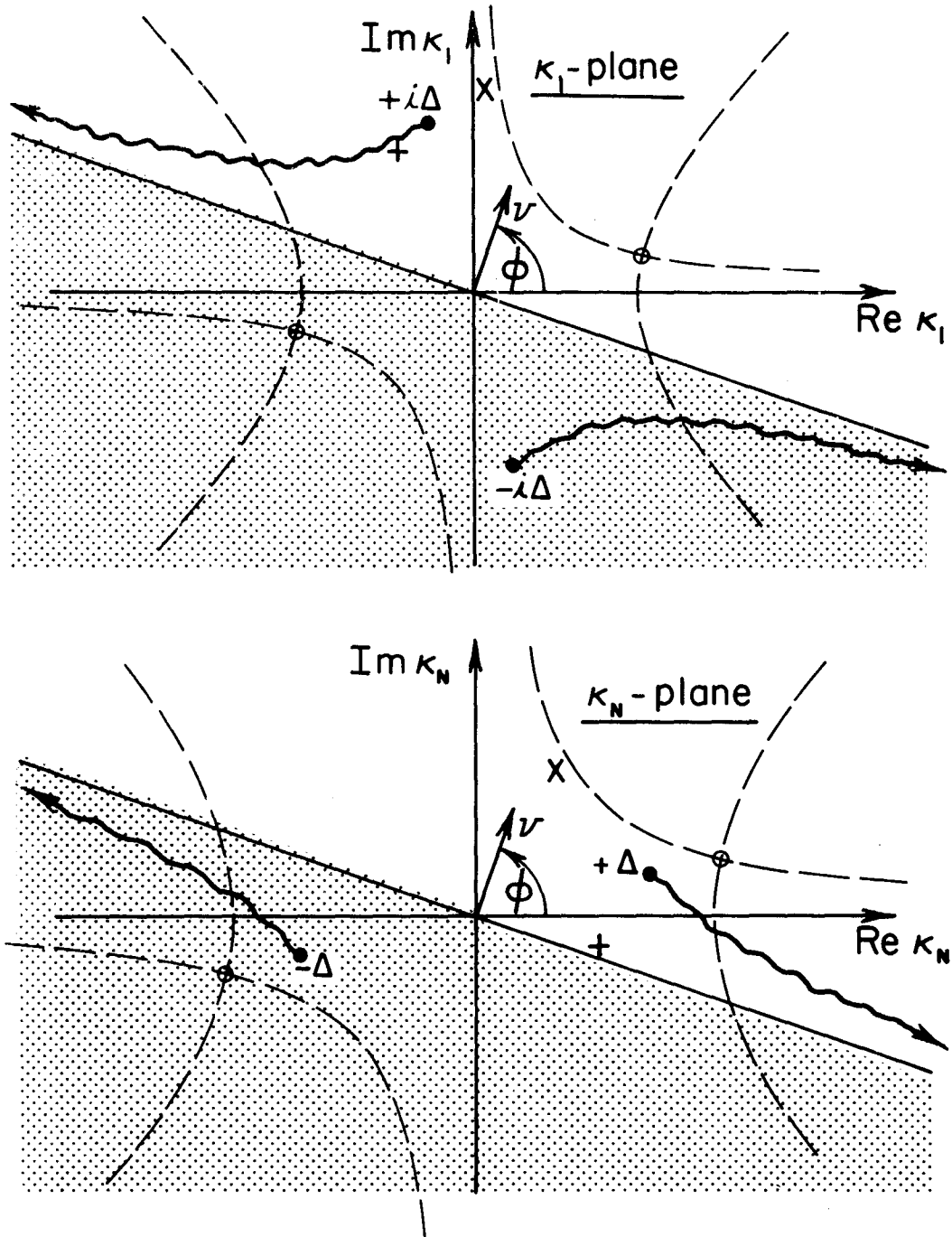


Figure 3.6 Nonconventional branch specification in κ_1 and κ_N planes. Unit vector v points normally into unshaded principal branch half-plane. Leaky mode root, $+$, now appears on principal branch of κ_N , and on top sheet for κ_1 .

planes are unchanged. However, the plus sign for the leaky mode is not now circled, to indicate that it is located on the top sheet for the κ_1 -plane and on the principal branch for κ_N . Both bound and leaky modes (at least some of them) may now appear on the same branch. For example, if $\phi = \pi/4$ then all of regions 1 and 4 described in Sect. 3.2 are on the principal sheet.

The principal branch specification here is simply stated in terms of a unit vector \mathbf{v} , pointing normally into the principal half-plane, or by the angle ϕ relative to the real axis. For any arbitrary ϕ , the specification may be written as $\text{Re } \kappa \cos \phi + \text{Im } \kappa \sin \phi \geq 0$. Or, if \mathbf{v} and κ are considered as geometric vectors in the plane, their dot product is to be positive, $\vec{\mathbf{v}} \cdot \vec{\kappa} \geq 0$. This may be written as $\text{Re } \kappa \cdot \text{Re } \mathbf{v} + \text{Im } \kappa \cdot \text{Im } \mathbf{v} \equiv \text{Re } (\kappa \mathbf{v}^*) \geq 0$. For the conventional branch specification $\phi = \pi/2$; and for the positive-real half plane $\phi = 0$. For computation, values of κ on the principal branch are easily generated. Usually a library subroutine for a complex square root returns values with positive real part. For such a value of κ the branch specification is tested, and if not true the sign of κ is simply reversed.

As shown in Fig. 3.5 the corresponding branch cuts in the β^2 -plane are oriented at an angle 2ϕ . Any rotation of the branch boundaries in the κ -planes results in the branch cuts in the β^2 -plane being rotated by twice as much. If ϕ is changed by π the cuts in β^2 rotate by 2π , returning to the same position; but the Riemann sheets for each κ will have been interchanged, and the designation of the principal and second branch plane for κ will be exchanged.

In these figures the same branch specifications have been used for both κ_1 and κ_N . This is not at all necessary. It is emphasized that the branches for κ_1 and κ_N may be independently specified. For example, modes may be restricted to those which are leaky into only one semi-infinite layer, for

which $\phi \approx \pi/4$ might be used; but a conventional branch, $\phi = \pi/2$, would be used for the other semi-infinite layer. If different specifications are used for κ_L and κ_N the corresponding Figs. (3.5) and (3.6) become more complicated. It is then possible to have the branch cuts in β^2 and β cross each other, and in Fig. (3.4) the branch cuts for one κ could cross the branch boundary for the other κ . When branch cuts cross each other it is particularly difficult to visualize the four Riemann sheets involved.

The use of arbitrarily positioned branches has proved very useful. It has contributed greatly to the efficiency in finding sets of roots. For, it is much more efficient to find a root in several iterations and later reject it as not of interest, than it is to spend five times as many iterations in a futile attempt at finding that root just beyond the branch cut. From the point of view of the root searching, on the analytic domain of the four Riemann sheets, the branch cuts are only artificially imposed barriers. For any choice of branches it is easy to make runs for the four possible choices of branches and find roots on all four sheets in some region of the β^2 -plane; say to the right of the real axis. The resulting modes can be plotted in the respective planes without regard to branch cuts, just as Figs. (3.1) and (3.2). That is, in four runs the same results will be obtained regardless of how the branch cuts were chosen. An example of a very complicated set of loci in the full κ_L -plane, obtained in this manner for a relatively simple 4-layer structure, is shown later in Fig. 7.2.

Note that the nonconventional branch cuts are not suggested as being relevant to any integral representations. They are only for convenience in the calculation of location of the roots for the discrete modes. Deformation of the integration paths to lie along these cuts would not lead to convergence of the integration in general. However, the cuts shown in Figs. 3.5

and 3.6 could be used in the near-plane, and the integrals would converge provided that the cuts in the far plane approached infinity along the negative real axis for β^2 , and along the positive imaginary axis for β , just as in Fig. 3.3.

3.4 Modes of the Continuous Spectrum

Expansion of a general solution for a layered structure, as a sum over a finite number of bound eigenmodes plus one or two integrals over a continuous spectrum, is familiar [1, pp. 98-106; 2, pp. 87-40]. This spectral representation may be described as the result of deformation of the contour of integration (in the β -plane) of an integral representation for the solution [5, pp. 464-470]. A particular solution, arising from some specific excitation, is determined by the values of the expansion coefficients in the sum and in the integral contribution. This report concerns the calculation of the discrete eigenmodes (including unbounded improper modes), but the field solutions associated with the continuous spectrum (of β -values) are an important part of a complete representation of a general solution. It is appropriate to describe these continuous or radiation modes at this point because they are not eigenmodes of the transverse problem. Rather, they are solutions to the field equations for a continuous range of β -values, and always include both an outgoing and incoming wave in one or both of the semi-infinite layers.

The integral contributions arise from separately integrating along the conventional branch cuts for κ_1 and κ_N in the complex β -plane. See Fig. 3.3. These two parts of the deformed integration contour come from infinity in the upper half plane, in along one side of a cut, around the branch points at n_1 or n_N , and out to infinity along the other side of each cut [78, p. 312].

The branch cuts for this purpose are defined by $\text{Im } \kappa_1 = 0$ and $\text{Im } \kappa_N = 0$, and integration is necessarily on the principal Riemann sheet of β for both κ_1 and κ_2 . For values of β on each cut κ is real; and the opposite sides of the cut (and the contributions to the integral therefrom) correspond to the negative and positive halves of the real line of each κ . Therefore, κ can be used as a real variable of integration along the cut. The two solutions corresponding to the two signs of κ (the contribution from the integration along opposite sides of the cut) can be combined into a single function, a mode of the continuous spectrum.

There are two spectra involved, one for each semi-infinite layer, and the two must be considered separately in the general case of complex and unequal n_1 and n_N . Each spectrum consists of the points of β along the corresponding branch cut, or equivalently to points on the positive real line of κ . For each point in the spectrum there is a solution or mode function defined. It is composed of solutions for both positive and negative values of the respective κ . That is, in that semi-infinite layer both outgoing and incoming waves are present; so some external excitation is always implied. In considering all points of one spectrum, say κ_1 , and all values of β on the cut, then the other κ_N is single-valued and always on its principal sheet. That is, the solution in the opposite semi-infinite layer always consists of the single outward solution, having exponential decay.

Therefore, we adopt the following definition for the modes of the two continuous spectra. Each spectrum consists of the one-dimensional domain of points in β along the respective branch cut, or equivalently the positive real line of κ , for one semi-infinite layer. For any point in the spectrum the field solution is defined as having a single outward decaying solution in the opposite semi-infinite layer. The solution is thus being defined by means

of a single boundary condition corresponding to one or the other of Eqs. (3.1), taken separately. One spectrum may be described as the set of all β for which $0 \leq \kappa_1 \equiv +(n_1^2 - \beta^2)^{1/2}$ is real; and the solutions for which $F_z + Y_N F_y = 0$ at x_N , Eq. (3.1b). The other spectrum consists of the set of β for which $0 \leq \kappa_N \equiv +(n_N^2 - \beta^2)^{1/2}$ is real; and the solutions for which $F_z - Y_1 F_y = 0$ at x_0 , Eq. (3.1a). Each boundary condition, with some arbitrary normalization, serves as an initial condition at x_N or x_0 respectively; and by transformation across the structure each solution is uniquely defined everywhere.

Most treatments of dielectric waveguides assume that n_1^2 and n_N^2 are real. Consequently, the branch cuts and the continuous spectra of β lie along a portion of the real axis below n_1 or n_N , and along all the positive imaginary axis. For real β between n_1 and n_N then only one continuous spectrum is present. But for β less than both n_1 and n_N , and for the imaginary axis, the two branch cuts and spectra are superimposed. (For values of β on the imaginary axis the modes are strictly evanescent in the z direction.) For any point β in this superimposed region, there is a two fold degeneracy in the mode functions; two modes of the continuous spectrum exist, and these may be taken in other arbitrary linear combinations. Several workers have constructed the modes for the continuous spectrum of 3-layer guides in such a way that they reduce to functions of odd and even symmetry when the structure is reduced to a symmetric structure (if not originally symmetric) [1, p. 25, 29; 2, p. 48]. This seems to be a rather artificial construction, and not useful for general structures which can be very nonsymmetrical.

There are further questions about normalization of the continuum modes, and about the orthogonality between modes in the two continuous spectra, and

orthogonality between them and the discrete modes. These questions are not considered here. It is possible that the continuous modes, as defined here (in terms of outward-only solutions separately in the two outer layers) may in fact satisfy some orthogonality requirements [23, 87, p. 241]. This has not been checked.

The continuous modes are discussed here only because they can be easily included by a minor extension of the formulation. In any program to calculate general solutions (no boundary conditions) or eigenfunctions (two boundary conditions), it is only necessary to provide the input options to calculate solutions from each of the two boundary conditions of Eq. (3.1) separately. This is easily done. It is of course possible to generate two such solutions for any value of β in the complex plane, but most will not have any physical significance. Only for points corresponding to the real lines of κ_1 or κ_N will a solution be a mode function of the continuous spectrum.

In the literature points in the continuum of the spectral variable are frequently referred to as eigenvalues, and the mode functions as eigenfunctions of the continuous spectrum (of the operator $-i\partial/\partial z$). This can be misleading because these are not solutions of the transverse eigenvalue problem in the sense of two-point boundary value problems. Modes of the continuous spectrum are required to satisfy only one boundary condition at one end of the structure; there is no characteristic function in the usual sense, whose roots define the eigenvalues. It is emphasized that the continuous spectrum and the discrete spectrum are solutions to two different boundary value problems. The boundary conditions imposed are different.

The simple case of plane waves, incident on the structure from the semi-infinite layers, is very closely related to the continuous spectrum. If the

outer two layers are lossless, the domain of β (real $\beta < n_1$, or n_N) and the field solutions are the same for both. If the outer layers are lossy then an outward plane wave implies that $\beta/\kappa = \tan w$ is real, with w being the angle of propagation with respect to x . That is, κ and β have the same ratio between their real and imaginary parts, and in their own complex planes each lies on the line between the origin and the point n_1 or n_N . These points then differ from the continuous spectrum when n_1 or n_N are complex.

For a plane wave incident on one side, the solutions are obtained by imposing the boundary condition of Eq. (3.1) corresponding to the other outer boundary (just as for the continuous spectrum, but for possibly different values of β). That is, since the reflected wave on the incident side is not known until the solution is obtained, the solutions are most easily defined and calculated by specifying only an outward transmitted wave on the opposite side. As for discrete modes the normalization is arbitrary.

Therefore any computer program using the present formulation can easily include the options for calculating the fields in multi-layered thin-film optical filters, including lossy layers. Likewise the fields for plane radio waves incident on arbitrarily complicated models of layered earth may be found.

3.5 Constant Surface-Impedance Boundary Conditions

In some applications it is useful to approximate a boundary by a surface having a fixed value of surface impedance or admittance. That is, at some surfaces in a field problem, the ratio of the tangential fields on one side of a boundary is taken to be approximately constant. This assumption replaces the need to consider the fields in the region beyond the boundary [5, p. 545].

For the layered structure, constant admittance/impedance surfaces at the outer boundaries x_1 and x_{N-1} may be used; by simply taking Y_1 and Y_N , in the boundary conditions (3.1), to be fixed values, not dependent on β^2 . A sense of direction is still implied, with Y_1 and Y_N being admittances "seen" looking outward, from the interior of the structure, toward the outer boundaries. The effect of the semi-infinite layers is replaced by the assumed values for Y_1 and Y_N . These boundary conditions are also equivalent to assuming a fixed complex reflection coefficient, at the outer boundary, for outward exponential solutions from within the adjacent finite layer.

The practical use of surface-impedance concepts is somewhat limited, because in few situations are the values reasonably constant, and because of difficulty in determining the appropriate values. Two limiting cases, of zero or infinite impedance, are nevertheless useful. If Y_1 or Y_N are zero, then $F_z = 0$, and the boundary corresponds to a magnetic wall for the TE case and to an electric wall for a TM case. The converse, of an electric wall for TE and a magnetic wall for TM cases, corresponds to Y_1 or Y_N being infinite. For computation it is then better to write the boundary conditions in terms of the impedance(TE)/admittance(TM); namely, with $Z \equiv 1/Y$, as $ZF_z \pm F_y = 0$. The limiting cases are useful for metal walls at microwave frequencies. Thus the formulation here is directly applicable for completely arbitrary plane layered, inhomogeneously filled, planar metal waveguides.

Another useful application is to symmetrical layered structures, where a factor of two economy in calculating the modes is possible. All eigenmodes will be odd or even about the midplane of symmetry for the structure. Calculations can then be made using only half the structure, with the midplane being replaced by an outer boundary having a zero surface admittance or impedance. The other boundary remains open as for the original symmetrical

structure. Modes of even symmetry are calculated by taking $Y = 0$ at the midplane boundary; for, then $F_y \neq 0$ there, and F_y will be an even function of x . Odd modes are calculated by taking $Z \equiv 1/Y = 0$ at the midplane. (The odd and even symmetry refers to that of F_y ; the symmetry of F_z will be the opposite type.) The value of κ in the one open semi-infinite layer of the half structure must also represent the value for κ in the other semi-infinite layer of the full structure. By symmetry, the two are equal; they are taken on the same branch. Therefore, if κ_1 and κ_N are to be taken on different branches, the solutions cannot be obtained by this method. The modes may then not have either odd or even symmetry.

It should be noted that assumption of a fixed surface-impedance at both outer boundaries greatly simplifies the eigenmode problem. Since the boundary conditions do not depend on β^2 , then there are no branch points or cuts in the β^2 -plane for any aspect of the problem. In particular, the characteristic function for the eigenvalues in β^2 (see next sections) has no branch cuts; it is a single-valued function on a single Riemann sheet for β^2 . (The same is true for the Green's function for the structure, [5, p. 456].) The numerical search for eigenvalues should be more efficient. The waveguide is closed and all modes are physically acceptable regardless of how complex or complicated is the layered interior structure. If only one boundary is closed, then the problem is simplified by half. Only for the one open boundary and semi-infinite layer is it necessary to consider the branch singularity, specification and mode classification.

4. THE CHARACTERISTIC EQUATION

Given the differential equation and its matrix solutions, the imposition of the outer boundary conditions gives rise to the transverse eigenvalue problem. The present section considers the formulation of the characteristic equation whose roots, in β^2 , are the eigenmodes for the structure. Several approaches to the equation are given to show its mathematical significance, to provide some physical insight, to show its relation to the transverse resonance method, and to point out some of the numerical considerations.

4.1 For a General Homogeneous Two-Point Boundary Problem

A general linear eigenvalue problem, in a variable parameter λ , may be stated in the form of a homogeneous differential equation

$$L[\lambda, f(t)] \equiv f'(t) - A(\lambda, t) \cdot f(t) = 0, \quad (4.1)$$

and the homogeneous boundary conditions

$$B_a(\lambda) \cdot f(a) + B_b(\lambda) \cdot f(b) = 0 \quad (4.2)$$

for $a < t < b$ [69, p. 146; 88, p. 142; 89, Chapt. 3]. Here the dependent variable, $f(t)$, is an n -vector, and $A(\lambda, t)$, $B_a(\lambda)$, and $B_b(\lambda)$ are $n \times n$ matrices. The differential operator $L[\lambda, f(t)]$, as well as the boundary condition matrices, all may depend on λ , the eigenvalue parameter. The dependence may be non-linear, but is assumed to be analytic. In addition, the coefficient functions may depend analytically on other parameters of the problem. All quantities except the independent variable, t , may be complex, and the assumption of a finite interval $[a, b]$ is important.

Equation (4.2) represents the most general possible linear boundary conditions. Depending on the structure of the matrices B_a and B_b , it allows

separated, mixed, and even periodic boundary conditions. To have an eigenvalue problem at all, there must be n linearly independent boundary conditions. This is stated as requiring in general that for the adjoined $n \times 2n$ matrix $[B_a, B_b]$,

$$r = \text{rank } [B_a, B_b] = n.$$

Otherwise, if the rank $r < n$ regardless of λ , then $n - r$ solutions always exist for any λ [69, p. 155; 89, p. 39]. With these assumptions, Eqs. (4.1) and (4.2) form a well-posed eigenvalue problem; that is, for what values of the parameter λ do solutions $f(t)$ exist?

For Eq. (4.1), by itself, fundamental matrix solutions (sets of n linearly independent column vector solutions) always exist and are also analytic in λ . A fundamental matrix solution, $F(\lambda, t)$, may be defined by specifying at some point t_0 , $a < t_0 < b$, that $F(\lambda, t_0) = I$, the unit matrix. The matrix on the right could be any other orthogonal matrix, but this greater generality is not needed. Most frequently t_0 is chosen to be $t_0 = a$, and sometimes $t_0 = b$, but nothing in the problem depends on a specific choice for t_0 within the interval. For any choice of λ , let $F(\lambda, t)$ be a fundamental matrix solution; then any vector solution $f(t)$ may be written in the form [68, p. 324; 69, p. 45]

$$f(t) = F(\lambda, t) \cdot c,$$

where c is some constant vector. Obtaining solutions to the eigenvalue problem depends on finding values of λ , and corresponding vectors $c(\lambda)$, such that $f(t)$ also satisfies the boundary conditions, Eq. (4.2). This will be true if, and only if, the matrix equation (obtained by substituting $f(t)$ above into Eq. (4.2)),

$$Q(\lambda) \cdot c \equiv [B_a(\lambda) \cdot F(\lambda, a) + B_b(\lambda) \cdot F(\lambda, b)] \cdot c = 0, \quad (4.3)$$

is satisfied. The $n \times n$ matrix $Q(\lambda)$ is called the characteristic matrix for the boundary problem, and under the assumptions made, it is analytic in λ . If for a given λ , $Q(\lambda)$ is non-singular, then no solutions for the vector c or for $f(t)$ exist [89, p. 40].

Therefore, Eq. (4.3) has a non-trivial solution for c only for those specific values of λ for which the determinant equation is satisfied,

$$D(\lambda) = \det Q(\lambda) = 0 \quad (4.4)$$

This is the characteristic equation for the eigenvalue problem in the parameter λ . $D(\lambda)$ is a determinant of order n , and it is analytic in λ whenever the other matrices are analytic. Because of the analyticity, then either D is identically zero and every λ is an eigenvalue, or else the eigenvalues λ form at most a denumerably infinite set with no finite limit point. That is, the eigenvalues are distinct, and there is no continuous part to the spectrum of the eigenvalue problem [89, p. 39]. It is possible, however, to have degeneracy and multiplicity of an eigenvalue. This multiplicity can at most be equal to n .

The characteristic equation (4.4) does not depend on the particular fundamental matrix $F(\lambda, t)$ used in constructing the characteristic matrix $Q(\lambda)$. For, although fundamental matrices are not unique, they can differ at most by multiplication on the right by a constant non-singular matrix (having a non-zero determinant). Therefore, though $Q(\lambda)$ and the vector c for any solutions will be changed by any such matrix multiplier, the characteristic equation (4.4) is only multiplied by a scalar constant, the determinant of the constant matrix. The choice of fundamental matrix can thus be based on convenience of

calculation and numerical considerations.

To obtain the value of the characteristic function $D(\lambda)$, evaluation of any fundamental matrix is needed only at the end points a and b . For example, if $C(\lambda; b, a)$ is a transformation matrix between solutions $f(a)$ and $f(b)$ at the end points, then

$$f(b) = C(\lambda; b, a) \cdot f(a),$$

$$f(a) = C^{-1}(\lambda; b, a) \cdot f(b) \equiv C(\lambda; a, b) \cdot f(b);$$

where $C(\lambda; b, a) \equiv F(\lambda, b) \cdot F^{-1}(\lambda, a),$

regardless of the choice for $F(\lambda, t)$. That is, the matrix transformation of f between any two points is unique, and it may be determined from any fundamental matrix whose value is known at the two points. Then the characteristic equation may be written as

$$D(\lambda) \equiv \det [B_a(\lambda) \cdot C(\lambda; a, b) + B_b(\lambda)] = 0, \quad (4.5a)$$

or as $D(\lambda) \equiv \det [B_a(\lambda) + B_b(\lambda) \cdot C(\lambda; b, a)] = 0; \quad (4.5b)$

and in fact C may be factored at any interior point t to write

$$D(\lambda) \equiv \det [B_a(\lambda) \cdot C(\lambda; a, t) + B_b(\lambda) \cdot C(\lambda; b, t)] = 0, \quad (4.5c)$$

independent of t . Although similar to the expression for $Q(\lambda)$ in terms of $F(\lambda, t)$, as defined in Eq. (4.3), this equation emphasizes that $D(\lambda)$ is independent of the choice for $F(\lambda, t)$; except for multiplication by a constant.

The formulation above is presented to emphasize some general conclusions. These are, first, that the construction of general solutions between the two end points, and the specification of the outer boundary condition and the characteristic equation, are two separate parts of the eigenvalue problem.

General solutions (depending on the parameter λ) can always be constructed to satisfy the differential equation throughout the interval, without considering the outer boundary condition; and the characteristic function can be defined and evaluated for any λ regardless of how the solutions were constructed. For example, in an n -th order system, there are n linearly independent solutions; in any interior region it does not matter how these or any linear combination of these are chosen. Further, at any points of discontinuity, the interior boundary-matching conditions may be considered to be a part of the definition of the differential operator, or a part of the construction of a general solution. They are not a part of the specification of the characteristic function. For these reasons the characteristic function can always be reduced to an n -th order determinant, regardless of the complexity of the structure leading to the differential equation. Secondly, the analytic properties of the coefficients of the differential equation and the boundary conditions carry over to $D(\lambda)$. This permits conclusions about properties of the roots. That $D(\lambda)$ is analytic in λ , whenever the coefficient matrices are analytic, is very important to the possible methods for numerical root-searching. Further, there is assurance that $D(\lambda)$ is an analytic function of other parameters of the problem, and in consequence the eigenvalue roots (and the eigenfunctions) are continuous functions of the parameters [69, p. 40].

This description has not made use of any self-adjointness properties for the problem, nor has it been necessary to assume any boundedness or square-integrability properties for the eigenfunctions. These additional assumptions may be required for physically acceptable solutions. Often the boundary conditions themselves can be prescribed in such a way that only physically reasonable solutions are included in the set of eigenfunctions. But it should be recognized that these additional conditions constitute a restriction on the

domain (of functions) of the differential operator. Mathematically there is nothing in the differential equation or the boundary conditions which requires these added restrictions; they are based on physical grounds.

For the layered structure the transverse eigenvalue problem in x is easily stated in the above form, with two important exceptions. The order is $n = 2$, the eigenvalue parameter is $\lambda \rightarrow \beta^2$, and the independent variable is $\tau \rightarrow x$ (or ξ). The differential operator is given by Eq. (2.5), with the coefficient matrix $K(\beta^2)$ being piecewise constant and analytic within each homogeneous layer. The boundary matching conditions of Eq. (2.2) are considered a part of the differential equation. For any value of β^2 then, single vector solutions, or fundamental matrix solutions, are easily generated for any choice of initial conditions anywhere in x . In particular, the transformation matrix between the first and last boundaries (or the inverse) may be easily generated by the chain multiplication of the individual layer matrices. If the boundary field values are saved at each interior boundary, x_ℓ , this may be considered to generate a solution, but need not be done. The differential equation and the matrix solutions are all analytic functions of β^2 and of the other material and dimensional parameters of the problem.

The two important exceptions to the previous assumptions are that, 1) the boundary condition equations are not analytic for all values of β^2 , and 2) the interval of the independent variable (a,b) is not finite, but is the whole infinite line. The second aspect must be considered with care before the boundary conditions can be applied in such a way that most of the previous conclusions apply. Ordinarily, a differential equation defined on an infinite domain, with coefficients that do not vanish at infinity, is considered to have an irregular singular point; and a much more complicated theory is required [89, p. 53]. In the present case, because the coefficients become

constant in the semi-infinite layers, and by restricting the domain of solutions, it is possible to impose the impedance type boundary conditions at finite values of x and obtain the exact solutions even though the domain is infinite. Under these circumstances most of the conclusions from problems on a finite interval remain valid [89, p. 56].

Thus, at some $a \leq x_1$, and $b \geq x_N$ the boundary conditions of Eq. (3.1) may be written as

$$B_a \cdot f(a) = \begin{bmatrix} Y_1 & 1 \\ 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} F_y(a) \\ F_z(a) \end{bmatrix} = 0, \quad \begin{matrix} (4.6a) \\ (3.1a) \end{matrix}$$

$$B_b \cdot f(b) = \begin{bmatrix} 0 & 0 \\ Y_N & -1 \end{bmatrix} \cdot \begin{bmatrix} F_y(b) \\ F_z(b) \end{bmatrix} = 0; \quad \begin{matrix} (4.6b) \\ (3.1b) \end{matrix}$$

where Y_1 and Y_N depend on β^2 , and some fixed specification of principal branch for κ_1 and κ_N used.

For the adjoined boundary matrix,

$$\text{rank } [B_a, B_b] = \text{rank} \begin{bmatrix} +Y_1 & 1 & 0 & 0 \\ 0 & 0 & +Y_N & -1 \end{bmatrix} = 2;$$

and in fact $\text{rank } B_a = \text{rank } B_b = 1$, since each has only one row. These are separated boundary conditions, because each row of the equation involves F_y and F_z at only one or the other of the boundaries. Though applied at finite x , these boundary conditions are equivalent to their being applied at infinity; because, if they are satisfied anywhere, they are satisfied uniformly throughout the semi-infinite layer.

Y_1 and Y_N are functions of the eigenvalue parameter β^2 and have branch points at n_1^2 and n_N^2 respectively. They are not analytic at the branch point, or on any fixed branch cut which may be imposed in the β^2 plane. This lack of analyticity cannot be avoided, and it compromises the assumptions made for the general model. In particular, the characteristic function $D(\beta^2)$ is discontinuous at the branch cuts; or else it must be defined on a set of four Riemann sheets for the β^2 -plane, and β^2 allowed to move onto the other branches of Y_1 and Y_N . Except at the two branch points, the previous conclusions about the analytic properties of $D(\lambda)$, and the eigenfunctions, remain valid on the four Riemann sheets for β^2 . On these extended planes the eigenvalues remain distinct, and are analytic functions of all parameters. Near the branch point, however, for some values of the physical parameters, it is possible for two eigenvalues to coalesce into one.

An explicit expression is easily written for the characteristic function in terms of the transition matrix from x_0 to x_N . Let the elements of the matrix be

$$C^+ = \begin{bmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{bmatrix}.$$

The characteristic matrix $Q(\beta^2)$, as defined by Eqs. (4.3) and (4.5b), will be

$$Q(\beta^2) = \begin{bmatrix} Y_1 & 1 \\ 0 & 0 \end{bmatrix} \cdot I + \begin{bmatrix} 0 & 0 \\ Y_N & -1 \end{bmatrix} \cdot \begin{bmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{bmatrix}$$

$$= \begin{bmatrix} Y_1 & 1 \\ (Y_N C_{11} - C_{21}) & (Y_N C_{12} - C_{22}) \end{bmatrix}$$

and the characteristic equation is

$$D(\beta^2) = \det Q = (Y_1 Y_N C_{12} - Y_1 C_{22} - Y_N C_{11} + C_{21}) = 0. \quad (4.7)$$

This is the equation of central interest in this formulation-- the eigenvalue equation (in β^2) for complex eigenmodes of the layered structure. All quantities are transcendental functions of β^2 , and the practical problem of calculating the roots remain. For even the most complicated structure, once the overall transition matrix is calculated, the characteristic equation has only these four terms. This equation is for outward-only solutions in each semi-infinite layer. For the opposite choice in either layer (inward-only solutions) the characteristic equation is obtained by simply changing the sign before Y_1 or Y_N , respectively, as they appear in Eq. (4.7). If the characteristic equation were to be written in terms of the elements of the inverse matrix C^- , for the transformation from F_N back to F_0 , then the position of C_{11} and C_{22} would be interchanged, and signs before C_{12} and C_{21} would be reversed.

4.2 As Elements of Reciprocal Transmission and Reflection Coefficients

Some physical interpretation of the characteristic equation is possible if the reflection and transmission of "waves" incident from the outside of the structure is considered. If a reflection or transmission coefficient for a structure is found to have a pole in some variable parameter, this implies the existence of outgoing waves in the absence of any incoming waves; i.e. a

solution to the source-free, homogeneous, problem-- or the eigenmodes. The Green's function for a structure can be interpreted as a transmission coefficient between source and observation point, and it is well known that poles of the Green's function, as a function of the variable parameters, correspond to the eigenmodes of a structure-- solutions in the absence of a source [5, Sect. 3.3]. In the present case the "waves" in the semi-infinite layers, for which the reflection and transmission coefficients are defined, are not, in general, real transversely propagating waves. For bound modes the solutions are nearly pure real exponentials, though for complex modes the solutions will also have some components of transverse phase propagation. For the most general complex case it is still useful to consider the amplitudes of the two exponential solutions in the semi-infinite layers, and to define the ratios of these complex amplitudes as generalized reflection and transmission coefficients.

Rather than use the T-matrix, which contains terms in $1/Y_1$ or $1/Y_N$, a re-normalized form for the wave-transmission matrix will be used. This form, denoted by S, avoids the possible infinities in these terms, provides greater symmetry between the forward and backward transformations, and leads to characteristic functions of the same form as Eq. (4.7). In fact, it is found that the four elements of this matrix are the four possible characteristic equations for the different choices of inward or outward solutions in layers 1 and N.

Let the forward and reverse matrices S^+ and S^- be defined by

$$S^+ = \begin{bmatrix} Y_N & 1 \\ Y_N & -1 \end{bmatrix} \cdot C^+ \cdot \begin{bmatrix} 1 & 1 \\ Y_1 & -Y_1 \end{bmatrix} \equiv (2Y_N)[_N^T 1] \quad (4.8+)$$

$$S^- = \begin{bmatrix} Y_1 & 1 \\ Y_1 & -1 \end{bmatrix} \cdot C^- \cdot \begin{bmatrix} 1 & 1 \\ Y_N & -Y_N \end{bmatrix} \equiv (2Y_1) [{}_1 T_N] \quad (4.8-)$$

Using these (rather than the T-matrices of Sect. 2.5) the amplitude coefficients A_1 and A_N are related by

$$(2Y_N) \begin{bmatrix} A_N^+ \\ A_N^- \end{bmatrix} = S^+ \cdot \begin{bmatrix} A_1^+ \\ A_1^- \end{bmatrix}, \quad (4.9)$$

$$S^- \cdot \begin{bmatrix} A_N^+ \\ A_N^- \end{bmatrix} = (2Y_1) \begin{bmatrix} A_1^+ \\ A_1^- \end{bmatrix}.$$

The determinants are

$$\det S^+ = \det S^- = 4Y_1 Y_N,$$

so that S^+ and S^- are both singular at $\beta^2 = n_1^2$ and $\beta^2 = n_N^2$ ($\kappa_1 = 0$, or $\kappa_N = 0$). However, there is no need to consider their inverses. Thus S^+ and S^- are not inverses of each other; rather,

$$S^+ \cdot S^- \equiv S^- \cdot S^+ = (4Y_1 Y_N) I.$$

At the singular points, $Y_1 = 0$ or $Y_N = 0$, their product is zero, but both S^+ and S^- are finite and nonzero. The S-matrices may also be described as the finite parts of the ${}_N T_1$ or ${}_1 T_N$ matrices, with the poles at $Y_N = 0$ or $Y_1 = 0$ having been explicitly factored out.

It would be possible to normalize a wave transmission matrix to be non-singular and with unit determinant. This would be the same normalization required if the A-coefficients were to represent the square root of power, with the transverse Poynting power being $S_x = |A|^2$. To do so requires division or multiplication of the T, S, and A variables by $(Y_1)^{1/2}$ and $(Y_N)^{1/2}$, which requires a further branch specification and leaves all quantities being a function of the fourth-root of $(n^2 - \beta^2)$ in each of the outer layers. That is, now four branches and sixteen Riemann sheets for all field quantities as a function of β^2 . This normalization appears to offer no advantage over that used here, is more complicated, and is probably intolerable for numerical purposes. The normalization chosen leads to four simple expressions for the elements of both S^+ and S^- in terms of Y_1 , Y_N , and the elements of the overall C-matrices.

The elements of the S-matrices may be written explicitly, using the elements of C^+ say, as

$$\begin{aligned}
 S_{11}^+ &= (C_{11}Y_N + C_{12}Y_1Y_N + C_{21} + C_{22}Y_1) = +S_{22}^- \\
 S_{12}^+ &= (C_{11}Y_N - C_{12}Y_1Y_N + C_{21} - C_{22}Y_1) = -S_{12}^- \\
 S_{21}^+ &= (C_{11}Y_N + C_{12}Y_1Y_N - C_{21} - C_{22}Y_1) = -S_{21}^- \\
 S_{22}^+ &= (C_{11}Y_N - C_{12}Y_1Y_N - C_{21} + C_{22}Y_1) = +S_{11}^-
 \end{aligned} \tag{4.10}$$

The same four terms appear in each of the four elements of both S^+ and S^- ; only the signs of the terms differ. Any two elements differ by the simultaneous change of the signs of two terms, and all possible permutations of the sign changes (taken in pairs) are represented. If the signs of S_{21}^+ and S_{22}^+ were reversed in the above definitions, then the sign changes between the

four elements correspond precisely to changing the signs before Y_1 and Y_N separately. Thus these four elements of S^+ and S^- correspond to the four possible choices of inward and outward types of boundary conditions.

Note that the S_{22} element is precisely the same as $D(\beta^2)$ of Eq. (4.7), and the characteristic equation may be written as

$$S_{22}(\beta^2) \equiv D(\beta^2) = 0 .$$

That is, the eigenvalues are the zeros of S_{22} as a function of β^2 .

From the viewpoint of the transmission coefficients defined before we have $t^- \equiv 1/T_{22} = 2Y_N/S_{22}$; so the zeros of S_{22} are the poles of t^- . This fact may be described directly in terms of the A^\pm amplitudes. For some fixed branch specification, take A_1^+ and A_N^- to represent the inward (exciting) solutions, and set these to be zero. And assume the outward solutions (A_1^-, A_N^+) to be nonzero. Then from (4.9) we have

$$(2Y_N) \begin{bmatrix} A_N^+ \\ 0 \end{bmatrix} = S^+ \cdot \begin{bmatrix} 0 \\ A_1^- \end{bmatrix} ,$$

or

$$\begin{aligned} 2Y_N A_N^+ &= S_{12} A_1^- \\ 0 &= S_{22} A_1^- . \end{aligned}$$

For nonzero solutions to exist ($A_1^- \neq 0$) then requires that $S_{22} = 0$, the eigencondition.

Only one other element of S^+ is relevant to these solutions; it gives the ratio of the two amplitudes at the outer boundaries. $A_N^+/A_1^- = S_{12}/2Y_N$. (This

ratio remains finite even as $Y_N = 0$, because then also $S_{12} = S_{22} = 0$, as may be seen from the first two of Eqs. (4.10).)

The remarkable property of the S-matrix is that the other elements constitute the characteristic function for other choices of the boundary conditions. The S-matrix is a matrix of four possible characteristic functions, corresponding to the four Riemann sheets of the β^2 -plane.

If the conventional branch specification is used, for example, and complex modes leaky into layer 1 are now of interest, then in that layer $A_1^- = 0$ and $A_1^+ \neq 0$ for "inward" solutions (outward exponential growth). The relations (4.9) between the amplitudes become

$$(2Y_N) \begin{bmatrix} A_N^+ \\ 0 \end{bmatrix} = S^+ \cdot \begin{bmatrix} A_1^+ \\ 0 \end{bmatrix},$$

$$2Y_N A_N^+ = S_{11} A_1^+$$

$$0 = S_{21} A_1^+.$$

For nonzero solutions to exist ($A_1^+ \neq 0$) then the characteristic equation is now

$$S_{21}(\beta^2) = 0,$$

and the ratio of the amplitudes is given by $A_N^+/A_1^+ = S_{11}/2Y_N$.

The following table summarizes the four possible cases of the eigenvalue problem, each using one of the four elements of the S-matrix for the characteristic equation. The solutions are described with respect to the conventional branch specifications for κ_1 and κ_N . The array of four blocks corresponds to the four elements of S^+ , which in the first line constitute the

Layer N Layer 1	Inward Improper, Leaky Waves	Outward Proper, Bound Waves
Inward Improper, Leaky Waves	$S_{11}(\beta^2) = 0$ $A_1^- \equiv A_N^+ \equiv 0$ $A_1^+, A_N^- \neq 0$ $A_N^-/A_1^+ = S_{21}/2Y_N$ $= (C_{11} + C_{12}Y_1)$	$S_{12}(\beta^2) = 0$ $A_1^+ \equiv A_N^+ \equiv 0$ $A_1^-, A_N^- \neq 0$ $A_N^-/A_1^- = S_{22}/2Y_N$ $= (C_{11} - C_{12}Y_1)$
	$S_{21}(\beta^2) = 0$ $A_1^- \equiv A_N^- \equiv 0$ $A_1^+, A_N^+ \neq 0$ $A_N^+/A_1^+ = S_{11}/2Y_N$ $= (C_{11} + C_{12}Y_1)$	$S_{22}(\beta^2) = 0$ $A_1^+ \equiv A_N^- \equiv 0$ $A_1^-, A_N^+ \neq 0$ $A_N^+/A_1^- = S_{12}/2Y_N$ $= (C_{11} - C_{12}Y_1)$

Table 4.1 The four possible characteristic equations for inward and outward solutions in the semi-infinite layers. The first line is the characteristic equation in terms of the elements of matrix S^+ . The two columns correspond to the two possible choices for solutions in layer 1. The two rows correspond to the two possible choices in layer N.

characteristic equation. The next two lines show the conditions on the amplitudes, and the last two lines show the ratio of the nonzero amplitudes. Elements of C^+ appear in the last line. (Which implicitly assumes the characteristic equation is satisfied, and which could be written in a different form. For example, in the 2-2 case the ratio is $A_N^+/A_1^- = (C_{11} - C_{12}Y_1) = (C_{21} - C_{22}Y_1)/Y_N$; the second equality is simply a restatement of the characteristic equation.)

Representation of the characteristic equation in terms of the elements of the S matrix have proved very useful. It is convenient to program. From the C^+ matrix, calculated by the chain matrix multiplication, then S^+ is calculated by two additional matrix products, Eq. (4.8+). This may be done for any specification of principal branches for κ_1 and κ_2 . The choice of outward or inward solutions in each outer layer is easily controlled by two input parameters. These are used to select which element of S to be used as the characteristic function. With the added freedom provided by the nonconventional branch specifications (Sect. 3.3) there is complete flexibility in choosing the types of solutions to be represented by the characteristic equation.

4.3 As a Wronskian Determinant

Yet another viewpoint on the characteristic equation is possible. It offers further physical insight on the nature of the eigenfunction solutions, and has a direct relationship to the transverse resonance method.

We consider a specially constructed matrix solution of the differential equation. In contrast to fundamental matrix solutions, let each of the two columns now separately satisfy initial conditions at two different values of x . In particular, the two vector-solutions are taken to separately satisfy

the boundary condition at opposite ends of the interval. Thus, for any value of β^2 , let the vector solution $F^-(x)$ satisfy the boundary condition at x_0 , and let the vector $F^+(x)$ satisfy the boundary condition at x_N . For example, assuming outward solutions at each boundary, $F^-(x_0) = \text{col}[1, -Y_1]$ and $F^+(x_N) = \text{col}[1, +Y_N]$. (The superscript sign implies the outer boundary at which the boundary condition is used as an initial condition.) Starting at each respective boundary, by means of chain multiplication by the layer transition matrices, each solution may be propagated across the structure to the opposite boundary. But there, in general, each solution will not satisfy the other boundary condition. The two vector solutions F^+ and F^- may be adjoined to form a matrix solution

$$F(x) = [F^+(x), F^-(x)] ,$$

which is well defined everywhere in x ; and we consider its Wronskian determinant.

The Wronskian, $W[F(x)]$, is constant in x , and in general is nonzero. At either outer boundary, for most arbitrary β^2 , one or the other vector solution will not satisfy the required boundary condition; therefore the two columns are linearly independent there (and everywhere), neither one is an eigenfunction in x , and the Wronskian is not zero, $W[F(x)] \neq 0$. However, $W[F(x)]$ is a function of β^2 . For some particular values of β^2 each solution may come to satisfy the unfulfilled boundary condition (which, by definition, is already satisfied by the other solution), and the two solutions would then become proportional, and $W[F(x)]$ becomes zero. Conversely, at those values of β^2 for which $W[F(x)] = 0$, then the two solutions are necessarily linearly dependent (proportional); they must both satisfy the two boundary conditions, and are both the same eigenfunction. Therefore, one representation for the

characteristic function is simply the Wronskian determinant of this specially constructed matrix solution. The characteristic equation is

$$D(\beta^2) = W[F^+(x), F^-(x)] = \det \begin{bmatrix} F_y^+ & F_y^- \\ F_z^+ & F_z^- \end{bmatrix} = 0 ,$$

or

$$D(\beta^2) = F_y^+ F_z^- - F_y^- F_z^+ = 0 , \quad (4.11)$$

at any x.

To evaluate $D(\beta^2)$ for any β^2 , the two solutions F^+ and F^- need not be generated for all x , only from the outer boundaries x_0 and x_N inward toward some common position, x , at which the determinant is to be calculated. Most commonly F^- is calculated forward to x_N , at which F^+ has just its starting value. Just as easily F^+ may be calculated backwards toward x_0 , at which the characteristic equation may be defined. More generally F^- may be calculated forward from x_0 , and F^+ backward from x_N , to whatever common intermediate x may be chosen, conveniently at a boundary. The same number of matrix multiplications is needed in any case. It should also be noted that only a single vector solution is being calculated across the layers, not a matrix solution as in the previous representations. The complete matrix $F(x)$ here is calculated only at the common interior boundary. However, if the full matrix were calculated, the Wronskian may be evaluated at all interior boundaries and these could serve as a numerical check. Even further, for numerical purpose it is possible to define the characteristic equation as the average of $D(\beta^2) = W[F^+, F^-]$ over all the interior boundaries at which it may be calculated.

For the four possible choices of boundary conditions, four different Wronskian determinants are defined. It is possible to display these four determinants as a 2×2 matrix, and in fact will be entirely equivalent to the S-matrix. If the determinants are evaluated at some interior point, then this will be equivalent to evaluating the S-matrix at the interior point. For example, in Eq. (4.8+) C^+ can be partitioned at some interior boundary x_ℓ , $C^+ = {}_N C_\ell \cdot {}_\ell C_1$. The product of the first factor in (4.8+) and ${}_N C_\ell$ can be evaluated numerically, separately from the product of ${}_\ell C_1$ and the last factor. The rows of the first product (transposed to column vectors) will constitute the solutions transformed backward from x_N to x_ℓ , and the columns of the second product will constitute the solutions transformed from x_0 to x_ℓ . The product of these two separate factors will then complete the evaluation of S^+ in (4.8+), and can be shown to constitute just the four Wronskian determinants between the two sets of solutions.

The following somewhat more physical viewpoint is also possible for the eigenmode problem. As for the modes of the continuous spectrum, and for modes arising from plane-wave excitation in Sect. 3.5, two linearly independent field solutions defined as above exist for nearly all values of β^2 . As β^2 is varied though (by changing the form of excitation say), it is found that values of β^2 exist at which these two solutions degenerate to the same solution, an eigenmode. As an eigenvalue of β^2 is approached, less and less excitation is required to maintain the same normalized amplitude within the structure; and the two types of excitations, corresponding to the two separate boundary conditions, give rise to solutions which are less and less distinguishable. This is a resonance situation, where a large response is determined more and more by the properties of the system, rather than by the form of the excitation. In the limit of an eigenvalue, the two vanishing excitations produce the same

nonzero and finite field solution. (Of course the excitations referred to may not be physically realizable. Also, for an eigenvalue β^2 , a second linearly independent solution must still exist. It is only the two solutions generated as prescribed that do not remain independent.)

4.4 Relationship to Transverse Resonance Method

The characteristic equation for the transverse resonance method is most directly related to the form just described. Equation (4.11), at any x , may be written as

$$F_y^+ F_z^- = F_y^- F_z^+ . \quad (4.12)$$

If neither F_y^+ nor F_y^- are zero, then the equation may be divided by their product to give for the characteristic equation

$$\vec{Y} \equiv \frac{F_z^+}{F_y^+} = \frac{F_z^-}{F_y^-} \equiv -\overleftarrow{Y} . \quad (4.13)$$

The definitions of \overleftarrow{Y} and \vec{Y} follow from the construction of F^\pm in the previous section. Since F^+ consists of only an outward solution at x_N , it corresponds, at any other x , to the fields when "looking" toward positive x . Likewise, F^- consists of only an outward solution at x_0 , and at any interior x it corresponds to the fields when "looking" toward negative x . The negative sign for \overleftarrow{Y} is necessary for the proper directional sense for the wave admittance. Therefore, the characteristic equation may be written in the familiar form [2, p. 108; 5, p. 215].

$$\overleftarrow{Y} \equiv \vec{Y} + \overleftarrow{Y} = 0 ;$$

where all Y are understood to be a function of β^2 , and also depend on the

choice of x .

That F_y^+ and F_y^- not be zero for the division leading to Eq. (4.12) is very important. By accident of choice of x , close to a node of an eigenfunction, it would be possible for the F_y to be near zero. At worst, this could lead to fatal numerical overflow, and at best there could be considerable loss of significant digits, as the characteristic equation may become indeterminate in the form of $(\infty - \infty)$ at the eigenvalue. Also, it is difficult to set up a reasonable convergence criteria when the two terms in the equation can be arbitrarily large or small.

But most importantly, and regardless of the choice of x , there will always exist values of β^2 for which F_y^+ and F_y^- will in fact become zero. These zeros of $F_y^+(\beta^2)$ and $F_y^-(\beta^2)$ will nearly always be independent of each other and will depend on x . At a zero for either one, the respective \vec{Y} or \vec{Y} will become infinite; as will the characteristic function $\vec{Y}(x, \beta^2)$, which thus must be considered a function of x . In lossless structures, for example, a real β^2 greater than n_1^2 and n_N^2 will lead to real oscillatory functions of x within any layers of large n^2 . At a fixed x , and with changing β^2 , these zeros will move past the point of x . Also, the conditions for which $F_y^+ = 0$ and $F_y^- = 0$ may be interpreted as a new boundary condition imposed at x , with the structure remaining unchanged on either side. The structure may then be viewed as having been partitioned into two separate and isolated structures, each with its own set of eigenvalues in the β^2 -plane. That is, the zeros at $F_y^+(\beta^2) = 0$, and of $F_y^-(\beta^2) = 0$, correspond to the roots of the equations $1/\vec{Y}(x, \beta^2) = 0$ and $1/\vec{Y}(x, \beta^2) = 0$; which are the characteristic equations for the two partial structures. Unless the structure is symmetric, and x is the midplane, the two sets of roots will be unrelated. It is likely that the two sets of roots together will about equal the number of eigenvalues for the whole structure. In

the general direction of the negative imaginary axis of β^2 , for example, there will be an infinite number of poles for \overleftrightarrow{Y} .

We emphasize then that the traditional characteristic function for the well known transverse resonance method,

$$\overleftrightarrow{Y}(x, \beta^2) = \overleftarrow{Y}(x, \beta^2) + \overrightarrow{Y}(x, \beta^2) ,$$

has poles in the complex plane of the eigenvalue parameter, β^2 (or β). Although the roots of the equation $\overleftrightarrow{Y} = 0$ do not depend on the location x at which the function is defined, the function itself and the location of the poles do depend directly on x . It is conjectured that the poles and zeros exist in about equal numbers and are probably interspersed. In the exceptional case of x at a node of F_y for some eigenmode, then the root β^2 and the β^2 for two poles, with opposite sign, will coalesce. The two poles cancel, leaving the characteristic equation in the numerically indeterminate form just mentioned, $(\infty - \infty) = 0$.

This lack of analyticity of $\overleftrightarrow{Y}(\beta^2)$ does not appear to have been recognized in the literature before. It is very important to the problem of complex root searching in β^2 , whatever method is used. It is sufficient reason to avoid the use of the transverse resonance form of the characteristic equation for numerical applications. The problems of dealing with $\overleftrightarrow{Y}(x, \beta^2)$ correspond to the problems of using $Y(x)$ as a field variable as discussed in Sect. 2.7.

Actually, Eq. (4.11) can still be considered as a transverse resonance condition, but stated in terms of an analytic function of β^2 and independent of x . The transformation of $D(\beta^2)$ to $\overleftrightarrow{Y}(x, \beta^2)$, through multiplication by $1/F_y^+ F_y^-$, is another example of undesirable transformations of characteristic functions mentioned in Sect. 1.2. The concept of transverse resonance condition can be retained if F_y^- , F_z^- and F_y^+ , F_z^+ (rather than \overleftarrow{Y} and \overrightarrow{Y}) are taken to

be the quantities observed when "looking" in the negative and positive directions at x . That is, with the structure separated at x , these are the fields observed when a test "wave" is incident in the two directions at the opened plane x .

4.5 Explicit Expressions for the Characteristic Equation

For the 2-layer structure there is only a single interface, $x_0 \equiv x_N$, and C^+ is the unit matrix. The characteristic equation (4.7 or 4.11) reduces to simply

$$Y_1 + Y_N = 0 .$$

(just as for the transverse resonance form).

For the TE modes in dielectric layers, with $\mu = 1$ in both, the equation becomes

$$\kappa_1 \equiv (n_1^2 - \beta^2)^{1/2} = -(n_2^2 - \beta^2)^{1/2} \equiv -\kappa_2$$

Because of the negative sign, there clearly can be no solution if the principal branches for κ_1 and κ_2 are chosen in the same way. The two sides of the equation can have the same sign only if the opposite choice for principal branch, or assumption of an inward solution, is made for one layer. Then a solution exists only for $n_1^2 = n_2^2$, and is any value of β . That is, the trivial case of no dielectric discontinuity, and a wave propagating through at any angle.

For the TM modes the characteristic equation becomes (with $\mu = 1$)

$$\frac{\kappa_1}{\epsilon_1} \equiv \frac{(\epsilon_1 - \beta^2)^{1/2}}{\epsilon_1} = \frac{-(\epsilon_2 - \beta^2)^{1/2}}{\epsilon_2} = \frac{-\kappa_2}{\epsilon_2},$$

since $\epsilon \equiv n^2$. Now, if either ϵ_1 or ϵ_2 are negative, solutions can exist even when the same principal branch specification is used for both κ_1 and κ_2 . The solution for β^2 is given by

$$\beta^2 = (1/\epsilon_1 + 1/\epsilon_2)^{-1}$$

If ϵ_2 is taken as negative (a metal) and $\epsilon_2 < -\epsilon_1$, then β^2 is positive for real propagating waves; $\epsilon_1 \leq \beta^2 \leq -\epsilon_2$ and $n_1 \leq \beta \leq -in_2$; and both κ_1 and κ_2 are pure positive imaginary. If ϵ_1 and ϵ_2 are complex then more careful consideration of the real and imaginary parts of the characteristic equation is needed.

For the very familiar 3-layer structure the C-matrix is just that for the single central layer. With $C_{11} \equiv C_{22} = \cos \theta_2$, and $C_{12} = (i/Y_2) \sin \theta_2$, $C_{21} = (iY_2) \sin \theta_2$, the characteristic equation becomes

$$(Y_1 Y_3 / Y_2 + Y_2) \sin \theta_2 + i (Y_1 + Y_3) \cos \theta_2 = 0; \quad (4.14)$$

where all quantities are functions of β^2 through the respective κ_ℓ . For real bound modes in lossless materials, Y_1 and Y_3 are pure imaginary and the equation is pure real. The equation depends on the choice of branch for κ_1 and κ_N ; but it is an even function of κ_2 (through Y_2 and θ_2), so it does not depend on the choice of branch for κ_2 . This equation is in a rather unfamiliar form, but for use with a general root search algorithm it has significant numerical advantages over the form listed in Fig. 1.2.

The familiar form for the characteristic equation is obtained by dividing through by $\cos \theta_2$ and by the first factor on the left,

$$\tan \theta_2 = - \frac{i(Y_1 + Y_3)}{Y_2 + Y_1 Y_3 / Y_2} = \tan (\phi_1 + \phi_3) ;$$

with

$$\phi_1 = \text{Tan}^{-1}(Y_2/iY_1), \quad \phi_3 = \text{Tan}^{-1}(Y_2/iY_3) ,$$

and the principal branch for complex Tan^{-1} is implied. Taking the Arc-tangent of both sides and assuming the m th branch for θ_2 , yields the final form (all on the left side)

$$f(\beta^2) = \theta_2 - \pi m - \phi_1 - \phi_2 = 0 .$$

Recall that $\theta \equiv \kappa_2 k_0 t_2$; this is just the phase integral over the one thickness t_2 .

The great advantage of this familiar form is that it allows a physical interpretation of the terms in the equation: phase shifts at the boundaries, ϕ_1, ϕ_2 ; total phase propagation across the layer θ_2 ; all to add to an integral multiple of π . Perhaps best of all it permits a specification of the mode number, m , as part of the eigenvalue equation. The root research can be carried out for a specific mode. For no other form of the equation, nor for any structure of more than three layers, can this apparently be done without rather restrictive assumptions.

For the fully complex case, when a root search procedure may range freely over the complex β^2 plane, the familiar form has several disadvantages -- additional singularities have been introduced. For a given m , the equation now depends on the sign of κ_2 ; $f(\beta^2)$ then has a branch point and cut associated with the definition of κ_2 . Only by also reversing the sign of m whenever the sign of κ_2 changes, or when the branch cut is crossed, can this

problem be fully avoided. The Arctan definitions for ϕ_1 and ϕ_2 introduce additional branch points and cuts, though these may not be in a region of the β^2 -plane which is important. (The branch points of Arctan z are at $z = \pm i$, and the branch cuts are normally taken outward along the imaginary axis.) Nevertheless, any singularities in the near β^2 -plane can significantly slow down the rate of convergence of any complex root searching procedure which is based on a low order approximation to the characteristic function. For these reasons the familiar expression of Fig. 1.2 and the above is not as desirable in the fully complex case as is the form of Eqs. (4.7) and (4.14).

The four-layer structure has two finite interior layers. Using the transformation matrices for these layers, the characteristic matrix Q is conveniently defined at the central boundary, x_2 , in the form of Eqs. (4.3) and (4.5c).

$$Q(\beta^2) = B_1 \cdot C_2^{-1} + B_4 \cdot C_3 ,$$

where B_1 and B_4 are the boundary condition matrices at $x_0 \equiv x_1$ and at $x_3 \equiv x_4$. Then

$$\begin{aligned} Q(\beta^2) &= \begin{bmatrix} Y_1 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} c_2 & -(i/Y_2)s_2 \\ -(iY_2)s_2 & c_2 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ Y_4 & -1 \end{bmatrix} \begin{bmatrix} c_3 & (i/Y_3)s_3 \\ (iY_3)s_3 & c_3 \end{bmatrix} \\ &= \begin{bmatrix} [Y_1 c_2 - (iY_2)s_2] [-Y_1 (i/Y_2)s_2 + c_2] \\ [Y_4 c_3 - (iY_3)s_3] [+Y_4 (i/Y_3)s_3 - c_3] \end{bmatrix} , \end{aligned}$$

where for compactness $c_\ell \equiv \cos \theta_\ell$, and $s_\ell \equiv \sin \theta_\ell$, $\ell = 2, 3$, have been used.

The characteristic equation becomes, with some collecting of terms,

$$\begin{aligned}
D(\beta^2) = & [Y_2/Y_3]Y_4 + (Y_1/Y_2)Y_3] s_2 s_3 \\
& - (Y_1 + Y_4) c_2 c_3 \\
& + i[(Y_1/Y_2)Y_4 + Y_2] s_2 c_3 \\
& + i[(Y_1/Y_3)Y_4 + Y_3] c_2 s_3 = 0 .
\end{aligned} \tag{4.13}$$

Many different forms for this equation can be obtained by collecting the terms in different ways, and also by using trigonometric identities to convert the various products of sines and cosines into functions of the sums and differences, $\theta_2 \pm \theta_3$. Further, the $\sin \theta$ and $\cos \theta$ factors can be converted to complex exponentials in θ_2 and θ_3 . The resulting expressions will be similar to those obtained by assuming exponential solutions in each layer as done by Harris [83] and Ward [54]. The expression here does not have the extraneous singularities and zeros which are present in their characteristic equation. It is not clear which form is most convenient. Only by making some a priori assumptions about one or the other inner layer being the guide layer, or being evanescent or cut-off, can Eq. (4.13) be manipulated into a form resembling the familiar 3-layer equation (e.g. to permit physical interpretation of some of the terms). Taking all layers on an equal basis, with no a priori assumption about which indices n_ℓ are high or low, then Eq. (4.13) appears more direct, simpler, and more useful than any extensions of the 3-layer expressions. It has few enough terms that it could be calculated explicitly (i.e., without 2x2 matrix multiplications, which may still use fewer arithmetic operations).

The explicit expressions given here show the relationship to other forms of the characteristic equation, and give some insight to the analytic properties. For more than four layers there appears to be little purpose in

writing out explicit forms. With increasing N the number of terms increase as 2^N , and the number of factors in each term increases as N . Clearly, say for N more than five or six, the number of operations necessary to calculate an explicit expression for $D(\beta^2)$ becomes prohibitive. Also, the programming logic required to sequence through all the permutations of the factors in the terms can be rather intricate.

The chain matrix multiplication method (or some equivalent recursive method) provides the only practicable way to evaluate the characteristic function for structure of more than a few layers. The number of calculation operations increase only linearly with N , and the programming required to implement it is transparently simple. It is well known in numerical mathematics that recursive function definitions and calculations can be very efficient and compact.

4.6 Discussion

The characteristic functions described from the different viewpoints are all entirely equivalent, apart from normalization of individual terms leading to the final value. Analytically they are the same function, defined in the β^2 -plane, and have as singularities only the branch points and cuts indicated in Fig. 3.5. Elsewhere in the plane, $D(\beta^2)$ is analytic, on four Riemann sheets, with simple isolated roots. (Except for rare particular combinations of parameters when two roots may coalesce.) There are no poles in the finite part of the plane, and no zeros which are not eigenvalues for the system. As evident in Figs. 3.3 and 3.5, if $D(\beta^2)$ is considered to be a function of β , then there are twice as many branch points, branch cuts, and zeros in the β -plane as there are in the β^2 -plane. It is suggested that this $D(\beta^2)$ has optimum analytic properties, and could be adopted as a standard

representation for the characteristic function for the layered structure. Any further transformations of $D(\beta^2)$ can only degrade its analytic properties.

For numerical purposes there can be some differences in convenience and accuracy when $D(\beta^2)$ is calculated in different ways. The simplest method appears to be to first calculate C^+ : by indexing through the layers 2 to N, calculating the layer parameters, each layer matrix, and accumulating the product to obtain C^+ at the end. Then $D(\beta^2)$ is evaluated according to Eqs. (4.7) for outward solution boundary conditions. Or the S^+ -matrix for the four possible boundary conditions may be calculated according to Eqs. (4.8+) or (4.10). Calculation of S^+ involves only a few more multiplications, and provides some additional information about the magnitude of $D(\beta^2)$ away from its roots. This calculation has been programmed, and it works very well except in the indeterminate situations described below.

$D(\beta^2)$ can effectively be evaluated at any x , as indicated in Eqs. (4.3), (4.5c) or (4.11). The difference is one of normalization. The use of the C^+ or S^+ matrix corresponds to a normalization of $F_y = 1$ at either x_0 or x_N , and evaluation of $D(\beta^2)$ at the other. At any intermediate x , however, the fields can be much smaller or greater than the nominal unit magnitudes at the boundaries. A strongly guided mode may have fields at the center of the guide which are much greater, say 10^3 , than at the outer boundaries. Then the terms making up $D(\beta^2)$, when evaluated at an interior x as in Eq. 4.11 (or Eq. 4.3), will be 10^6 larger than if evaluated at the outer boundaries. A significant difference in round off error can result. As evident in Eq. (4.11), $D(\beta^2)$ actually has the dimensions of the product of fields. Hence, with any renormalization of the fields, or as the fields vary with x , the individual terms in D will vary as the square of the fields.

An alternative, to the implied unit normalization of the fields at the outer boundaries, is to assume nominally unit fields at some interior boundary, x_ℓ . This could be an extra boundary, introduced for this purpose, at the center of a guiding layer. (That is, with no actual material discontinuity at x_ℓ .) A unit matrix at x_ℓ may be transformed to the outer boundaries at x_1 and x_N by the partial matrices ${}_1C_\ell$ and ${}_NC_\ell$. These two then are actually a fundamental matrix solution, $F(x)$, evaluated at the end points. $F(x_1) = {}_1C_\ell$, and $F(x_N) = {}_NC_\ell$, and these may be used as in Eqs. (4.3) and (4.5c) to calculate $D(\beta^2)$. The corresponding calculation for all the elements of S^+ at an interior boundary can also be done, as sketched in Sect. 4.3.

The only difference in these methods for calculating D is in the magnitudes of the numbers involved. All matrix multiplications involve sums and differences of products of terms. And the order in which the sums and differences of terms are calculated can greatly affect the round off error and numerical stability in difficult cases. A capability to evaluate D at any boundary would be very helpful in solving difficult problems. If round off error was suspected, the accuracy of the result could be checked by solving the problem with D evaluated at two or more of the boundaries. When evaluation at only one end of the structure is provided, then a simple test is to rerun the case with the order of the layers reversed.

The nominal magnitude of $D(\beta^2)$ away from or between roots is very important to the numerical solution of the characteristic equation. For, in practice, the characteristic equation is not $D(\beta^2) = 0$, but rather that $D(\beta^2) \leq \epsilon$, where ϵ is a small quantity used as convergence criteria. It is then important whether, between roots, D is on the order of 10^4 or 10^{-4} , say. In the first case the convergence test may be very difficult to satisfy, but

in the second case it may be too easily satisfied by poor values of β^2 . It would be desirable to use a convergence test which is relative to some representative magnitude for D . The above criteria is an absolute test; that D be small compared to unity.

One attempt was made to define a normalized characteristic function. The final value of D results from the sums and differences of four terms, as evident in Eqs. (4.7) and (4.10). It can be shown that the sums of the squared magnitudes of the four terms is the same as the sum of squared magnitudes of the four elements of the S matrix. (A consequence of $\text{Det } C = 1$.) It is natural to normalize (divide) D by this r.m.s. magnitude. The best solution that can then be expected is that D be zero in comparison to the average magnitude of the four terms; that the renormalized D be zero compared to unity. This is equivalent to finding, for the chosen set of boundary conditions (one element of S), that D is zero in comparison to the other elements of S (for the other possible boundary conditions). The renormalized D was found to be unusable for root searching, because many more iterations were needed for convergence. This is attributable to the fact that the normalizing factor is not anywhere an analytic function of β^2 . (Since $|f(z)|^2$ and $|f(z)|$ are nowhere analytic functions of z .)

An alternative to renormalizing $D(\beta^2)$ is to incorporate the normalizing factor into the convergence criteria as noted in Sect. 5.4. But this has not been done.

Regardless of the care in calculating $D(\beta^2)$, there easily exist layered structures and modes for which the eigenvalue problem is indeterminate. These cases arise when there is one (or more) relatively thick layer, within which κ has a large imaginary part. This occurs for modes with β^2 large compared to n^2 in the layer. Such layers may be referred to as evanescent or exponential layers, because the fields vary as real exponentials. If the

layer is thick, then the fields can change by many powers of ten from one part of the structure to the other. The matrix C^+ for the structure then becomes nearly singular and the problem is indeterminate. This may be seen by letting $t = -i\theta$ be large and real, for a thick exponential layer. Then the diagonal elements of C for the layer (and the structure) take the form of $\cosh t$, and the off-diagonal terms will be $\sinh t$. For large t these are nearly equal and very large. The determinant for C becomes $\det C = \cosh^2 t - \sinh^2 t$. Although mathematically this is unity, it is calculated as the difference between two large numbers. If $t \approx 10$, for example, then each term is about 10^8 ; and if using an 8 digit floating point number, all significant digits are lost in calculating $\det C$.

For numerical purposes the matrix C^+ for the structure is then nearly singular, and the problem is indeterminate, regardless of the method for calculating D . All representations for $D(\beta^2)$ suffer the same problem, D will retain few if any significant digits.

Physically, the indeterminate cases correspond to an overall physical system composed of noninteracting subsystems. Consider, for example, two guiding layers separated by a thick exponential layer. In either guide, modes may then propagate nearly independently, with little effect due to the presence of the other guide. For the complete structure, the eigenvalue problem is then poorly defined. Any linear combination of the modes in the individual guides would, within some numerical criteria, satisfy the eigenconditions equally well. Another viewpoint is that in the thick exponential layer the fields of the guides can approach zero. There the differential equation and the (homogeneous) boundary-matching condition could be well satisfied numerically by the near zero fields.

A similar indeterminate case arises if a thick exponential layer separates a guiding layer from either of the outer boundaries which define the overall structure. For example, in Fig. 2.1, the boundaries x_0 or x_N for the outer boundary conditions may be moved far out from x_1 and x_{N-1} . Or the layers 2 and $N-1$ may be thick and exponential, on either side of a strongly guiding region. Then, for large β^2 , the fields can become essentially zero at the outer boundaries, and the (homogeneous) outer boundary condition are well satisfied. When the fields go to zero, there is no distinction between inward and outward solutions. The present eigenvalue problem can be described as that for a physical system (the interior structure) interacting with its environment (the semi-infinite layers). When the physical system is isolated from its environment the eigenvalue problem becomes indeterminate.

Usually a case will be indeterminate only for lower order modes of a structure; for β^2 much larger than the smallest n^2 in the structure. For sufficiently higher order modes β^2 becomes smaller and more comparable to the smallest n^2 , and the problem becomes better defined.

Problems of numerical indeterminacy can be recognized by the following symptoms. These are all relative to the resolution of the floating point representation used for calculations. The imaginary part of the phase integral is large, say on the order of 5 to 10. The elements of the C^+ matrix for the structure are large compared to unity. For example, using 8 digit numbers, if the product of the diagonal elements of C , and the product of the off-diagonal elements, are on the order of 10^8 then complete loss of significant digits can be expected in calculating $D(\beta^2)$. The same symptoms are recognized by examining the determinant of C , which should be unity. If $\det C = 1$ only to a few significant digits, then this is all the accuracy which can be expected in the calculation of $D(\beta^2)$. And the eigenvalue equa-

tion $D = 0$ can be solved only to this accuracy. These quantities should always be available for examination in troublesome cases. Often the problem can be attributed to the phase thickness and C matrix of one particular layer. Finally, for a poorly converged root, an indeterminacy of the second kind is evidenced by two elements of S^+ being small at once.

There appears to be no way to incorporate the mode index into the definition of the characteristic equation. That is, for the general structure, it is not possible to define the characteristic equation and solve it for a mode of some given index, m , specified ahead of time. When sets of several modes are being solved for, it is very useful to order them on the basis of the real part of the phase integral and on the magnitude of β^2 . This is possible for bound modes when β^2 is mostly real. When the complex root search misses finding one mode, it can often be readily noticed by a gap in the ordered modes which are found. In the vicinity of cut-off, as roots pass near the branch point at n_1^2 or n_N^2 , and move onto other sheets of β^2 and branches of κ_1 and κ_N (with changing frequency or other parameters), modes can be uniquely identified only by tracing their locus in the complex planes [86]. This is illustrated by the TE_2 mode in a four layer structure in Fig. (7.2).

An ineffective effort was made to incorporate the mode index, as defined from the phase integral, into a modified characteristic function. This was done by multiplication of $D(\beta^2)$ by a weighting function, which is proportional to the squared difference between the phase integral and the intended mode index. The intention was to bias the root search toward the zero for the intended mode, by making the modified D much larger in the vicinity of other modes. This method is again suspect because such a weighting function is not an analytic function of β^2 . Limited trials showed

that there was little effect on which roots were found, and two to three times as many iterations were needed. The slowed convergence rate is attributed to the non-analyticity of the modified D.

5. COMPLEX ROOT SEARCH; MULLER-TRAUB METHOD

Given a constructive definition of the characteristic function $D(\beta^2)$, the roots can be found only by direct numerical methods. Even for the three-layer case the function is transcendental, and for more than three layers or for complex parameters it is not possible to use graphical methods.

The choice of root searching method is dominated by two properties of $D(\beta^2)$. Firstly, it is expensive to calculate; the number of steps in evaluating D , for each value of β^2 , far exceeds the number of steps in calculating any iterative formulas. Each calculation of D requires evaluation of complex square roots, sines, and cosines for all layers, and N multiplications of 2×2 matrices. Secondly, there is no feasible way to calculate the derivative of D . Therefore, it is not possible to use the well known Newton's method with its rapid convergence properties. The dependence of D on β^2 is embedded in all the $\kappa(\beta^2)$ for all layers, and thereby in all the Y_x , $\sin \theta$, and $\cos \theta$ for all layers, and the derivative requires an N -fold matrix product for each of N terms. An analytic expression for the derivative is impossible. Any derivative information needed must be obtained by numerical approximation. Of less importance, but of some benefit, is that the roots of D are nearly always isolated, so there is no problem with multiple roots. Also there is considerable knowledge of where useful roots are expected to be found; namely, in the range of β^2 between zero and the largest value of n^2 for the structure, and of imaginary part somewhat smaller than n^2 . The presence of two branch points and cuts in the β^2 -plane, and an infinite row of roots in the direction of the negative real axis, is significant but unavoidable.

Under the circumstances the choice of possible methods is very limited, but one of these works exceptionally well. It is an iterative procedure originally proposed by Muller for use on the real line [90], but which in

fact is most naturally applied in the complex plane [91, 92]. It depends on a quadratic approximation to the function, based on three points near the root; a root of the quadratic is then used as the next best estimate of the true root, and the process is repeated iteratively. Traub [91, p. 154] describes it as an iteration formula with memory, since the previous three points are saved at each iteration. These points effectively provide derivative information without additional expensive function evaluation. Traub also showed that the iteration formulas used by Muller could be simplified by about half, being more economical and also reducing the possibility of loss of significant digits. Hence it is also called the Muller-Traub method. The order of convergence is 1.84, nearly as good as the order 2.0, or quadratic, convergence rate for Newton's method [91, p. 211].

Only one subroutine for Muller's method appears to have been published; it is an ALGOL program [93, 94]. Two Fortran subroutines are known which are parts of proprietary software libraries. One of these was known to be inefficient, requiring twice as many function evaluations as should have been needed, and the second was not initially available. Hence a Fortran subroutine was written to implement a complex root search using Muller's method. Several novel features were incorporated, two of which greatly improve the efficiency of the search. Other features permit much greater control of the root searching process than is available in the published or proprietary subroutines.

The next sections summarize the iteration formulas, the generation of initial guesses and initial iterates, and the convergence criteria used.

5.1 Iteration Formulas

Let a complex function be $f(z)$ (the characteristic function), whose roots are sought in a complex z -plane. And let $z = a, b, c$ be three values of z which are in the neighborhood of a root. At these points let f_a, f_b , and f_c be the values of the function. Assume that the point c is the best approximation to a root (c is closer to the root than is a or b , and $|f_c|$ is smallest), and let the quadratic approximation to $f(z)$ be taken about c :

$$F(z) = A(z-c)^2 + B(z-c) + C .$$

The coefficients are determined by requiring that $F(z) = f(z)$ at the three points $z = a, b, c$. The root of $F(z)$ nearest to c is then assumed to be the next best approximation to the root of $f(z)$.

In terms of a standard notation for divided differences [91], $f[a,b] \equiv (f_a - f_b)/(a-b)$, which is the slope of $f(z)$ between any two points a and b , the coefficients of $F(z)$ are given by:

$$\begin{aligned} A &= \frac{f[a,c] - f[b,c]}{(a-b)} \equiv \frac{f[a,b] - f[a,c]}{(b-c)} \\ &= \frac{f[a,b] - f[b,c]}{(a-c)} \equiv f[a,b,c] . \end{aligned}$$

The last term is the standard notation for the second divided difference. A is an estimate of half the second derivative of $f(z)$ at the point c . With the value of A calculated, then B is given by

$$\begin{aligned} B &= f[b,c] - (b-c)A = f[a,c] - (a-c)A \\ &\equiv f[b,c] - f[a,b] + f[a,c] . \end{aligned}$$

B is an estimate of the first derivative of $f(z)$ at $z = c$. It may be viewed as the approximate derivatives $f[b,c]$, or $f[a,c]$, but with a correction for

the effect of the second derivative. The coefficient C is simply

$$C \equiv f_c ,$$

the function itself at $z = c$. C is a measure of the discrepancy by which $f(z)$ is not zero-- c is not at the root. The correction to $z = c$, to reach the true root, may be expected to be proportional to C .

With values for A , B , and C , the roots of the polynomial $F(z)$ are

$$z_o = c + \delta, \quad \text{with}$$

$$\delta \equiv \frac{+B \pm \sqrt{B^2 - 4AC}}{2A} \equiv \frac{-2C}{-B \pm \sqrt{B^2 - 4AC}} .$$

The correction term, δ , especially in the second form, resembles the well known correction term $-f/f'$ of Newton's method. It is proportional to $f(z)$, and the denominator is an approximation to $2f'$. All quantities are complex.

The root z_o which lies closest to c is obtained by choosing the sign to make the magnitude of δ smallest. This is preferably done by using the second form, and choosing the sign which makes the magnitude of the denominator largest. The alternative is a sign choice to make the numerator of the first form smallest. This is certain to lead to problems of round off error, especially near convergence when the numerator must go to zero.

With z_o as a new approximation to the root for $f(z)$, the list of iterates is updated: a is discarded and replaced by b , b is replaced by c , and c is replaced by z_o . The associated values of f are updated, $f(z_o)$ being newly calculated to replace f_c . That is, a single function evaluation is needed for each iteration, and the two previous function values are saved. Then, subject to convergence tests and iteration limits, the iteration process is

repeated. This description is of the search for a single root, and it proceeds to rapid convergence if the initial iterates are within the neighborhood of a single root.

By a neighborhood it is meant that the distances between each iterate and the true root, and the distances between the iterates themselves, are all small compared to the distance to any other roots. Only if this is true will the rapid convergence rate of 1.84 be realized. Actually, because of the quadratic approximation, Muller's method accepts the presence of two true roots within the neighborhood of the iterates. What usually happens is that during the early stages the iterations improve slowly and erratically. This happens when the three iterates are relatively widely spaced, and within range of three or more roots. Then the quadratic approximation $F(z)$ may have little resemblance to $f(z)$, and there is no assurance that each iteration will reduce the magnitude of $f(z)$. Then in a final stage, as a single root is isolated, the convergence rate becomes very rapid, the number of significant digits nearly doubling with each iteration. Therefore the number and spacing of all roots in a region to be searched, and where the search is started, can greatly affect the rate at which roots can be calculated. Fortunately, some of the zeros of the function $f(z)$ may be removed, some exactly and others approximately, to give a modified function; for which the iteration process is much more efficient.

5.2 The Reduced Function

Any known roots of $f(z)$ can effectively be removed through division by a polynomial having those same roots. A polynomial denominator $P(z)$ is thus formed as

$$P(z) = \prod_m (z - z_m) ,$$

where the product is over a set $\{z_m\}$ of some known roots. The reduced function $g(z)$ is then defined as

$$g(z) = f(z)/P(z) .$$

The known roots may be said to have been divided out. Or $f(z)$ may be considered to have been multiplied by a function having poles at the location of some of its zeros, thereby cancelling them.

The iteration procedure then is actually carried out using $g(z)$ rather than $f(z)$. As each successive zero is found it is included in the set for $P(z)$. The reduction (or sometimes called deflation) of $f(z)$ to $g(z)$ is essential to avoid repeatedly calculating the same root; and it also makes $g(z)$ simpler, and the quadratic approximation more valid, for the remaining roots. For these reasons, roots are most efficiently found in sets, of say several to 10 at a time. For a large number of roots the procedure often appears to become slower, and increasingly difficult to obtain accurate convergence for the latter roots. All known implementations of Muller's method provide for finding roots in sets of several at a time, using a reduced function.

It can also be very useful, in the reduction of $f(z)$ and $g(z)$, to include poles which do not correspond exactly to zeros of $f(z)$. First, if the pole is approximately correct, then approximate pole-zero cancellation can still be very effective. At distances which are large compared to the pole-zero separation, the pair will be invisible to the search for other roots. Thus, even when convergence is not obtained, the last iterate might be reasonably close to a root, and should be included in the reduced function.

But it can also be useful to include poles which are only poor approximations to a root; or even sometimes to include a pole not related to a root, for the purposes of influencing the course of the iteration process. This use has not apparently been suggested in the literature; only the use of previously found roots. A provision was made in the present subroutine so that, if desired, any of the input guesses (at which the search for each root starts) could be included in the reduction of the function. In most cases a great savings in the number of iterations for most roots is realized.

Even crude pole-zero cancellation is useful when the zeros are reasonably well separated in a region of interest. If poles (at the input guesses) are inserted in the region, with about the right number and spacing, then the pole-zero cancellation will be effective. If there is a group of zeros, for example, then a similar number of poles inserted anywhere in the group, even midway between the zeros, would largely compensate most of the zeros. In the region to one side of the group, and at a moderate distance compared to the spacing between zeros and poles, the iteration procedure will be little affected by the zeros. In such regions the root search will be drawn rapidly to the nearest uncompensated zero. As each zero is found, the respective pole-zero cancellation becomes exact.

A pole of $g(z)$, unrelated to a zero of $f(z)$, can also be useful by repelling the root search from a region which it is desired to avoid. This is an additional justification for including a unconverged last iterate as a pole for $g(z)$, as described later. But it can also be useful to place a few arbitrary poles, say along a branch cut, or in the present example along the imaginary axis for β^2 , to discourage the root search from approaching such regions. These poles may be included as part of the array of input guesses, but with a control parameter which causes no corresponding search to be made.

5.3 Generation of Initial Iterates; Ordering of Iterates.

The iterative procedure just described requires three values of z for each step; and to start the search for each root these iterates must initially be generated in some arbitrary way. After the first three iterations the initial iterates will have been replaced by three successively calculated iterates.

All known descriptions of Muller's method take for granted that the iterates are ordered so that a is the poorest and c is the best approximation to a root. The iterates are accepted in the order calculated, with the most recent being used for c because it is presumably the best. This is very frequently not true. It is certainly unlikely to be true for the initial arbitrary iterates, and it can easily fail to be true during the course of iterations. Only if the three iterates are in the neighborhood of an isolated root will the successive iterates always be smaller and the convergence order of 1.84 be realized.

During the early stages each iteration does not always lead to a smaller magnitude for $f(z)$. The root of $F(z)$ nearest to c , or even both roots of $F(z)$, may actually be farther from a true root of $f(z)$. Then $|f(z)|$ for a new iterate can easily be larger than $f(c)$. This has frequently been observed to happen in the first few iterations, and has often occurred as late as the fifth iteration.

The implementation of Muller's method here explicitly reorders the initial iterates on the basis of $|f(z)|$, so that $f(a)$ is in fact the largest and $f(c)$ the smallest. And during iteration this order is preserved by checking $f(z)$ for each new iteration against $f(c)$. If $f(z_0)$ is not smaller, then c is retained, and the new iterate is instead used to replace a or b , preserving the order. The largest iterate, a , is always discarded. The

reordering affects the evolution of the iterations in two ways. Use of the root of $F(z)$ nearest the smallest iterate is now guaranteed. And the number of times an iterate is used in subsequent calculations depends on its quality. Normally each iterate is used three times, progressing up the list before being discarded. But a poor iterate placed farther up the list now is used only twice or once, and the better iterates remaining lower on the list are used more than three times. A few tests on polynomials with five to twenty roots showed that reordering occurred frequently for the first several iterations, and savings of one or two iterations always occurred. Usually a savings of three or four iterations was observed, which represented a factor of two improvement. For the present problem this is a significant saving.

To generate the initial iterates, some starting point or neighborhood must be designated. This point will be called the initial guess. The choice of initial iterates about this guess is wholly arbitrary. It is very important to be able to control the distance of the three points about the initial guess. It is convenient to choose a radius which is a negative power of ten, say 10^{-k} , where k is chosen to reflect the quality of the guess. A poor guess may use a k of about 0 to 2, while an excellent guess may justify a k of 3 to 5. The radius should be larger than the convergence criteria being used, and it should be smaller than the expected spacing between roots.

A novel method for generating these iterates has been used. It is based on an unfamiliar metric, or measure of distance, in the complex plane. This metric is more justified and described later for use as a convergence test, but it also offers some advantages for generation of the initial iterates.

Let z_0 now be an initial guess. It may be based on previous knowledge about the expected location of a root, or it may be located only generally in a region in which roots are sought. Three values z_j , $j = 1, 2, 3$, are to be

generated about z_0 for use as initial iterates. These are taken to be spaced about equally on a circle about z_0 ; but the circle is not necessarily centered on z_0 , and the "distance" from z_0 is measured on the Riemann sphere for the complex z plane. This is called the chordal metric on the sphere [75, 76].

For any two points z and z_0 , the metric, d , is given by [75, p. 311]

$$d^2(z, z_0) \equiv 4|z - z_0|^2 / (1 + |z|^2)(1 + |z_0|^2) .$$

For points very close to the origin, d reduces to the Euclidean metric $|z - z_0|$; but for large z , d is much less, and in fact is always finite. The maximum distance between any two points is $d = 2$, the diameter of the unit sphere. This is the distance between the origin and the point at infinity, between any two points on opposite sides of the unit circle, or between any two points z and z_0 for which $z z_0^* = z^* z_0 = -1$.

The advantage of this metric is that it remains invariant under a large class of (conformal) Mobius transformations of the z -plane. These transformations correspond to rigid rotations of the Riemann sphere, and have the form [75]

$$z \rightarrow w(z) = M:z \equiv \frac{\alpha z - \beta}{\beta^* z + \alpha^*} ;$$

where α and β are two complex parameters of the transformation, and M is a matrix

$$M = \begin{bmatrix} \alpha & -\beta \\ \beta^* & \alpha^* \end{bmatrix} .$$

M : is an operator notation for the transformation (also mentioned in Sect. 2.7). M is considered normalized if $|\alpha|^2 + |\beta|^2 = 1$, but the transformation is not affected by the normalization. The rigid rotations of the sphere, and the invariance of d , correspond to the normalized M being a unitary matrix [75]. It is well known that Mobius transformations map circles and lines (as degenerate circles) into circles and lines. The circle of initial iterates about z_0 is obtained here by such a transformation.

The unitary transformations are important because many properties of polynomials in particular, and of rational fraction approximations for functions in general, remain invariant. For example, the distances between roots, or between roots and singularities, and the accuracy of function approximations, all remain invariant when expressed in the chordal metric [76]. One transformation, often used in finding (large) roots of a polynomial in z , is the substitution $z = 1/w$. If the initial iterates and convergence tests are based on the chordal metric, then roots searches conducted in either the z or w planes should lead to the essentially the same results in terms of accuracy.

Consider then a complex plane of w , and three points on a circle of radius r_w centered on the origin. These three points are transformed to points on a circle about z_0 (the origin of w maps to the point z_0) by a transformation

$$z(w) = \frac{w + z_0}{1 - w \bar{z}_0^*}, \quad w(z) = \frac{z - z_0}{1 + z \bar{z}_0^*}.$$

So z_0 itself is the single parameter determining the transformation.

The chordal metric, d , between any point w and the origin, or between the corresponding z and z_0 , is of course identical;

$$\begin{aligned}
d^2(w, 0) &\equiv d^2(z, z_0) = 4|w|^2/(1+|w|^2) = 4r_w^2/(1+r_w^2) \\
&= 4|z-z_0|^2/(1+|z|^2)(1+|z_0|^2) .
\end{aligned}$$

The circles about z_0 , obtained from circles about the origin of w , are not centered on z_0 except in the limit of very small radius. For some radius r_w , the circle about z_0 in fact degenerates to a straight line through infinity. The straight line and the corresponding radius r_w can be found by noting that $z = \infty$ maps to become $w = 1/z_0^*$, on the circle of radius $r_w = 1/r_0$ about the origin of w , where $r_0 \equiv |z_0|$. The diametrically opposite point, $w = -1/z_0^*$, maps to become the point $z' = (z_0 - 1/z_0^*)/2$, through which the line to infinity must also pass (perpendicularly to the line joining all the points $z = 0, \pm z_0, \pm 1/z_0^*$). To avoid this degenerate case it is necessary to limit the radius r_w to be less than some $r_{\max} < 1/r_0$. For large z_0 a factor of a half is useful, say $r_{\max} = 1/2r_0$. But for z_0 near the origin even this r_{\max} becomes arbitrarily large; so it is also desirable to limit r_{\max} , to be no greater than unity say, when $r_0 = z_0 = 0$.

Let r_{\max} then be defined arbitrarily by

$$r_{\max} \equiv 1/(1+2r_0) < \min[1, 1/2r_0] .$$

The initial iterates are defined on a circle of radius r_w , starting at any point w_0 on that circle, by

$$r_w = 10^{-k} r_{\max} ,$$

and

$$w_j = R^j w_0 ; \quad j = 1, 2, 3 ;$$

where k is an input integer, and R is a complex rotation factor with an angle of about 120° , say $R = -0.6 + i0.8$. The three points w_j are then transformed to become points about z_0 by the Mobius transformation

$$z_j = \frac{w_j + z_0}{1 - w_j z_0^*} \quad j = 1, 2, 3$$

Together with $f(z_j)$, evaluated at the three points, these serve as the initial iterates with which to start Muller's method.

The initial guess z_0 may sometimes be an excellent guess. If a root is available from a previous calculation, and only small changes are being made in parameters, then z_0 may in fact be closer to the root than any of the three initial iterates; that is, if r_w is chosen too large, k too small. To cover this case it seems worthwhile (though debatable) to incur a fourth function evaluation to obtain $f(z_0)$. z_0 is then included in the initial re-ordering with the other iterates, the worst one is discarded, and the best three kept. The retention of z_0 in preference to one of the other initial iterates frequently occurs, but the amount of benefit is not known.

5.4 Convergence Criteria and Iteration Limits

The criteria for deciding that a root has been found with sufficient accuracy, and the iteration process stopped, is important; but a particular choice is largely arbitrary. Many strategies are found in the literature.

Since the roots are defined by $f(z) = 0$, then the most directly relevant convergence criteria would be that

$$|f(z)| \leq \epsilon_f N_f ,$$

where ϵ_f is some small positive number chosen to set the level for acceptance of a root. N_f is a normalization factor representing the nominal range of magnitude expected for $f(z)$ away from the roots. The need for N_f is rarely acknowledged in discussion of root searching methods; it is usually assumed to be unity. But it is important to recognize that in different problems the range of values for $f(z)$ can be very different. For example in one case $f(z)$ may have values on the order of 10^{-3} say, but the definition of $f(z)$ in another problem may lead to values on the order of 10^3 . If the same value of ϵ_f is used for both problems and $N_f = 1$, then the above convergence test represents very different criteria for the two problems. In the absence of any information about expected magnitudes the $N_f = 1$ may be used. But if any information is available it should be used to provide a value for N_f , however crude.

It is sometimes argued that since the iteration process is based on the reduced function $g(z)$, then the convergence criteria should also be based on $g(z)$, rather than on $f(z)$. This would be that

$$|g(z)| \leq \epsilon_f N_g ,$$

where a normalization value N_g may or may not be available for $g(z)$. However, the range of values for $g(z)$ is even more unpredictable than for $f(z)$, and it varies from root to root, because of the magnitude of the reducing polynomial. For example, if roots are spaced apart on the order of 10 (or 0.1) units in z , then, in dividing out 5 roots, the magnitude of the polynomial can be on the order of 10^5 (or 10^{-5}). Thus the significance of the convergence test using $g(z)$ can vary wildly with the problem, the root spacing, and number of roots being divided out.

A convergence criteria more directly related to the users interest in the accuracy of the roots would be that

$$|\delta| \leq \epsilon_z, \quad \text{or perhaps } |\delta/z| \leq \epsilon_z .$$

δ is the difference between the last two values of z , namely the increment in z of the last iteration. The first form is an absolute test comparing $|\delta|$ to unity, and the second form is a relative test comparing the fractional increment in z . The latter test is reasonable for large z , but it breaks down for roots very near zero.

To obtain a convergence test having some invariant properties, for z large or small, the chordal metric described in the previous section has been used. The motivation and justification for doing so is valid mostly for polynomial root searching rather than the transcendental eigenvalue problem here. But the program was intended to be a high quality general purpose subroutine, which is often tested and judged on polynomial root searches. And the chordal metric has some desirable properties for any problem.

If z_o is now the most recent iterate, and $z = c$ is the previous one, the chordal metric is

$$d_z^2 = 4|z_o - c|^2 / (1 + |z_o|^2)(1 + |z|^2)$$

as before. But $z_o - c \equiv \delta$, and in the last stages of convergence, δ is very small; then z_o and z are essentially equal, and the metric for use in the convergence test is taken to be

$$d_z = 2|\delta|/(1+|z_o|^2) .$$

The convergence test then becomes

$$d_z \leq \epsilon_z .$$

For $|z_o|^2 \ll 1$, then $d_z = |\delta|$, and the convergence is based on $|\delta|$ relative to unity. But for large z_o the test is based on δ relative to $|z_o|^2$ (not relative to $|z_o|$). For very large $|z_o|$ this is appropriate though. For, consider a root which is effectively at infinity; let $f(z) = 1/z$. Then, at some iterate z , the increment will be $\delta = -f(z)/f'(z) = +z$, and the convergence test becomes

$$d_z = 1/|z| \leq \epsilon .$$

Hence, for $f = 1/z$ each iteration doubles z (a slow way to reach infinity), but the convergence test will be satisfied for $|z| \geq 1/\epsilon_z$. That is, by the chordal metric, the point $z = 1/\epsilon_z$ is within ϵ_z of the point at infinity; and the convergence test stops any further efforts to reach the point at infinity.

The two convergence tests, on $|f|$ or $|\delta|$, are related by the derivative of f ; for, $\delta \approx -f/f'$. Which test is more liberal or restrictive depends on the magnitude of f' near the root, as well as on ϵ_f and ϵ_z . One situation to keep in mind is that f' can be nearly zero, near a double root for example. Then f can be very small and the convergence criteria for f may be satisfied; but δ will not be small, and a convergence test in z will never be satisfied. In such a case accurate solutions for a root may not be possible, even though the equation $f(z) = 0$ can be satisfied within a very small ϵ_f .

For double roots Muller's method has an advantage over Newton's method in that the two roots can be found exactly. But still, the above situation exists then for a triple root. On the other hand, when f' is large near a root, then δ can be very small and the convergence test in z will be satisfied, even though $f(z)$ is still significant. In general it is not possible to provide any one convergence test which can assure that a root is known to some desired accuracy.

The program written here uses all three convergence tests, and the last iterate is accepted as a root if any one test is satisfied. An output integer is set to indicate which test was satisfied. This choice is arbitrary and subject to change. A more stringent criteria would be that the test on $|f|$ and the test on $|\delta|$ must both be satisfied. The emphasis on one or the other can be controlled by appropriate choice of ϵ_f and ϵ_z .

A limit on the maximum number of iterations for each root is essential, and is usually determined by an input integer. When an iteration limit is reached without convergence most routines abandon any further search for other roots. Here the last iterate is retained as an approximate root, but the output integer is set to indicate nonconvergence. Only if the iteration limit is reached for two successive roots is the further search for other roots abandoned. More importantly, all roots which have been attempted, even those for which the iteration limit is reached without convergence, are divided out in forming the reduced function. If a root is approximately correct then the pole-zero cancellation will be good. If the last iterate

is not near a root, for whatever cause of nonconvergence, then the reduced function will have a pole at that point. This pole will tend to repel any subsequent root search from that region. Then, whatever the cause of the search going to the region where convergence was not obtained, subsequent searches will likely not try it again. If a second iteration limit occurs, this is taken as a sign that no further progress can be expected. This strategy has worked extremely well for the layered structure. Though nonconvergence does often happen, the subsequent root search has never been abandoned because it happened twice in succession.

For the present problem iteration limits of 10 to 15 have been used. Lack of convergence within this limit sometimes happens. In every case that has been checked, the root search was then entangled in a branch cut. Successive iterations were close to and on opposite sides of the cut. This emphasizes the importance of positioning the branch cut. In some cases the iteration limit has been reached when in the vicinity of the branch point.

5.5 Generation of Initial Guesses

The set of guesses, at which the search for each root is started, is the single most important factor in determining which roots are found, and the order in which they are calculated. Also, the number of iterations needed for convergence depends greatly on the ability to provide approximate guesses in the region of interest. Even though it is not usually possible to estimate the locations of any one specific root, it is important to generate guesses in about the right number and spacing in the region. The guesses must be based on knowledge of the structure represented by $f(z)$, and cannot be provided by the root searching method.

One crude set of guesses is to make them all the same. A starting value of β^2 equal to the largest n^2 in the structure is useful, or some mean value of n^2 may be better. Such guesses will lead to eventual convergence for roots, but the number of iterations required can be very large.

In the present problem the phase integral provides a basis for generating quite good guesses for most complex modes of interest. Sect. 2.8 described the phase integral defined for any β^2 , and it may be used for labeling and indexing the modes. The converse purpose here is to generate approximate values for β^2 , corresponding to desired mode indices. This may be done as follows.

For simplicity let β^2 be represented now by q , and consider several values in the neighborhood of the real axis. (A fixed imaginary part for β^2 may be chosen arbitrarily and supplied as an input parameter.) For every value of q the phase integral Φ_R is defined as in Sect. 2.8. Let $p(q) \equiv \Phi_R/\pi$ be the real phase integral, in units of π , on a scale to be used for mode indexing. For three representative values of q , the three values of $p(q)$ may be calculated, and then used to obtain a quadratic approximation for the inverse relationship of q vs p . This quadratic is then used to calculate estimated values of $q = \text{Re } \beta^2$ for any number of intended mode indices on the scale of p . The quantities here are all real.

The specific formulas are as follows. Let the three values of $q = \text{Re } \beta^2$ be defined as:

$$q_3 = \max(\text{Re } n^2) \text{ over the inner layers,}$$

$$q_1 = \text{input value, say } q = 0, \text{ or } q = \min(\text{Re } n^2) \text{ over the inner layers,}$$

$$q_2 = \text{average of } q_3 \text{ and } q_1.$$

For each q_i , $i = 1, 2, 3$, let $p_i \equiv p(q_i) = \Phi_R(q_i)/\pi$, be calculated. The quad-

ratic fit to these three points is then written as

$$q(p) = q_3 - A_1 p - A_2 p^2;$$

where the coefficients are given by

$$D_1 \equiv (q_3 - q_1)/p_1, \quad D_2 \equiv (q_3 - q_2)/p_2,$$

$$A_1 = (p_1 D_2 - p_2 D_1)/(p_1 - p_2),$$

$$A_2 = (D_1 - D_2)/(p_1 - p_2).$$

The particular form for the quadratic reflects the fact that, for lossless dielectrics with positive n^2 , the values of Φ_R increase monotonically with decreasing β^2 ; q decreases with increasing p ; and A_1 , A_2 , D_1 , and D_2 are all positive coefficients. Also it is assumed that $q(0) = q_3$; reflecting the fact that Φ_R goes to zero for β^2 equal to the maximum value of n^2 for the inner layers. It may be noted that p , the phase integral, is a function of q as an independent variable; however, the quadratic represents an inverse relation of q vs p (an inverse interpolation function). For any intended value of phase integral, p (a continuous mode index), the quadratic returns a value for $q(p) = \beta^2$, for use as a starting guess.

A relationship between p and any intended integer mode index, m , is still needed. For simple guiding structures, as noted in Sect. 2.8, the modes are expected at unit intervals in p , but offset at some constant value corresponding to the phase shifts at the boundaries. For flexibility in generating the initial guesses, input parameters may be provided to specify the average spacing of the modes in p , and also the constant offset. Thus, for every intended mode index, m , in some range of interest, the expected phase integral p_m is prescribed as

$$p_m = ms + p_o,$$

where s is the mode spacing, often unity, and p_0 is the offset or bias. For simple guiding structures $p_0 = 1/4$ to $1/2$; but for a structure of three guides $p_0 = 3/2$ may be more reasonable, and for the three lowest order modes s may easily be much less than unity. The values of p_m are then used in the quadratic interpolation expression above to generate the guesses.

An additional refinement step in calculating the quadratic has been incorporated in the process of generating the guesses. Usually a range of modes is to be calculated. Let m be the center value of this range, and p_m be the corresponding p . This may be used to generate a corresponding guess q_m using the quadratic. This q is now used to replace the q_2 value initially used to generate the quadratic; and the quadratic formula for $q(p)$ is recalculated. That is, the new value of q_2 (now based on the actual range of modes desired) is used to calculate a new p_2 , and the coefficients of the quadratic are recalculated. This refinement process has proved very worthwhile.

It must be emphasized that the guesses are only estimates with respect to particular mode indices. It is not possible, a priori, to ensure that the guess is close to the root for a particular value of m ; nor is it possible to assure that a particular mode is actually found. When some structure is being studied, the first several runs will quickly provide information about average mode spacing, s , and the offset, p_0 , in the region of interest. These may be used to provide much better guesses for subsequent calculation. Recall that q_1 is also available as an input parameter for controlling the guesses generated.

This procedure for generating guesses has worked very well. The primary virtue is that a set of values for $q = \beta^2$ is generated with about proper spacing and number, in order of increasing m and decreasing β^2 , in the region of interest. For simple structures and low order modes, the guesses have

been excellent, permitting convergence in only a few iterations. In nearly all cases it is very advantageous to divide out all guesses. The number of iterations for convergence is much greater if the guesses are not included as poles in the reduced function.

Guesses generated by this method become poorer for modes having a significant imaginary part for β^2 . The assumptions leading to this method are not valid when n^2 in some layers has a large imaginary part or is negative (a metal). And when β^2 has a large imaginary part the real phase integral is less satisfactory for ordering and indexing the modes. Also, the method does not provide a variable imaginary part for the guesses. Nevertheless, in all but the most difficult cases the present method provides a useful set of guesses at which to start.

Provision is easily made for the set of guesses to be supplied as input values by the user. This may be used in the more difficult cases. When a familiar structure is being studied, approximate values for the roots are often known. It is then very worthwhile to supply these as input values, rather than to generate guesses.

It is also easy to provide that the set of roots from a previous case is retained as starting guesses for a subsequent case. This is extremely valuable when small changes are being made in the parameters from case to case. This is desirable, for example, in developing dispersion curves for β^2 vs. frequency, or vs. a thickness or permittivity of a layer. Only one or a few iterations may then be needed for each root with each increment of the parameter.

5.6 Discussion

Without extensive comparisons it is difficult to make quantitative statements about the quality of an algorithm. But it is believed that the subroutine written here is the most efficient one available. This is attributed to the ordering of iterates, and provision for dividing out initial guesses and even unconverged roots. With relatively well distributed guesses, and searching for sets of 3 to 7 roots at a time, convergence in the present problem is often obtained in 2 to 3 iterations. Most roots are found in 4 to 7 iterations each, and otherwise an iteration limit of 10 to 15 is reached without convergence. If the initial guesses are not divided out the number of iterations is considerably greater, sometimes by more than a factor of two. If all guesses are started at the same point a very large number of iterations is usually needed.

The number of iterations needed depends, of course, on the convergence criteria used. A value of ϵ of 10^{-9} to 10^{-15} has usually been used, with the latter value requiring only one or two iteration more than the first. These values are possible because a floating point number of 14 digits was being used. To force a more accurate determination of β^2 , the ϵ_f for the convergence test on $D(\beta^2)$ was often made 10^{-3} smaller than the ϵ_z , for the test on the increment in β^2 .

The economics of root searching becomes more and more important as the numbers of layers increases. For only three layers, and a few modes, a factor of two in the number of iterations may not be significant. But for many layers, say 10, and more than a few modes, the efficiency of the root search can be a very significant factor. It can make the difference in how extensively a range of parameter values for some particular structure can be explored.

The fact that the mode index, m , cannot be made a parameter of the characteristic equation is unfortunate. As a consequence it is not always possible to guarantee that all the desired modes have been found. When there are several modes of interest, and some of them are near cut-off or are improper, the situation can become confusing. Some strategic exploration and tricks may be necessary to understand the situation. If it is suspected that a root has been missed, then the case can be rerun with the known roots as input guesses, plus one or two new guesses inserted in the region of interest. That is, a search is made for additional roots in the same region. If no other roots exist there, the search will wander off and likely find new roots beyond the region of the previously found roots.

If a search is started with several different sets of starting guesses in a region of β^2 , and exactly the same roots are found each time, that is strong evidence that there are no other roots present. When the same roots are found several times, from several different sets of starting guesses, these may be compared to show directly the accuracy with which the roots are being determined. It is sometimes very illuminating to rerun cases with some small changes in the parameters of the problem, particularly the frequency. Since roots are always continuous functions of the parameters, the resulting changes in the location of the roots can be very helpful in making proper identification. Modes in the vicinity of cut-off are particularly sensitive to parameter changes.

The specification of boundary conditions and orientations of the branch cuts in β^2 , and branch boundaries in κ_1 and κ_N , is very important. If more than a few roots reach an iteration limit without convergence, then it likely that the search is reaching for roots on the other side of the branch boundaries. It is emphasized that any search can be carried out only in one half

of each of the κ_1 and κ_N planes at a time. Any non-converged roots may be plotted in the κ -planes, and will likely be found to lie near the boundary for either κ_1 or κ_N . This is a sign that roots lie nearby, but in the other half plane. If these roots are of interest, then the branch boundary must be rotated or opposite boundary conditions must be specified.

It is worth keeping in mind the relationship between the branch cuts and boundaries and the location of the initial guesses. There is little point in starting the root search in the immediate neighborhood of the branch cuts in the β^2 plane. The initial iterates may fall on opposite sides of the cut, leading to little progress in earlier iterations.

The number of roots is a conserved quantity for most familiar guiding structures. Roots do not cease to exist, or mysteriously appear and disappear with changing parameters. If, with a variation in some parameter, some particular root can no longer be found by the search, then it has moved across the branch boundary. A mode may move onto a nonphysical branch or into a branch which is not of interest. But mathematically the root always moves continuously in the κ and β^2 planes. By changing the branch specifications or boundary conditions as necessary most roots can be uniquely identified, and tracked throughout the complex planes.

It is more distinctive and illuminating to plot the locations of roots in the κ_1 and κ_N planes than in the β^2 plane. The values of κ_1 and κ_N , for a converged root or the final iteration, should always be available. These values, when plotted in the κ -planes, reveal immediately in which half-plane they are located, whatever the branch specification may be. But the value for a root located in the β^2 plane cannot by itself show which Riemann sheet is intended. The values of κ uniquely determine β^2 ; but not conversely, without consulting the branch specification and boundary condition.

One feature not described yet has also been incorporated in the root searching algorithm. This concerns a strategy to be used when multiple roots are present, and is probably not important in the present problem. When there is a multiple root, and one of these, z_0 , has been found, then a subsequent root search will approach the same root again. In doing so, the reducing polynomial $P(z) \approx (z-z_0)$ can approach zero; but not exactly as $f(z)$ approaches zero, since z_0 may not be exact. Then the reduced function $g(z)$ can become infinite or indeterminate. In Ref. [94] it is suggested that if any iterate, z , approaches a previously found root, z_0 , within the convergence criteria, ϵ_z , then z should be accepted as a new root without further convergence tests. This is easily done during the formation of the reducing polynomial, $P(z)$; but it adds some overhead to the calculation, and the benefits are uncertain.

6. FIELD SOLUTIONS AND POWER FLOW

A great advantage of the 2×2 representation for the fields is that the same algorithm, a sequence of matrix multiplications, serves to calculate both the characteristic function and the actual field distributions. No separate procedure need be formulated for calculating the fields once the discrete mode propagation constants are found.

6.1 Tangential Fields at the Boundaries

The tangential fields F_y and F_z at all the boundaries are sufficient to completely characterize the field solution throughout the structure. They are a set of $2N-2$ values (which may be thought to correspond to the same number of amplitude coefficients required if exponential solutions were used in each layer). For any value of β^2 , for a discrete or continuous mode, the boundary fields are easily calculated by the sequence of multiplications by layer matrices. The process may be started at either or both of the outer boundaries, as described in Sect. 4.3. That is, at x_1 the tangential fields may be taken to be $F_y = 1$, and $F_z = -Y_1$. Or at x_{N-1} they may be taken to be $F_y = 1$, and $F_z = +Y_N$. These are transformed forward or backward, respectively, across the structure, saving the values of F_y and F_z at each boundary. This is a trivial operation compared to the use of Cramer's rule.

For true discrete modes these two sets are equivalent, and either one may be used as the eigenfunction (Sect. 4.3). If both sets of field values are calculated, then the Wronskian determinant can be calculated at all the boundaries as a numerical check on the accuracy to which the characteristic equation is satisfied. The Wronskian should be very small, corresponding to the convergence criteria used, and it should be the same value at all

boundaries. If the determinant is not the same at all boundaries, it indicates that the numerical problem is, to some degree, indeterminate relative to the floating point resolution of the computation. If the determinant is the same at all boundaries, and not small, then the problem is well defined, but greater accuracy for β^2 could easily be obtained in the root search. The average of the two separately calculated field solutions can be used as the eigenfunction with some improvement in accuracy.

For modes other than the discrete modes the Wronskian determinant will usually not be small, but it should be constant as required by reciprocity. The two different field solutions are then linearly independent and must be considered separately and used as needed.

The normal field component, F_x , is not necessarily continuous at the boundaries. It is calculated as $F_x = Y_z F_y$, using the possibly different values of Y_z in the two adjacent layers. See Table 2.2.

Normalization of the field solutions is arbitrary. For bound modes the solutions are often normalized to have unit total propagating power (per unit width in y). There is no particular need for doing this, and for improper modes it is not possible. For numerical purposes, and for any type of mode, it is more convenient to normalize for nominally unit mean squared field magnitudes when averaged over all the boundaries. When the total power is finite, it may be calculated, and listed separately for use when needed (Sect. 6.3). This renormalization of the initially calculated fields is easily provided. A real normalizing constant G is calculated as

$$G^2 = \sum (|F_y|^2 + |F_z|^2) / 2(N-1) .$$

The summation is over all the $N-1$ boundaries, and an extra factor of 2 appears because both F_y and F_z are included. The field values as calculated

above are then divided by G . The mean squared value over all tangential fields will be unity. In regions where the power is concentrated the values can be considerably larger, but in other regions the fields will be much less.

Because all fields can be complex-valued it is useful to also standardize the fields so that F_y is pure real at some selected boundary. This is easily done at an interior boundary, where fields are expected to be large, by multiplying all field values by an appropriate phase factor. For cases of no real transverse power flow (bound modes in lossless structures) F_z is pure imaginary, and the quadrature between F_y and F_z holds across the structure. Small departures from this condition become more obvious if the complex phase standardization is used.

6.2 Field Distributions

A set of field values at equally spaced points in x may be needed for graphical purposes or for numerical integration. The fields may be calculated at a set of points in each layer, ℓ , given by $x(n) = x_{\ell-1} + nh$, where h is a small increment in x . By defining a layer matrix corresponding to the increment, the successive field values can be generated by repeated matrix multiplication. As for any layer, the incremental matrix can be defined as

$$C_\delta = \begin{bmatrix} \cos\theta_\delta & +(i/Y_x)\sin\theta_\delta \\ +(iY_x)\sin\theta_\delta & \cos\theta_\delta \end{bmatrix}$$

where $\delta \equiv k_0 h$ is now the thickness of the incremental layer on the scale of ξ , and $\theta_\delta \equiv \kappa\delta \equiv \kappa k_0 h$. An index ℓ for the different layer parameters is always implied. Then the vector fields $F(n)$ may be calculated iteratively

within layer ℓ , at the points $x(n)$, as

$$\begin{aligned} F(0) &= F_{\ell-1}, & F(n+1) &= C_{\delta} \cdot F_n, & F(n) &= C_{\delta}^n \cdot F_0, \\ x(0) &= x_{\ell-1}, & x(n+1) &= x(n) + h, & x(n) &= x_{\ell-1} + nh, \end{aligned}$$

for $n = 0$ until nh exceeds the thickness of the layer. The starting values $F_{\ell-1}$, at the lower boundary of each layer, have presumably been calculated previously.

The advantage of this method is that only four complex multiplications are needed for each increment, and both F_y and F_z are calculated. The alternative is to evaluate and apply the matrix for the transformation from $x_{\ell-1}$ to each x_n in turn. The same number of matrix multiplications is required, but evaluation of the complex $\cos\theta$ and $\sin\theta$ for each point can require ten to a hundred times as many additional multiplications. The incremental method corresponds, of course, to the use of the trigonometric identities for sums of angles; $\cos \kappa(\xi+\delta) = \cos \kappa\xi \cos \kappa\delta - \sin \kappa\xi \sin \kappa\delta$, and $\sin \kappa(\xi+\delta) = \sin \kappa\xi \cos \kappa\delta + \cos \kappa\xi \sin \kappa\delta$.

6.3 Power and Energy Relations

Values for the transverse, S_x , and longitudinal, S_z , Poynting power densities are easily calculated whenever field values are calculated. At any point in x , at the boundaries or at incremental points, then (Table 2.1)

$$S_x = \frac{1}{2} F_y F_z^*, \quad \text{and} \quad S_z = \frac{1}{2} F_x^* F_y = \frac{1}{2} Y_z^* |F_y|^2.$$

S_x is continuous at all boundaries, but S_z can be discontinuous because F_x changes magnitude by any step change in $1/\mu$ or $1/\epsilon$ at the boundary. The calculation of S_x and S_z may actually be considered a part of the field calculations.

Similarly, the energy densities W_x , W_y , and W_z , may be easily calculated at any plane in x where field values are available. These are defined in Table 2.1. For reasons given below, it is worthwhile to keep these three terms separate. For complex material parameters the energy density can be complex, the imaginary part representing the rate of energy absorption or gain.

Total propagating power in each layer and, when finite, the total propagating power in the structure are important quantities. These permit the renormalization of the fields to unit total power, and identification of the fraction of power propagating in each layer. Similarly, the energy density may be integrated to obtain the fraction of energy stored in each layer, including absorption loss or gain in each layer. These quantities, together with the transverse Poynting power, are all related as pointed out below.

The given expressions for S_z and the different W 's are easily integrated across any layer, but their calculation has not yet been incorporated

into the program. A particular difficulty encountered concerns a layer very near cut off, $\kappa\tau_g \ll 1$. Just as for evaluation of a layer matrix, the expressions for the power and energy become numerically indeterminate (though finite) in this limit. These expressions have four terms (since the fields anywhere depend linearly on two parameters, say the tangential fields at the nearest boundary). One of the terms is finite; two terms are numerically indeterminate in the form of $(1-1)$, with the first remaining term proportional to $\kappa\tau^2$; and one term is indeterminate even to first order in $\kappa\tau$, with remaining term proportional to $\kappa^2\tau^3$. For $\kappa\tau$ small but not negligible, these terms are not necessarily small because the thickness, τ , can be arbitrarily large. For accurate calculations of the integrated power in this situation it is necessary to obtain several power series expansions, but these have turned out to be quite complicated. This is an area for future extension of the formulation, and which is yet needed in the program. Here we limit ourselves to indicating the direction and format it might take.

We first point out that there have been some recent extensions, to open multi-region dielectric guides, of some generally known relations between group velocity and power flow and energy density in a waveguide [95, 96, 97]. One set of relations is summarized by Kawakami [97]. In these, the fractional part of the propagating power in each dielectric region plays an important role. The relation between phase and group velocity, as well as an orthogonality relation, can be written as an average of $k^2 = \omega^2\mu\epsilon$ over all the regions, each weighted by the fraction of the power propagating in that region. These relations were presented for lossless dielectrics and real β . However, for proper modes with finite total energy, all the quantities remain defined for complex modes also. Extension of these relations to complex modes should be explored. The needed quantities should be easy to calculate in the present model. The group velocity, when defined, may

probably be more accurately calculated in this manner than by approximating the derivative $d\omega/d\beta = v_g$.

The group velocity, v_g , when it is defined, relates the total power flow, P , and stored energy, W (per unit length) as [2, p. 42, 99, Eq. 39];

$$P = v_g W .$$

The relation holds for a wide variety of lossless guides. We point out that P and W are still defined, though complex, for modes of lossy guides, provided only that the mode is bounded. Hence the above relation could be used as a definition for v_g , although it would be complex. Group velocity is only a first order concept ($d\omega/d\beta$ constant over the bandwidth of a signal), and care should be taken in interpreting it too literally. In particular, no physical interpretation appears to have been suggested for a complex v_g , but perhaps some significance could be given to the imaginary part.

Another, exact, relationship exists between the phase velocity and the stored energy terms.

$$P = \omega/\beta (U_t - U_z)$$

where $\omega/\beta = v_p$ is the phase velocity for a mode, and P is the total propagating power. U_t is the total energy stored in the transverse fields, and U_z is the energy stored in the longitudinal field components [2, Eq. 2.2, 89; 98; 99, Sect. IV]. This is one of two independent relations valid for closed and open lossless dielectric waveguides even with material dispersion. In [100] it is shown that the $(U_t - U_z)$ can be interpreted as a electromagnetic momentum flow.

Of more interest to the present problem is the fact that these two relations (theorems) can be generalized to waveguides of fully complex

material parameters, and for complex ω and β [101, 102]. These were derived simply from Maxwell's equations, but were limited to closed waveguides having arbitrary but lossless impedance boundary conditions.

Here we present the two independent relations in terms of the normalized variables of Table 2.1, and valid for either polarization. Also, the results of references [101] and [102] are extended so that the theorems are useful also for open structures and unbound modes. At any plane x

$$\beta S_z = 2\omega_r W_x \quad (6.1)$$

$$\beta^* S_z + i dS_x/d\xi = 2(\omega_r^* W_y^* - \omega_r W_z) \quad (6.2)$$

These may be obtained directly from Maxwell's equations. Substitution of the definitions for S and W reduce (6.1) to a simple identity, and (6.2) can be proved by using the two differential equations of Table 2.2. This simplicity belies the importance of these two relations. Their difference is, in fact, Poynting's theorem in differential form, $\nabla \cdot S = i2\omega(W_m - W_e)$; where W_m and W_e are the magnetic and electric energy density (TE modes). And their sum, apart from the terms in S_x , leads to the relation given above for the phase velocity.

When Eqs. (6.1) and (6.2) are integrated between any two planes x_1 and x_2 , then

$$\beta P_z = 2\omega_r U_x \quad (6.3)$$

$$\beta^* P_z + i(S_{x2} - S_{x1}) = 2(\omega_r^* U_y^* - \omega_r U_z) \quad (6.4)$$

P_z is the total propagating power between the two planes, and U_x , U_y , and U_z are the total energy (per unit length) associated with each of the three field components. These two equations hold for any two planes of the structure; in particular for each finite layer, and for the whole structure.

Except for the term in S_x , Eqs. (6.3) and (6.4) correspond to Eqs. (10) and (11) of [101], and Eqs. (9) and (10) of [102]. $(S_{x2}-S_{x1})$ is the net Poynting power which flows transversely out of the region between x_1 and x_2 ; it is easily available from the boundary field values without integration. Inclusion of this term makes the equations valid for arbitrary complex modes. For closed waveguides, or for bound modes in open waveguides with x_1 and x_2 at infinity, the net transverse power outflow is zero; and Eqs. (6.3) and (6.4) reduce to those in [101, 102]. And for lossless materials these are also equivalent to Eqs. (48) and (49) of [99].

These equations have the dimensions of power per unit length of the guide, and may be considered as power balance equations. By taking sums and differences between the two equations, it is possible to write four relations, involving the real and imaginary parts of β and P_z separately [101, 102].

With the calculation of P_z , and U_x , U_y , U_z for each layer, it is then possible, using Eqs. (6.2) and (6.4), to make rather complete statements concerning the power flow in each layer, the power flow across layers, and the power dissipated or gained in each layer. And for the whole structure it is possible to identify the attenuation of the propagating power as being due to material absorption or due to transverse power leakage out of the structure. The imaginary part of β , of course, gives the total attenuation rate, but cannot be used to identify what fraction is due to radiation or to absorption. Also, although $(S_{x2}-S_{x1})$ is easily calculated to give the net transverse power flow into or out of a layer, it is not very meaningful until the total propagating power flow within the layer is also known.

As a final note, it is important to realize that the familiar concept of orthogonality of the modes, over the cross section of the guides, does not

usually hold for complex modes. In the first place, orthogonality is defined only for bound modes; or, with the help of the delta-function, also for the plane wave spectrum of continuous modes [1, p. 24]. For improper modes, because they are unbounded, the integrals used in defining orthogonality do not in general exist. But even for bound modes, which are complex as a result of complex material parameters, the modes are not orthogonal to each other. In particular, the modes are not orthogonal in the power sense, where the cross product between two different modes is taken in the same form as a time average Poynting vector, with one of the field values conjugated [1, p. 30; 3, p. 231]. Rather, a mathematically more correct definition of orthogonality might be used, with no conjugation [3, pp. 229-231].

But more generally it should be recognized that the transverse eigenvalue problem here is not a self-adjoint problem [5, p. 241; 69, Chapt. 8]. The eigenvalues, β , are not real; the eigenfunctions (the discrete modes) are not orthogonal to each other. Instead it is necessary to consider the adjoint problem, involving both the adjoint differential operator and adjoint boundary conditions [5, p. 53; 69, p. 139, Chapt. 10; 87, p. 148]. Eigenfunctions of this adjoint problem then exist. The eigenfunctions of the original problem are then orthogonal to the adjoint eigenfunctions rather than to each other; that is, biorthogonality. The present problem is further complicated by the open boundary conditions, which depend on the eigenvalue parameter. The adjoint boundary conditions can then be quite different. For these reasons the orthogonality of the discrete modes is not further discussed.

7. EXAMPLE RESULTS AND DISCUSSION

The present formulation, using the program described in Part II, has been tested on a variety of problems. Few published results, for 3 and 4-layer cases, include numerical results to more than a few significant digits. This makes it difficult to verify the accuracy of the program. For several published results there is agreement to the available significant digits. Comparison with other locally available programs for calculating 3 and 4 layer cases also show agreement to the 6 to 8 significant digits available.

There may be a need for some standard test cases by which calculations by different workers can be compared for accuracy. An artificial four-layer case has been used to preset all input variables for the program; this default case can be run with a null set of input cards. Propagation constants accurate to 8 decimal places are listed in Part II, and may be used for accuracy comparisons.

Here we present two examples to demonstrate the ability to provide complete complex solutions to general problems. These are complicated, either because of the way the roots vary with changing parameters, or because there are many layers, including two guides and two exponentially thick layers.

7.1 Gain and Loss in Simple GaAs Double Heterostructure Laser

A four-layer model for a GaAs DH laser is shown in Fig. 7.1. It was used by Streifer, Burnham, and Sciefers [28] in studying the effect of substrate radiation losses on the laser threshold for different modes. It is a simple structure, with gain assumed throughout the higher index guiding layer, 2. But losses into the substrate layer 4 are deliberately introduced

by using a thin isolation or tunneling layer 3. The radiation loss to the substrate is greater for the higher order modes, and the intention is to suppress the lasing of these modes in favor of the lowest order mode. Their objective was to calculate, for each mode, the threshold gain required in layer 2. Several approximate methods of calculation were compared; the best one could be applied iteratively, and if repeated to convergence it could give exact results. These are perhaps the only published results which include effects of loss and gain in different layers as well as radiation.

This case was calculated using program MODEIG to check that results consistent with theirs could be obtained. In [28] results were given for the threshold gain to five significant digits for three modes, but no values for β were listed. Using their parameters, and threshold gain values, the propagation constant, β , was calculated for the three modes. The resulting imaginary part of β was negative, indicating mode gain, and it corresponded precisely to that needed to make up the mirror reflection loss which had been assumed. That is, agreement was obtained, and was consistent within the available significant digits.

Subsequently, W. Streifer kindly provided some further results for complex β , to many significant digits, for several values of gain and thicknesses of layer 3. These same cases were also calculated using MODEIG. For many different combinations of parameters there was always agreement to 7 significant digits, and in most cases to 8 decimal places for both real and imaginary parts for β . This is considered as a direct and reciprocal confirmation of the exactness of both calculations, made by very different methods.

An unanticipated result was the rather complicated situation that emerged concerning the TE_2 mode, which is near cut off into the top layer 1.

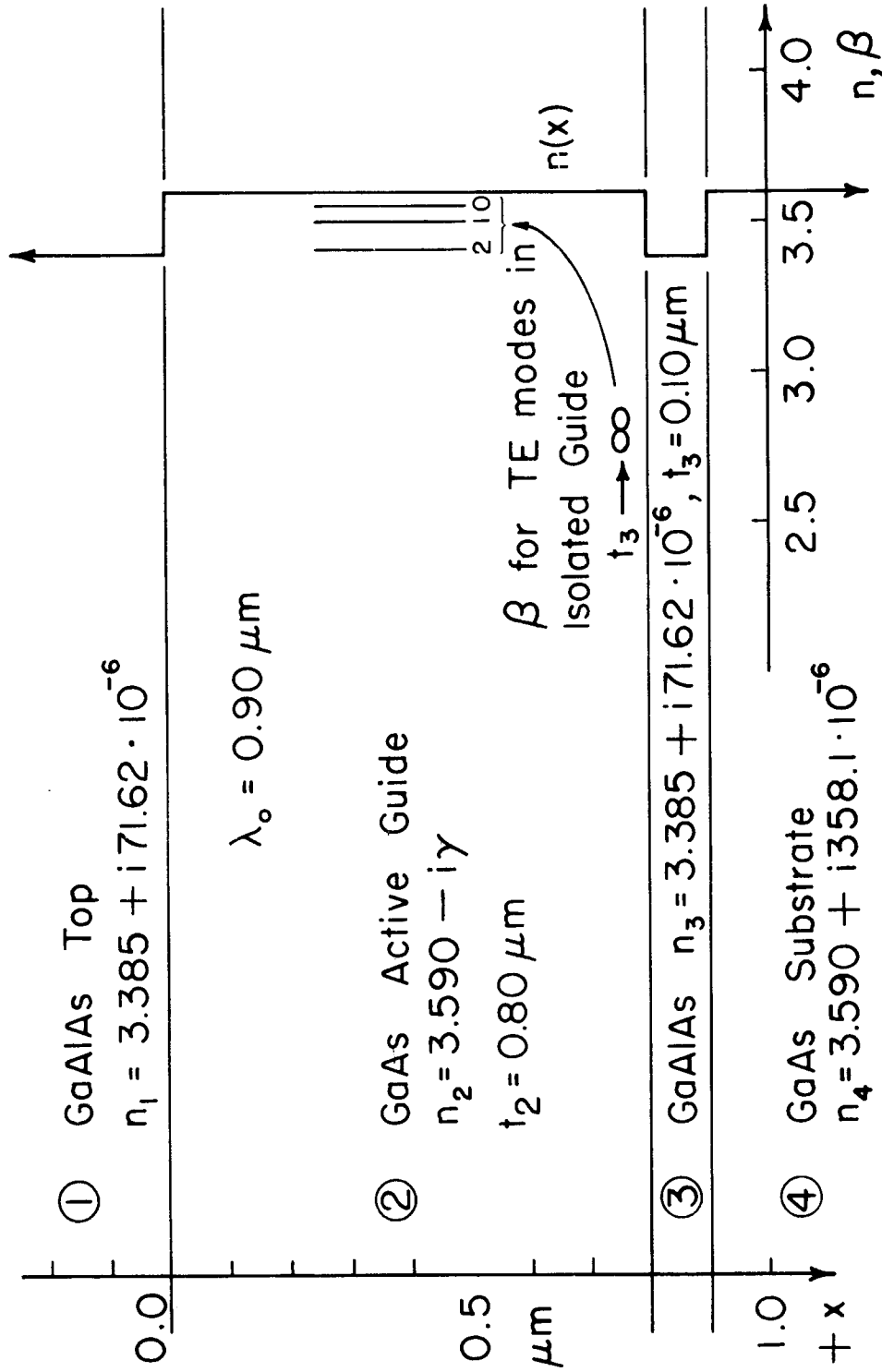


Figure 7.1 Four-layer GaAs DH laser model of W. Streifer, et al. [28]. Mode lines shown are for the isolated guide with $t_3 \rightarrow \infty$. For finite t_3 all modes are leaky into the substrate.

It was first observed that the solution for the TE_2 mode which was found by Streifer et al. was in fact derived from a root which, for lower gain, was strictly nonphysical. A different proper root for a TE_2 mode also existed which had a lower threshold gain. Subsequently, calculations of β were made for three or four modes, for a wide range of values of relative frequency and gain for the structure as shown in Fig. 7.1.

The results are shown in Fig. 7.2, displayed in the κ_1 -plane for the top layer. Thus, the modes are being described by their properties in the top semi-infinite layer. It is emphasized that all these modes are, in addition, leaky and improper in the substrate layer. The parameter values are shown in Fig. 7.1. Bulk attenuation is present in the three non-guide layers. Imaginary parts of n in layers 1 and 3 correspond to a bulk attenuation constant of $\alpha = 1.0 \text{ mm}^{-1}$. In layer 4 the value is $\alpha = 5.0 \text{ mm}^{-1}$. These are not very significant on the scale shown in Fig. 7.2; mode attenuation is primarily due to the substrate radiation. In the guide layer γ denotes the imaginary part of n , which is zero or negative representing bulk recombination gain. Results were calculated for three values of gain, denoted as g_1 , g_2 , and g_3 in Fig. 7.2. The g 's are intended to represent a negative value of α in units of mm^{-1} . The relationship to the imaginary part of n , say n_i , is that $\gamma \equiv -n_i = -\alpha/2k_0 \equiv g/2k_0$. The values represented by g_1 , g_2 , g_3 of Fig. 7.2 are

	$g = -\alpha$	$\gamma = -n_i$
g_1	293.22 mm^{-1}	$21.000 \cdot 10^{-3}$
g_2	363.03 mm^{-1}	$26.000 \cdot 10^{-3}$
g_3	568.34 mm^{-1}	$40.704 \cdot 10^{-3}$

These are listed for $\lambda_0 = 0.90 \text{ } \mu\text{m}$, $k_0 = 6.98132 \text{ } \mu\text{m}^{-1}$.

The principal features of Fig. 7.2 are the loci for the values of κ_1 with changing parameters. These are shown for three modes, for the different values of gain, including $g = 0$, and for a range of relative frequency $0.75 \leq \omega_r \leq 1.25$. With changing frequency, the value of $\kappa_1 \equiv k_x/k_o$ is defined using the fixed value of k_o corresponding to $\lambda_o = 0.90$.

Fig. 7.2 should be studied while keeping in mind the different regions of the plane shown in Fig. 3.2 and the mode classifications of Sect. 3.3. Fig. 3.6 is also relevant. The losses in layer 1 are not significant on the scale shown, so regions 2 and 3 of Fig. 3.2 reduce to the axes. Recall that in quadrants 1 and 3 modes will have gain in the direction of propagation, $\text{Im } \beta < 0$, and that leaky modes lie below the real axis on the right. The upper half plane is the proper branch of κ_1 , for modes which are bound in layer 1. Any formulations or calculations which are limited to this conventional branch specification would be blind to the behavior of the root loci shown in the lower half plane. The maps of the axes of the β^2 -plane, and the branch cuts corresponding to κ_4 , as shown in Fig. 3.6, all lie outside the region shown in Fig. 7.2. So these are not of concern here.

No branch boundary is indicated in the figure, because it is not relevant. Many of the points were calculated using the orientation shown by the line at 45 degrees. See Fig. 3.6. Separate calculations of the roots were made in the two half planes on each side of this line. But several other orientations were also used, particularly when there were roots near the origin. It is emphasized that the locations of the roots shown in no way depends on the choice of branch specification.

The loci for the bound TE_0 and TE_1 modes are well behaved; they lie near the positive imaginary axis for all parameter values. The TE_3 mode is a leaky mode for all values. But note that improper roots corresponding to

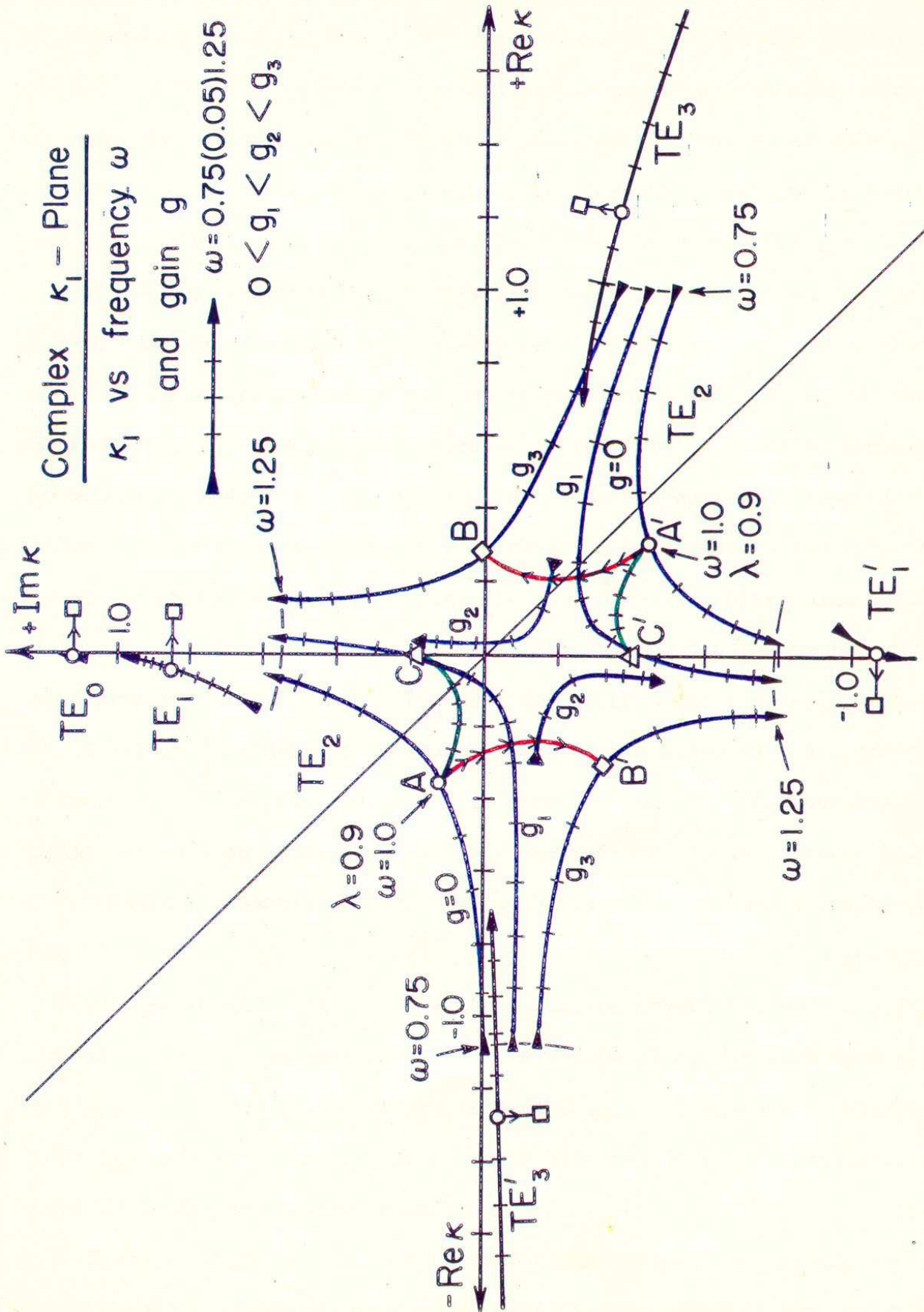


Figure 7.2 Locus of modes in the complex κ_1 -plane for top layer of DH laser, as a function of frequency and gain. Compare to Fig. 3.2. Central hyperbolic pattern is all associated with proper and improper TE_2 modes.

these modes also exist in some mathematical sense. These are labeled TE'_1 and TE'_3 . A TE'_0 root presumably exists also, but no special steps were taken to locate it. It may lie on the other sheet of this plane, associated with the other branch for κ_4 . The branch points for the branch cut in this plane (see Fig. 3.6) lie at $\Delta = \pm i 1.196$, just about where the TE'_0 root might be expected on the negative imaginary axis. Tamir [41] has shown that for a general layered structure roots always occur in pairs. One may be chosen, on the basis of branch specifications or physical arguments, to represent the mode. In the present case, because of the complex material parameters and substrate radiation, the pairs of roots do not have the symmetries noted by Tamir. But the number of existing roots is not affected though.

The remarkable feature of Fig. 7.2 is the central hyperbolic pattern. It is all associated with the TE_2 mode, showing how the two roots vary in the neighborhood of cut off. The case for no gain and a relative frequency of 1.0 may be considered a reference case, and is shown (for all modes) by open circles. The point labeled A is a proper root for TE_2 , but has a significant inward phase propagation. The point A' is an improper TE_2 root, with outward exponential growth dominating over the outward phase propagation.

With increasing thickness of the tunneling layer, t_3 , reducing the radiation loss to the substrate, the roots move along the loci from A and A' to the points C and C', marked by triangles on the imaginary axis. The point C is a truly bound TE_2 mode, along with the TE_0 and TE_1 modes. The point C' is strictly non-physical.

From the point A, now with increasing gain, the root crosses the real axis, becoming a mode with gain and moving to the point B' for the value of g_3 . The point A' moves upward with increasing gain, to become the point B

on the real axis. The point B is at threshold for the gain g_3 . The roots for all modes with $\omega = 1$, for gain g_3 , are shown by open squares. The TE_0 and TE_1 modes move into the first quadrant, becoming modes with considerable gain. The imaginary part for the leaky TE_3 mode is reduced, but not by much.

The value of gain for g_3 , in fact, is the threshold gain found by Streifer et al. for the TE_2 mode. The point B is their solution for the TE_2 mode at threshold and we agree to 8 digits in the value of β . But note that this solution derives, by a continuous variation of parameters, from the improper nonphysical root $C' \rightarrow A' \rightarrow B$. For this gain the other candidate root for the TE_2 mode is at B', improper and with considerable excess gain. But it, in fact, derives from the proper bound TE_2 mode at C and A. With gain increasing from zero, the root at A reaches the real axis, and threshold, at a gain of $g = 207.87 \text{ mm}^{-1}$, much lower than g_3 . Thus, the TE_2 mode root at A has a much lower threshold gain than was found by Streifer. For this reason it is proposed that the root at A is the more correct choice for the TE_2 mode.

With changing frequency, but now fixed gain, the roots move along the lines terminated by the solid triangles, which point in the direction of increasing frequency. All marks along these lines represent actual calculated points at intervals of 0.05; except along the line for g_2 , and the central part for g_1 , where the intervals are 0.01. The TE_0 and TE_1 roots are not very sensitive to frequency, but the TE_3 and especially the TE_2 modes are sensitive to frequency.

With increasing frequency, and no gain, the root at A moves up and toward the imaginary axis. The proper TE_2 mode thus becomes more bound, and farther from cutoff. The root at A' moves toward the negative imaginary

axis, becoming more "nonphysical". But, with frequency decreasing instead, it is the root of A' which moves to the right becoming more acceptable as the leaky TE_2 mode. And the root at A moves to the left; and in fact, crosses the real axis at about $\omega = 0.70$. Note that at $\omega = 0.75$ this root is in quadrant 3, implying a mode with gain; in spite of the fact that there is no gain in the system. So this root is not then acceptable to represent a TE_2 mode.

The behavior of the roots with changing gain also depends on frequency. For a frequency greater than about 1.02 the root from the locus of A crosses, not into quadrant 3, but into quadrant 1 as the gain is increased. Similarly, at the higher frequencies, the root from A' crosses into quadrant 3 with increasing gain, rather than into quadrant 1. So, a root may reach threshold either on the real or on the imaginary axis. The root from A attains threshold on the negative real axis for the lower frequencies, implying constant field amplitude in the transverse direction in the semi-infinite layer. But for the higher frequencies the same root reaches threshold on the imaginary axis, as do the TE_0 and TE_1 modes. This gives the very different, decaying exponential, behavior for the mode at threshold. Also note that a threshold condition on the negative real axis implies inward phase propagation; toward, rather than away from, the region of gain.

Clearly there is some problem in making a choice for which root is to be given a physical interpretation under different conditions of frequency and gain. This situation likely exists for any mode near cutoff. For some values of frequency and gain it may not be possible to make a choice. For example, at a frequency of about 1.02, and a gain slightly less than g_2 , both roots for TE_2 are located at about $\kappa_1 = -i 0.16$. (This is an example of the occurrence of a double root.) Both roots are strictly nonphysical

with pure outward exponential growth. Shevchenko [84, 85] has previously shown this situation to occur for the simpler symmetric slab guide. His results for the lossy slab guide [85] are the only other published work which resembles Fig. 7.2 here, and which demonstrates how complicated the situation for a mode near cutoff can be.

Even when there exists a choice, between the two different TE_2 roots, it may be difficult to make. For example, with zero gain and frequency decreasing from 1.25 to 0.75, the two roots trace out the loci through A and A'. The question then arises -- at what frequency does the TE_2 mode cease to be a proper mode, go past cutoff and become a leaky improper mode. If it is insisted that a TE_2 mode always "exists" then it is necessary, at some frequency, to switch attention from one locus to the other. The question cannot be answered by any fixed choice of principal branch specification. It may be seen that, whatever the orientation of branch boundary, there always exists a range of frequencies for which both TE_2 roots lie in the same, secondary, branch half-plane. The question does not necessarily have an answer because it oversimplifies the physical problem.

The mode concept is a mathematical construction, and individual modes offer only a partial description of any physical situation. Any actual problem must include sources or exciting fields, and observers; and the fields, which physically exist and are unique, can be given several mathematical representations. These may differ by having different choices of paths of integration for integral representations and different summations over discrete modes. One, both, or neither of the two TE_2 roots above might contribute to some representation. Only the complete summation and integral contribution has a unique physical interpretation. And great care must be taken in ascribing physical reality or existence to any single term in an

arbitrary representation.

The present example is somewhat unrealistic because the $t_3 = 0.10 \mu\text{m}$ is very thin and the radiation loss is excessive. The leaky modes, even the TE_0 and TE_1 , do not propagate sufficiently far to justify their usefulness as a discrete mode. This is certainly true for the TE_2 and TE_3 modes when they are leaky into both outer layers. The leaky mode concept is only useful when the imaginary part of β is a very small fraction (less than 0.001, say) of the real part. This can be realized to any degree by making t_3 thicker, such as 0.2 or 0.3 μm . But all the above descriptions of the root behavior would remain valid. The locus for the TE_2 would follow more closely the real and imaginary axes, and do so for smaller values of gain. The small value of t_3 has exaggerated the features in Fig. 7.2, and made them easier to calculate.

Note again, that in the absence of gain, the root for a proper bound mode is not necessarily the same root which becomes the leaky mode. It is proved here by example: the TE_2 mode with decreasing frequency. A similar behavior has been noted when the substrate is a lossy metal. This behavior was alluded to in Sect. 3.2, in the discussion of regions 1 to 4 of Fig. 3.2. It is likely that the bound and leaky mode roots remain on separate loci whenever the loss in the semi-infinite layer is less (in some sense) than the loss elsewhere in the guide or other semi-infinite layer.

This situation is emphasized here because it is not generally known. Often in the literature it is stated that proper bound modes pass beyond cutoff to become leaky modes. Or it is sometimes stated that leaky modes are obtained by analytic continuation of the proper root onto the improper plane (of β). This is certainly not generally true, as shown by the above examples. A simple case where the bound and leaky modes are part of the

same root locus is when the semi-infinite layer is lossy, with no other losses in the adjacent guiding structure. The locus would then likely lie in regions 2, 3, and 4 of Fig. 3.2.

The results for this example are presented to demonstrate the capability of the present method for readily calculating complex modes in very complicated situations. These results cannot be obtained by analytical means, and approximate methods are not likely to be successful. It would be very difficult to obtain these results for the TE_2 roots without the capability of the movable branch boundary. Also, roots very close to the branch point were found, with $\kappa < 0.1$. In the β^2 plane, where the root search is actually carried out, roots within 0.001 of the branch point were found (for example, with g_2 and $\omega = 1.03$). Further, there are two roots, very close to each other, and both close to the branch point. Once it is recognized that there are two roots in the vicinity, these are no more difficult to find than other roots. We believe that these capabilities of the present formulation and method are unique.

7.2 Modes of Seven-Layer Twin-Guide Semiconductor Laser

For an example of a more complicated structure, calculations were made of the modes in a seven-layer GaAlAs laser proposed and demonstrated by H. Suematsu et al. [29] and by Y. Kawanishi et al. [30]. All gain is provided by one guide which is parallel and distributively coupled to a second passive guide. Two designs are described. In [29] the active guide has reflecting end mirrors to form the laser cavity, and the passive guide serves only for output. In [30] the resonant cavity is formed instead by distributed Bragg reflectors at either end of the passive guide. Gain is provided by the strongly coupled active guide which has no end reflectors.

Their analysis was based on coupled mode theory, and on a first order perturbation analysis for the threshold gain. Here we present only some results for the true modes of the system of two coupled guides, and do not consider the effects of the end reflectors of either guide nor the effect of gain on the modes.

The structure is shown in the upper part of Fig. 7.3, where the dimensions and indices were taken from the model of Kawanishi, et al. [30, Fig. 1]. Two changes were made, however. Firstly, the thicknesses of the two tunneling layers, 2 and 6, were made smaller, $1.0\text{ }\mu\text{m}$. The original dimensions, 3.5 and $2.6\text{ }\mu\text{m}$, were sufficiently thick that no significant radiation occurred into the semi-infinite layers. That is, the problem was indeterminate in the sense described in Sect. 4.6, so it could be accurately solved instead as a 5 layer problem (layers 2 and 6 taken to be infinite). Reducing the thicknesses of layers 2 and 6 provides a more difficult test problem, of 7 layers with leaky complex modes. Secondly, some absorption loss was assumed for all layers; this had been ignored previously. Values for α were taken from the literature, corresponding to the Al concentration given in [30] for each layer. Values of $\alpha = 5.0\text{ mm}^{-1}$ were used in layers 1, 5, and 7. In layers 2 and 4, $\alpha = 1.0\text{ mm}^{-1}$; and in layer 3, the passive guide, $\alpha = 0.2\text{ mm}^{-1}$. For the following results no gain was assumed in layer 5, the active guide.

The values of β for the different TE modes are shown by lines superimposed in the different regions of Fig. 7.3. These values are on the same scale as n .

Mode lines in the two guide layers show β for the modes of the two guides when isolated from each other, by assuming that layer 4 is infinite. This is very easy to do with the program by specifying, for example, that

the right hand outer boundary condition is imposed at the boundary between layers 3 and 4. The rest of the structure to the right is then ignored. Similarly, the left hand outer boundary condition can instead be imposed at the boundary between layers 4 and 5, to calculate the modes in the active guide, ignoring the layers 1 to 3. Interestingly, these modes are all truly bound modes, in spite of the radiation leakage through the tunneling layer 2 or 6, respectively for the two separated guides. This is because of the bulk absorption loss in the semi-infinite layers; it is sufficient to absorb the tunneling energy, it does not radiate to infinity, and there is outward exponential decay for the fields. These occur in region 3 of Fig. 3.2, and might be called bound leaky modes. For thinner tunneling layers, and greater leakage of energy from the guide, this would probably not remain true.

The numerical values of β^2 for these modes were calculated to a convergence criteria of 10^{-10} , in 4 to 7 iterations per root, from the automatically generated starting guesses based on the phase integral. Only 8 decimal places are provided as output. The imaginary part of β , for the attenuation rate of these modes, was comparable to, but somewhat greater than, the imaginary part of the index in each guide layer. In the passive guide, for example, $\text{Im } n_3 = 10^{-5}$; and $\text{Im } \beta$ was on the order of 1.5 to $3.5 \cdot 10^{-5}$, and hence was known to 4 significant digits.

The dashed lines show modes which are beyond cutoff, and strongly leaky because there is no tunneling barrier. These leaky modes and the bound modes were calculated together as a set, with the branch boundary positioned to allow both types of modes on the same principal branch for κ of each of the semi-infinite layers 1, 4, or 7.

The mode lines for the complete structure, as shown, are indicated in layer 6. If the values of β^2 for the two separated guides, to two decimal

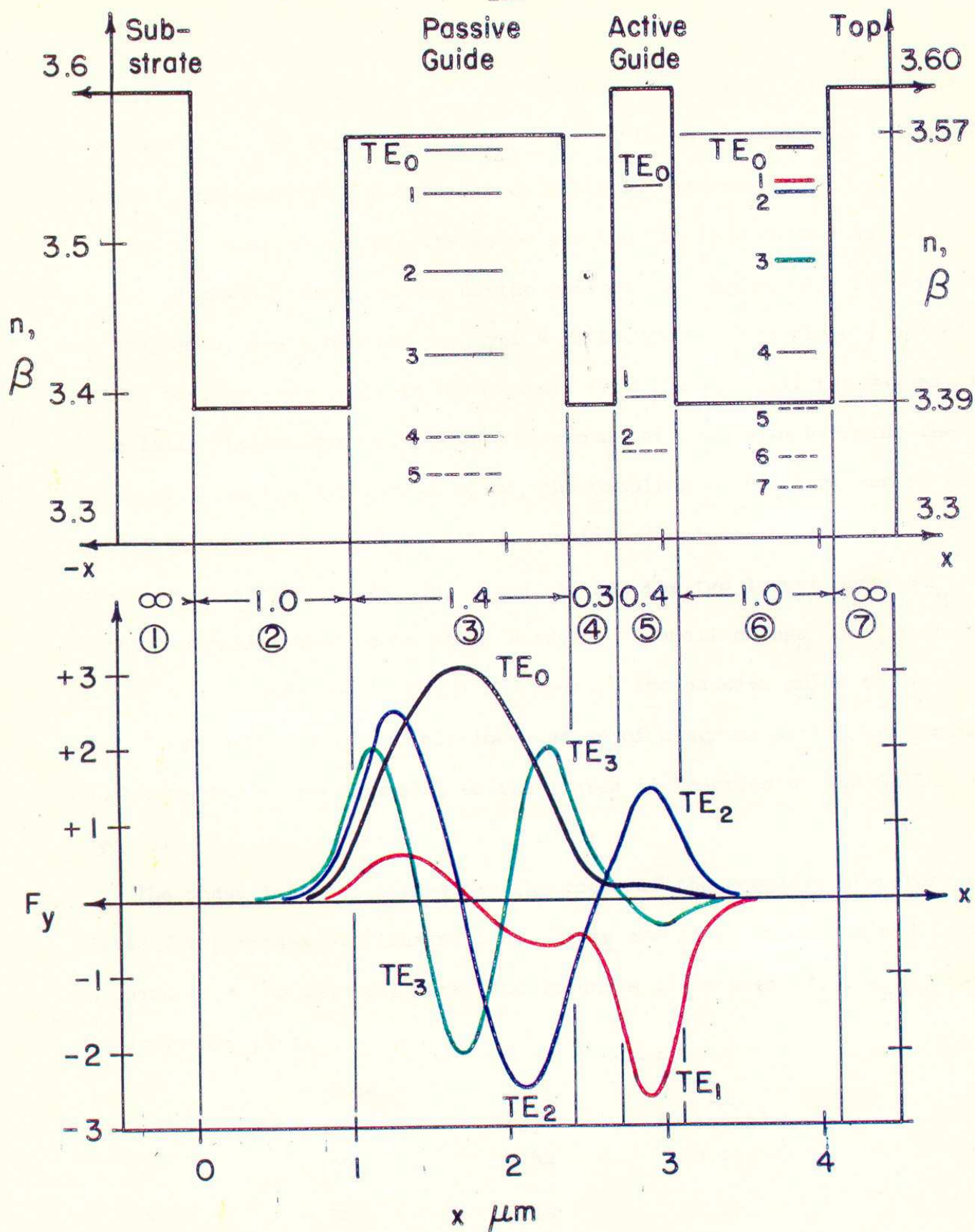


Figure 7.3 Seven-layer twin-guide GaAs laser of Suematsu and Kawaniski, et al. [30]. Index distribution and fields. Mode lines in layers 3 and 5 show values of β for the modes of the two separated guides, $t_u \rightarrow \infty$. Values of β for modes of complete structure are shown in region 6.

places, are used as starting guesses, convergence to 10^{-10} in β^2 is obtained in 3 iterations per root. This is considered to be a remarkably efficient, and exact, calculation for a rather complicated structure.

The TE_1 mode in the passive guide and the TE_0 mode of the active guide are nearly phase matched. And, in the concept of coupled mode theory, these are coupled by field overlap in layer 4 to become the two closely spaced TE_1 and TE_2 modes of the complete structure. From the original two values of β (especially their difference), and the amount of change in becoming the values of β for the two normal modes, the coupling coefficient can be calculated. There may be a mistake in the published values of n for this structure. The analysis in [29, 30] intended that the two lowest order TE_0 modes in the two guides were to be phase matched. A small change in n_3 from 3.57 to 3.55 would lower the β of the TE_0 mode in the passive guide to match that of the active guide. This lower value of n agrees better with published results for n corresponding to the listed Al fraction of the GaAlAs of layer 3.

The phase integral values for the modes of the complete structure are listed for purposes of illustration. These are given in normalized form, in units of π for the real part, and in units of decades ($\phi_I/\log_e 10$) for the imaginary part.

Mode	ϕ_R (π)	ϕ_I (Decades)
TE_0	1.34	7.95
TE_1	2.19	7.38
TE_2	2.36	7.21
TE_3	3.36	5.91
TE_4	4.31	3.55
TE_5	5.22	0.18

The first three modes are not spaced at integer numbers of π in Φ_R , and modes 1 and 2 are closely spaced. For the last three modes the integer part of Φ_R/π does correspond to the mode index. An imaginary part of about 7 for the first three modes shows that these may be somewhat indeterminate (due to the thick layers 2 and 6). With an 8 digit computer there may be difficulties with calculating these modes. Interestingly, the elements of the C^+ matrix for these modes were not large, probably because of approximate symmetry of the two thick layers.

The field distributions for the first four TE modes of the complete structure are shown in the lower part of Fig. 7.3. These are exact; rather than being based on coupled mode theory and linear combinations of the fields in the two separated guides, as usually encountered in the literature. Of course, the resemblance to the mode shapes in the individual guides is evident. The TE_0 and TE_3 modes are close to the TE_0 and TE_2 modes of the passive guide, with little field amplitude in the other guide. The TE_1 and TE_2 modes may be described approximately as the two possible linear combinations of the TE_1 mode of layer 3 and the TE_0 mode of layer 5. Each of these modes is normalized arbitrarily, and they do not represent the same amount of propagating power.

A more novel result, rarely mentioned in published examples, is the transverse power flow across the structure, shown in Fig. 7.4 for the first three modes. This transverse Poynting power density is routinely calculated whenever calculation of the field distributions is made. These results are for no gain in the active layer. The source of this transverse power flow is the propagating energy of each mode. Some fraction of the propagating energy diverges and flows transversely to supply the radiation and absorption losses outside the guiding layer. This implies a curvature of the

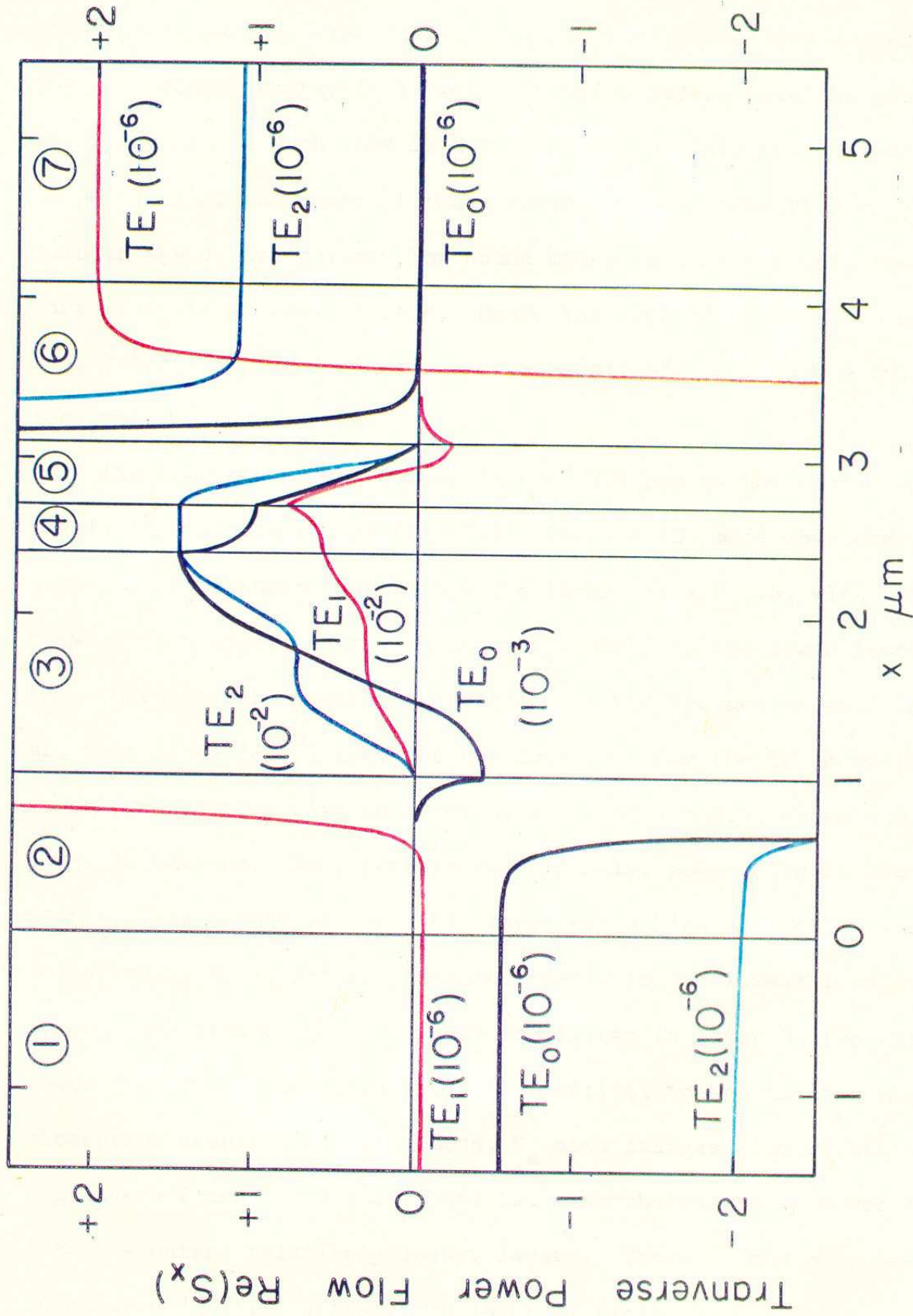


Figure 7.4 Transverse real power flow in twin-guide laser. No gain in active guide. Positive power flow is toward top layer.

phase fronts across the guide; the field quantities, F , do not have a constant phase factor. The shapes of these curves are very dependent on where the propagating energy is largest, on which layers have the greatest absorption, and on how much loss is due to radiation into the semi-infinite layers. In particular, the shape of these curves is very sensitive to the amount of gain in the active guide. For bound modes in lossless structures the real part of S_x is everywhere zero. Hence the type of information shown in Fig. 7.4 for a practical structure is available only from a fully complex treatment of the problem.

The features of the curves in Fig. 7.4 can be correlated somewhat with the field distribution of Fig. 7.3. For the TE_0 mode most energy is in layer 3. S_x changes sign within the layer, at $x \approx 1.5$, with power flow outward into upper layers, positive S_x , and into the lower layers, negative S_x . There is more power flow ($0.5 \cdot 10^{-6}$) into the nearer semi-infinite layer, than flows (10^{-8}) into the top layer 7. For the TE_1 mode the transverse power flow changes sign in layer 5, at about $x = 2.9$, where the propagating power is maximum. But, perhaps surprisingly, power flow is now toward this point. This occurs because this layer has a high absorption loss compared to layers 2, 3, 4, and 6. Because layer 3 is the lowest loss material, and a large fraction of the TE_1 power propagates in layer 3, the transverse power flow throughout this layer is positive, toward layer 5 where most absorption occurs. For this mode, S_x also changes sign within the tunneling layers 2 and 6; so that there is, nevertheless, some power flow outward into the outer, relatively lossy, layers. There is now more power flowing into layer 7 ($2 \cdot 10^{-6}$) than into layer 1, ($1 \cdot 10^{-7}$).

For the TE_2 mode more power propagates in layer 3, and S_x throughout the layer is toward the absorbing layer 5. S_x is nearly constant in layer 4.

This layer neither absorbs nor contributes to the transverse power flow across it. Its absorption is not large, and there is a node for the TE_2 mode within this layer (as seen in Fig. 7.3). Note that at other nodes in layer 3, for the TE_1 and the TE_2 modes ($x \approx 1.75$), S_x is also constant. For the TE_2 mode there is also a sign change in S_x at $x = 1.0$, but is not visible on the scale of the figure.

This type of information is uniquely available from a fully complex calculation of modes in a structure. It would be helpful, for example, in designing, or modifying the designs, of semiconductor laser structures by identifying regions contributing greatest power loss.

7.3 Conclusions

These examples show that the objectives of this work have been fully realized. Using the formulation, as programmed, it is possible to calculate any complex modes, propagation coefficients and field distributions, proper or improper, physical or nonphysical, for any arbitrary layered structure. Moreover, these may be calculated efficiently and to high accuracy.

This capability is made possible by: a) use of the 2×2 matrix method for calculating both the field distributions and the characteristic function, b) a characteristic function having maximum analytical properties, and c) an efficient complex root searching algorithm. The capability for accuracy is preserved by careful attention to detail, in avoiding variables and expressions which may inadvertently become indeterminate, and using a power series if necessary.

We believe that the results obtained, particularly program MODEIG, represent a powerful capability which has not previously existed. It

should prove valuable for the analysis of a large number of different planar structures, which are the prototypes of many practical integrated optics devices, or for other guiding or nonguiding layered structures.

Part II. FORTRAN PROGRAM MODEIG

The formulation described in Part I has been programmed in FORTRAN for rather complete case by case calculations of any arbitrary structure. The program follows very closely the analytic formulation. A large number of comment cards is included, so that the program is largely self-documenting. It should not be difficult to locate and follow the calculation steps if necessary.

1. Program Structure

The program consists of a group of subroutines which, for each case, are called in turn to perform various parts of the calculation. Each subroutine provides appropriate output associated with its function. Communication of variables between subroutines is almost entirely by means of labeled COMMON blocks. Following is a brief description of the various program units in the order of appearance in the listing in Sect. 3.

MODEIG Is the main program, and consists only of a sequence of calling statements to the other subroutines. It reads no input and prints no output. New cases are repeatedly called for and solved until a stop command is encountered or there is no more input.

BLOCK DATA BLOKOM Is a FORTRAN program unit in which all common-block data variables are declared, and preset to prescribed default values. A large block of comment cards is also included in which all input variables are described. These are listed within each of three NAMELIST groups.

Two example sets of actual input cards are also included as comment cards.

PUTSIN Is a main subroutine which reads input for each case, and calculates all needed variables and starting parameter values for use by other subroutines. NAMELIST groups are declared, input cards are read, and needed variables are preset or calculated according to TE or TM polarization. No other subroutines depend on type of polarization. A principal function is printing an output summary of the layered structure, with all important variables and calculated parameters for each case.

SEARCH Is the principal subroutine for calculation of discrete modes by calls to other subroutines. For non-eigen boundary conditions no search is made. It calculates initial guesses for complex root search, initializes necessary parameters, and calls CZEROM for the root search. For all discrete modes which are found it calculates all other mode parameters, matrices, propagation constants, admittances, and phase integral and writes summary for each mode.

COMPLEX FUNCTION EIGEQF Is a short subroutine to evaluate the characteristic function for any value of $QZ \equiv \beta^2$. Called only by CZEROM, it is used once for each iteration during the root search. It calls subroutine SYSMAT to obtain values of the $SM = S^+$ matrix, and then selects proper element for use as characteristic function, depending on inward/outward type of boundary conditions. Several modified or renormalized characteristic functions remain as options, but are not now recommended for use.

SYSMAT Is a core subroutine for the whole program. For any value of $QZ \equiv \beta^2$ ($WZ \equiv \beta^2$) it calculates phase thicknesses for all layers and accumulates

the phase integral. Calculates transform matrices for all layers, and by forward chain matrix multiplication calculates the $CM \equiv C^+$ matrix for whole structures. Calculates transverse propagation constants, $WX \equiv \kappa$, and wave admittances, $YX = Y_x$, of outer layers. Using the four combinations of outer boundary conditions it calculates the $SM = S^+$ matrix of four possible characteristic functions. Most calls come from EIGQF; but SYSMAT is also called by SEARCH and by FIELDS to obtain the same set of parameters for any given values of QZ for discrete or continuous modes.

FIELDS Calculates the set of tangential fields FY and FZ, and transverse Poynting power PX, at all boundaries, for each value of $QZ = \beta^2$ in an array QZM. These values may be discrete modes as found by subroutine SEARCH; or they may be arbitrary input values, as for the continuous spectrum or plane-wave spectrum for which no search is made. Two normalized sets of boundary field values are calculated (FY, FZ and GY, GZ), starting with the two opposite outer boundary conditions separately. Cross products (Wronskians) between these two sets are calculated as numerical checks on reciprocity and the characteristic equation. A summary output for these fields and checks is written. For discrete modes the average of the two fields is used. Calculates all fields, including PX, FX and the longitudinal propagating power, PZ, incrementally at a closely spaced set of points in x.

LAYMAT Is a short subroutine to calculate the layer transform matrix for any layer. Called only by FIELDS, for a full layer or for an incremental layer. Within SYSMAT a similar calculation is done in-line by a duplicate block of statements (more efficiently than by calling LAYMAT).

POWERS Is provided for future implementation of calculation of total propagating power in each layer, and if finite, the total propagating power in the structure. All common blocks and needed variables are provided, but no calculations are yet implemented. Called by FIELDS for each value of $QZ \equiv \beta^2$ after fields are calculated.

CZEROM(CFCN) Is a general purpose subroutine for calculations of complex roots of an arbitrary complex function $CFCN(Z,N)$. Called by SEARCH, with $CFCN = EIGEQF$, and $Z = QZ$. Muller-Traub method is used with additional improvements as described in Part I, Chapter 5. Each call to CZEROM calculates a set of roots, not just a single root. For each root, four calls are made to EIEQF in setting up the initial iterates, and then one call to EIGEQF if made for each iteration. Unlike most library subroutines, and for better efficiency, variables are communicated to and from the calling program by a COMMON block /CZECOM/.

MODEIG, altogether, is a rather large program. It was intended primarily for complete solutions on a case by case basis. Any change of parameter is considered a new case, and a complete solution is presented for each. Input cards for any number of cases can be submitted together, and it is only necessary to include those input values which are changed from each previous case. Some of the output for each case can be suppressed, at input option; or much more output can be requested, as for diagnostic purposes.

The program is not as efficient as it could be for calculation of dispersion curves, such as β vs. frequency, or for a large number of values

for any changing parameter such as a layer thickness or permittivity. No provision is made for incrementing any parameter; and for each new input value, the complete solution process, and output, is repeated. For very general structures it is not possible to anticipate which parameter it might be decided to increment.

A total of about 2100 cards appear in the listing in Sect. 3. About one third of these are comment cards. Nearly 200 of them appear in the BLOCK DATA unit to describe the input variables, and the rest are distributed throughout the program for self documentation and spacing. Together with a large number of type declarations for variables, common block declarations, and format statements, there may remain less than half the total cards as actual executable statements.

The program has only been compiled and executed on a CDC 6400 or CYBER 73 computer, using the CDC RUN FORTRAN compiler. A maximum of 44000 (Octal) words was required to compile (Subroutine FIELDS), and 33000 (Octal) is required for loading. The final length, loaded for execution with all library functions and input/output subroutines, is about 26000 (Octal) words. The RUN compiler does not provide a very high level optimization, and it is not known how much faster execution could be obtained using, for example, the CDC FTN compiler.

The CDC computers are ideal for this type of calculation, with the long word length providing 14.7 significant digits. On other computers, of say 8 significant digits, it will not be possible to solve as wide a range of problems. There appear to be no FORTRAN compilers which provide

double precision capability for complex variables. With 8 digits a problem can more easily become indeterminate.

The program is not considered to be complete nor in final form. It is believed that most options and alternatives have been tested and work as intended, but this cannot be guaranteed. Least tested are the various options for greater or abbreviated amounts of output from each subroutine. Hopefully, MODEIG will be used on a variety of problems; and with more experience some features may be found to be of little use, and it may be necessary to add other needed features. If the program is widely used, it would be worthwhile to eventually write a users manual.

are associated with indexing over layers or boundaries. Those starting with M are associated with modes, and those starting with I represent root searching iterations or parameters for incrementing x.

An attempt has been made to make the input foolproof so that some case is calculated with no fatal execution-time errors due to undefined variables or singular values. The first line of defense is all the preset default values. But in addition, there is considerable checking of input values. For example, all boundary locations $XL(L)$ are checked and reordered if necessary for increasing XL with increasing index L ; and all thicknesses $TL(L)$, if used for input, are made positive. Similarly many control parameters are checked to be positive; and, for example, the $L1$ and $L2$ for the outer boundary conditions are ordered so that $1 \leq L1 \leq L2 \leq LN$. The values are changed if necessary.

Modes are indexed internally, and in the output, by an index $M = 1$ to MN (and also for input values QZM and KM , if used). M is not the ordinarily understood mode index. An input bias parameter MO is available to define an intended mode index $MM = MO + M$, which is also used to label the output. MM is used explicitly only in the interpolation for starting guesses, and there is no assurance that MM will correspond to the index (if defined) of the modes actually found. Starting guesses (if $KGSS = 3$) are based on MM and input values for $PMFR$ and $PMDM$. Values of QZ are interpolated to give an intended real phase integral $PHM = MM * PMDM + PMFR$ in units of π . $QZNR$ and $QZNI$ are also important input parameters used in calculating the starting guesses. $QZNR$ should be on the order of the smallest value of PER in the structure.

The dimensions of the layered structure can be read in either by the locations of the boundaries $XL(L)$, or by the thicknesses of all the layers

TL(L), depending on KXTL. The total number of layers is LN. With the default KXTL = 1, then values of XL(L) are expected, and the thicknesses are calculated from their differences. But if KXTL = 2 is included in the input list of \$LAYERS then values of TL(L) from TL(2) to TL(LN-1) are expected in the list. Values of XL are then calculated from the thicknesses, starting with XL(1) = 0.0. Any units may be used for the dimensions, it is only necessary that WVL and XL or TL be expressed in the same units.

One useful provision allows the reference value for the free-space k_o to be specified by means of a wavelength or by a frequency. Two input parameters are provided-- a nominal wavelength, WVL, and a frequency factor, KC, which is allowed to be complex, and is actually read in (if used) by its real and imaginary parts, KCR and KCI, separately. WVL and KCR are preset to 1.0, and KCI to 0.0. To calculate cases for a set of different wavelengths, the different values of WVL would appear on input cards. Then, as usual, $k_o = KO = 2\pi/WVL$, provided that KC = 1.0 is unchanged. It may be desired instead to calculate cases for a sequence of frequency values rather than wavelength. Then a nominal value of WVL is first entered, and different values of KCR are entered as input for successive cases. The effective k_o is then given by $k_o = KC*KO = 2\pi KC/WVL$. That is, k_o depends on both WVL and KC. All propagation coefficients for modes and materials are normalized to this value of effective k_o . It should be kept in mind that if KC (that is, KCR) is not unity then the effective reference wavelength is not WVL, as input, but is multiplied by 1/KC.

KF is the relative frequency, ω_r of Sect. 2.2, and is also allowed to be complex. For input, it is read in by the real and imaginary parts separately, KFR and KFI, and these are preset to 1.0 and 0.0. That there are two complex frequency factors, KC and KF, can lead to confusion. Recall

that for different values of WVL (or KC) the propagation coefficients are always normalized to the different resulting values of k_o . But for fixed WVL, KC, and k_o , and changing values of $\omega_r = KF$, the resulting propagation coefficients are normalized to the fixed reference value of k_o . Either KC or KF may be used as the frequency parameters, depending on whether $\beta = WZ$ and $\kappa = WX$ are to be normalized to a variable or to a fixed value of k_o . Only if $\omega_r = KF = 1.0$ can WZ and WX be directly compared to the indices of refraction of the materials. If KF is not unity, then the relative wavelength is also different from the nominal input value, WVL.

Input for the material parameters of each layer is by means of the real and imaginary parts of the (relative) permittivity PER, PEI. A single value for the permeability, common to all layers, is also allowed to be complex, PMR, PMI. It is important to keep in mind the variation of the permittivity with frequency when using the frequency factors KC and KR. For careful quantitative calculations the desired values of PER and PEI must be obtained for each different frequency. These will depend, for example, on the model chosen to represent the material losses (or gain). A useful addition to the program would be a subroutine which, by input option, would calculate PER and PEI on the assumption of several possible models. These could include models assuming a constant conductivity, or a constant bulk attenuation coefficient, or a plasma model with parameters for resonant frequency and collision rate.

The outer boundary conditions may be imposed at any boundary specified by L1 and L2. At the start of any case these are set to $L1 = 1$, the first boundary, and $L2 = LN-1$, the last boundary. These may be changed by input values to any interior boundaries, $L1 \leq L2$, for calculations of any partial

structure. When either boundary condition is imposed at an interior boundary, then the adjacent outer layer is taken to be semi-infinite, ignoring its finite thickness and any other layers beyond. The type of boundary condition is specified by parameters KBC1 and KBC2. These determine whether the wave admittance YX in the semi-infinite layer is used ($KBC \leq 1$), or whether a fixed surface admittance $YB1$, $YB2$ is used ($KBC = 2$) or a surface impedance $ZB1$, $ZB2$ is used ($KBC = 3$). The directional sense for the solutions in the semi-infinite layers is specified by parameters KBD1 and KBD2: $= 1$ for inward, or $= 2$ for outward solutions. The principal branch specification for $WX(L)$ and $YX(L)$, in the outer layers $L = L2$, and $L = L2+1$, is determined by APB1 and APB2, the angles of the unit normal direction, ϕ , in units of π . See Sect. 3.3, Part I. The directional sense for the fixed surface admittance/impedances is also determined by KBD1 and KBD2. Either or both KBC1 and KBC2 may be zero to imply non-eigen conditions; no root search is then made, and both inward and outward solutions are allowed in the respective semi-infinite layers.

The use of input variables is best described by examples, which are given here for four different structures. Each set of input cards may include any number of cases, each starting with \$CASE, and also having cards for \$LAYERS and \$MODCON. After the last case in a set, a normal stop is made by a single \$CASE card containing KASE = 0, or KD00 = 0.

All examples below are direct card images, and start in column 2. There is a blank in column 1. All remaining 79 columns of a card may be used.

The default case, with all default parameters, may be calculated with the null set of input cards:

```
$CASE      $END
$LAYERS    $END
$MODCON    $END
$CASE KASE=0 $END
```

The same default case, but for TM modes, (KPOL = 2) is calculated by:

```
$CASE      $END
$LAYERS    $END
$MODCON KPOL=2 $END
$CASE KASE=0 $END
```

More TM modes, more stringent convergence criteria, and calculations of field distributions for the default case will be obtained by the set:

```
$CASE KASE= 5, MN=7,
KGCZ=4, EPS1=1.0E-10, EPS2=1.0E-10, IL=15,
KDOF=2, KOUF=4,
$END
$LAYERS    $END
$MODCON KPOL=2 $END
$CASE KASE=0 $END
```

These input cards were used to obtain the example of output shown in Sect. 2.3, next.

The following set of input cards includes six cases for the 4-layer DH laser of Sect. 7.1, Part I, for the relative frequency, KFR, decreasing from 1.0 to 0.75 in steps of 0.05. Layer 2 has gain, PEI(2) negative; and others are lossy, PEI positive. Note that PER(2) and PEI(2) overwrite the values just read in the previous two cards. The principal-branch boundary in the top layer is reoriented to 0.75π (APB1), and applies to all cases.


```

$CASE KASE= 703045,
MN=4, QZNR=10.0,
KGCZ=4, EPS1=1.0E-8, EPS2=1.0E-8, IL= 15,
$END
$LAYERS WVL=0.9,
XL(1)= 0.0,0.8,0.9,
PER(1)= 11.4582, 12.8880, 11.4582, 12.8881,
PEI(1)= 0.48486E-3, 0.51423E-3, 0.48486E-3, 2.5711E-3,
PER(2)= 12.88766, PEI(2)= -150.78E-3,
$END
$MODCON APB1=+0.75 $END
$CASE $END
$LAYERS KCR= 0.95 $END
$MODCON $END
$CASE $END
$LAYERS KCR= 0.90 $END
$MODCON $END
$CASE $END
$LAYERS KCR= 0.85 $END
$MODCON $END
$CASE $END
$LAYERS KCR= 0.80 $END
$MODCON $END
$CASE $END
$LAYERS KCR= 0.75 $END
$MODCON $END
$CASE KASE=0 $END

```

The 7-layer twin guide laser, of Sect. 7.2, Part I, is calculated for four cases by the following set of input. MN = 5, 3, or 7 modes are sought; no fields are calculated, KDOF = 0; thicknesses TL are read in since KXTL = 2; and all layers are lossy, PEI positive. The first case calculates only the partial structure for the first guide, layer L = 3; the second boundary condition is imposed at L2 = 3, and layer 4 is taken to be semi-infinite (ignoring the value for TL(4)). The second case calculates the partial structure for the second guide, layer L = 5; the first boundary condition is imposed at L1 = 4, again taking layer 4 to be semi-infinite. The next case calculates the full structure, L1 = 1 and L2 = 7 being reset internally. Input starting guesses are used, KGSS = 1, and these are provided by the MN = 7 complex values for QZM. All guesses are divided out, and initial

iterates are at a radius of 10^{-4} , $KM = 4$, for all seven values. The last case repeats the calculation with some gain in the active guide, $PEI(5)$ negative. Roots from the previous case, remaining is array $QZM(M)$ are used as guesses, all $KM(M)$ being reset by input to 4, as previously.

```

$CASE KASE= 703116,
MN=5, QZNR=10.0,
KGCZ=4, EPS1=1.0E-10, EPS2=1.0E-12, IL= 15,
KDOF= 0, KOUF= 0,
$END
$LAYERS WVL=0.86, LN=7,
KXTL=2, TL(2)= 1.0,1.4,0.3,0.4,1.0,
PER(1)= 12.9600,11.4921,12.7449,11.4921,12.9600,11.49210,12.9600,
PEI(1)= 2.46E-3,0.46E-3,0.10E-3,0.46E-3,2.46E-3,0.46E-3,2.46E-3,
$END
$MODCON L1=1, L2=3 $END
$CASE
MN=3, QZNR=10.0,
$END
$LAYERS $END
$MODCON L1=4, L2=6 $END
$CASE
MN=7, QZNR=10.0,
KGSS=1, QZM(1)= (12.68,0.0),(12.51,0.0),(12.47,0.0),(12.15,0.0),(11.73,0.0),
(11.49,0.0),(11.30,0.0),
KM(1)= 4,4,4,4,4,4,4,4,
$END
$LAYERS $END
$MODCON $END
$CASE KGSS=1, KM(1)= 4,4,4,4,4,4,4,4 $END
$LAYERS
PER(5)= 12.9600, PEI(5)= -1.23E-3,
$END
$MODCON $END
$CASE KASE=0 $END

```

The last example is for a stepped approximation to a quadratic permittivity profile, $n^2 = 9.0 - x^2/4$, and it illustrates the use of a fixed surface admittance/impedance. Nine layers are used to describe half the symmetric structure. A closed boundary condition, $KBC1 \geq 2$, is used at $XL(1) = 0.0$ to represent the midplane, and layer 1 is ignored. An open boundary condition is used ($KBC1 = 1$, as in all previous examples) at the last boundary $XL(9)$; so that layer 10 is taken to be semi-infinite, and truncates

the quadratic profile at $n^2 = 1.5$.

In the first case the even modes are calculated (FY symmetric about $x = 0.0$) by using a zero surface admittance(TE) at the midplane; that is, $KBC1 = 2$, $YB1 = 0.0$. In the second case the odd modes (FY an odd function about 0.0) are calculated by using a zero surface impedance(TE) at the midplane, $KBC1 = 3$ and $ZB1 = 0.0$. The fractional part of the phase integral, PMFR, as used in generating the initial guesses, is different in the two cases. The solutions correspond to a symmetric approximating structure of 16 finite layers plus the two outer semi-infinite layers. The values of $PER = n^2$ are taken at the levels of the mode values $\beta_m^2 = 9.0 - (m + 1/2)$, which are expected for the continuous profile. The values for XL are about midway between the turning points for these modes, but are calculated so that the average of n^2 between any two boundaries is in fact the same as that of the continuous profile.

```
$CASE KASE=704102,
  MN=5,
  PMFR= 0.25,
  KGCZ=4, EPS1=1.0E-8, EPS2=1.0E-12, IL= 15,
  KDOF=1, KOUF=4,
$END
$LAYERS
LN=10, WVL= 6.28318530,
XL(1)= 0.0, 0.942809, 1.978085, 2.820973, 3.460071,
3.997388, 4.470269, 4.897560, 5.290377,
PER(1)= 1.0, 9.0, 8.5, 7.5, 6.5, 5.5, 4.5, 3.5, 2.5, 1.5,
$END
$MODCON
KBC1=2, YB1=(0.0,0.0),
$END
$CASE
PMFR= 0.75,
$END
$LAYERS $END
$MODCON
KBC1=3, ZB1=(0.0,0.0),
$END
$CASE KASE=0 $END
```

2.2 Default Case

The default case is a four-layer structure ($LN = 4$) with simple values for permittivity (PER, PEI) comparable to glass. A guide layer is separated from a higher index semi-infinite layer by a low index air layer, as for a prism coupler. All material parameters are real. The dimensions are chosen so that there are two bound lossless modes, one complex mode which is weakly leaky into the high index semi-infinite layer, and additional modes which are leaky into both outer layers. About 8 modes exist for which $\text{Re } \beta^2$ is positive. The parameters for the structure are:

Layer (L)	Thickness (TL)	$\text{Re } \epsilon = n^2$ (PER = QN)	N (RN)	
1	inf.	2.25	1.5	Top
2	1.0	1.00	1.0	Air
3	2.0	2.56	1.6	Guide
4	inf.	1.96	1.4	Substrate

The structure is lossless, $\text{Im } \epsilon$ (PEI) is zero. The reference wavelength (WVL) is set to 1.0 which becomes the units in which $x_\ell = XL(L)$, and $t_\ell = TL(L)$ are expressed. The units of dimensions are immaterial, it is only necessary that λ_0 and x or t are expressed in the same units.

For the two bound modes, the imaginary part of β should be zero, as well as a large number of real or imaginary parts of other quantities. For example, all κ values should be pure real or imaginary, the imaginary part of F_y and real part of F_z should be zero, etc. Numerically, this will not be true due to inexact convergence to the real roots in β^2 , and due to round-off accumulation in the calculation of all variables. The magnitude of the

quantities which should be zero will then give direct and immediate evidence of the residual error in the calculations. It is not necessary to compare the results to known accurate values in order to estimate the fractional or absolute accuracy.

The default control parameters call for calculation of four ($MN = 4$) TE modes ($KPOL = 1$), at $\lambda_0 = 1.0$ ($WVL = 1.0$, $KC = (1.0, 0.0)$, $KF = (1.0, 0.0)$). The boundary conditions, applied at the outer boundaries ($L1 = 1$, $L2 = 3$), call for open boundary eigenconditions ($KBC1$, $KBC2 = 1$), and outward-only solutions ($KBD1$, $KBD2 = 2$). The principal-branch boundaries for $WX \equiv \kappa$ in the outer layers are oriented at $\phi \equiv APB1 = APB2 = 0.25\pi$ (Sect 3.3; Figs. 3.5 and 3.6).

Root search parameters are rather conservative. Iteration limit is $IL = 10$, and the convergence criteria are $\epsilon_z \equiv EPS1 = 10^{-6}$, $\epsilon_f \equiv EPS2 = 10^{-6}$. Initial guesses are calculated by phase-integral interpolation ($KGSS = 3$), initial guesses are not divided out ($KGCZ < 4$), and initial iterates are calculated at a radius of 10^{-3} ($KGCZ = 3$).

Field values are calculated only at the boundaries ($KDOF = 1$, $KOUF = 3$), and the Wronskian characteristic function is calculated for checking.

Propagation constants $WZ \equiv \beta$, for the first 7 seven modes of each polarization, to 8 decimal places, are:

Mode	Re β	Im β
TE_0	1.58562152	0.0
TE_1	1.54225504	0.0
TE_2	1.46994487	0.00000002
TE_3	1.37930840	0.01386909

Mode	Re β	Im β
TE ₄	1.21789538	0.04953175
TE ₅	0.99336621	0.08195785
TE ₆	0.87761217	0.06198096
TM ₀	1.58395407	0.0
TM ₁	1.53585442	0.0
TM ₂	1.45759329	0.00000001
TM ₃	1.36673381	0.02525407
TM ₄	1.21188610	0.08262072
TM ₅	1.02904091	0.12493319
TM ₆	0.83011683	0.15123624

(The values of β for the TM modes appear as WZ in parts 10. to 13. of the output samples in the next section.)

These same values are obtained using a convergence criteria of 10^{-6} , 10^{-8} , or 10^{-10} ; so there is confidence that the values are accurate to the 8 decimal places listed. These are offered for use as possible numerical checks of calculations made using other methods.

2.3 Output

The last six pages of this section show an example of the printed output from MODEIG. It is provided to show the format of the output and to explain some of the output variable names not explained elsewhere. The output is for the default case, with some changed parameters, obtained by the third example of input cards in Sect. 2.1.

Various parts of the output are identified by circled numbers, which correspond to descriptions below. Many of the variables are input quantities, these are identified by (I).

1. Summary of wavelength and relative frequency. WVL (I) is the wavelength λ_0 used to partially define the normalizing k_0 ; the definition is completed by the frequency factor $KC = (KCR, KCI)$ (I). All propagation constants WZ and WX below are normalized by the reference, free-space propagation constant $k_0 = 2\pi KC/WVL$. $KF = (KFR, KFI)$ (I) is the separately specified relative frequency, ω_r .
2. Summary of polarization conditions, determined by KPOL (I).
3. Description of layered structure and material parameters. L is used as an index for both the layers and the boundaries. The XL(L) are locations of boundaries; TL(L) are layer thicknesses, and are also shown in unit of WVL. L1 and L2 (I) identify outer boundaries; these are movable to other XL positions, to calculate modes in partial structures.
- 4-5. Material parameters. $PE(L) = (PER, PEI)$ (I) is the complex permittivity; $PM = (PMR, PMI)$ (I) is the permeability, the same for all layers. $QN = KF*KF*PE*PM$ is the normalized propagation constant k^2

- of the material at relative frequency KF . For unit KF then $QN = n^2$, and $RN = \sqrt{QN} = n$. $YN = 1/KF \cdot PM$ (TE) or $1/KF \cdot PE$ (TM) is a wave admittance/impedance factor, for later multiplication by WX and WZ to obtain $YX = WX \cdot YN = Y_x$ and $YZ = WZ \cdot YN = Y_z$. $PHO = KO \cdot RN \cdot TL$ is the complex phase thickness of each layer for $\beta^2 = QZ = 0$.
6. Summary of outer boundary conditions. Depends on $KBC1,2$ and $KBD1,2$ (see input). $APB = \phi = APB1, APB2$ (I) is angle of unit normal into principal-branch half-plane for WX in respective semi-infinite layers $L1$ and $L2+1$.
 7. Representative values of real $\beta^2 = QZR$, and real part of normalized phase integral $\Phi_R \equiv PHM$. These values form the basis for calculating initial guesses for the root search. Integer part of PHM for $QZR = 0.0$ provides an estimate for maximum possible number of (non-evanescent) modes of structure. Second value of QZR is from input variable $QZNR$, and the fourth QZR is the maximum value of QN from 4. above.
 8. Summary of starting values of QZ for root search. Here, with $KGSS = 3(I)$, the real parts are calculated by interpolation from the QZR , PHM values above. MM is the intended mode index. The imaginary part of QZ is determined by the default or input value of $QZNI$. PHM is the renormalized phase integral, in units of π and decades. KM is a control integer used by $CZEROM$ and is preset to the value of $KGCZ(I)$ in line above. Value of $KM = KGCZ = 4$ indicates that initial iterates are calculated at a radius of about 10^{-4} . And since $KM \geq 4$ the initial guesses will be divided out. Last line shows parameters for $CZEROM$: $NN = MN(I)$, $EPSZ = EPS1(I)$, $EPSF = EPS2(I)$, $II = IL(I)$, $DOUT = KOUZ(I)$.

9. Output from CZEROM during root search. This portion will not appear if KOUZ (I) = 0. KR = 7 indicates convergence of DZ to EPS1 = EPSZ. KR = 6 indicates convergence of F(Z) to EPS2 = EPSF. KR = 5 indicates similar convergence of F(Z)-reduced. If no convergence, KR = 4. I = number of iterations used for each root. DZ(I) is last increment of $Z(I) = QZ = \beta^2$. F(Z) = characteristic function, to be zero. F(Z)-reduced is F(Z) divided by polynomial of other roots and initial guesses. Initial guesses divided out only if KG CZ = KM \geq 4.
- 10-12. Summary output for each root found (or each input QZM for non-eigen conditions). MM is intended mode index; compare to integer part of Re(PHM). $QZ = \beta^2$ and $WZ = \beta$ (Re $\beta \geq 0$). Normalized phase integral PHM = (Real (PHR)/ π , Imag (PHI/ln 10)). KM is value of KR from CZEROM in 9. above. PHR and PHI are complex phase integrals, separately accumulated with positive real parts or with positive imaginary parts. ATQZ is polar (phase) angle of QZ in its complex plane. In units of $\pi/2$, the integer part of ATQZ is intended as a quadrant indicator in the QZ plane.
11. SM = S^+ matrix of Sect. 4.2, Part I, one element of which is the characteristic function; here it is SM(2,2) = SM(KBD2, KBD1), and corresponds to F(Z) in 9. above. CM = C^+ matrix of Sects. 2.4 and 4.1-2, Part I. DET(SM) = det S^+ ; and DET(CM) = det C^+ should equal unity, residual part is shown. DETNORM is the sum of the two terms whose difference is DET(CM). As a numerical check, DET(CM) - 1.0 should be small (comparable to floating point resolution) relative to DETNORM.

12. Transverse wave parameters in the two semi-infinite layers: $WX = \kappa$, $YX = WX*YN = Y_x$, and $QX = (WX)^2 = QN - QZ$. WX is obtained from QX , and depends on principal branch specification parameters in 6. above. $ATQX$ is polar angle in QX complex plane. It would be more convenient to instead exhibit the angle in the WX plane, and label it as $ATWX$ (this change is planned). It is intended as a quadrant indicator, to help identify the types of modes.
13. Start of output for field calculations for all modes; beginning with first mode ($M = 1$), the TM_0 mode ($MM = 0$), but check integer part of Real (PHM). Compare this part with 10. above. Here WX , YX , and PH for inner layers $L = 2,3$ also appear. Only the start of field distributions vs. x is shown for this mode.
- 14-21. Output from calculation of field distributions. Only the portion of output for the TM_2 mode ($MM = 2$) is shown complete.
14. Summary of propagation constants and phase integral for all layers. Repeats much of information shown in 12. above. If $KOUF \leq 2$, then only QZ , WZ information appears.
15. Calculation of two sets of boundary fields, and cross products for numerical checks. First two values of $DIFF$ are the characteristic equation at the two outer boundaries and should be zero for discrete modes. Third $DIFF$ is the difference between the first two, and is a reciprocity check. It should be zero for any value of QZ .
16. Display of both sets of tangential fields at all boundaries. For discrete modes, the F and G fields should differ only by a constant

phase factor. FY is real at L1 = 1, and GY is real at L2 = 3. Both sets are normalized in magnitude, but are not standardized in phase factor.

17. Various versions of numerical check of characteristic equation.
18. Summary of the tangential boundary fields, FY and FZ, and transverse Poynting power, PX, at all boundaries, as used for field distribution vs. x. Appears in this form only for true discrete modes. These are the average of the F and G fields (standardized in phase) of 16. above.
19. Field distributions vs. x. X is value of x; FY, FZ are field values, and PX the transverse Poynting power. FX, the normal field component, and the propagating power PZ, appear only if KOUF = 4. The X-increment is determined internally, and is proportional to $1/|\kappa|$ in each layer. An input parameter IDEN sets the nominal number of points per unit of $1/|\kappa|$; but the density of points is also limited to no more than IMAX (1) per layer. BDY identifies a boundary value for X at which fields values are from 18. above. *** identifies a value of X and fields which are calculated incrementally, but may be an extrapolation beyond the boundary and be outside the proper layer. Into the semi-infinite layers the fields are calculated for a distance of about INFX (I) units of $1/|\kappa|$.

```

*****
***** SUBROUTINE PUTSIN, KASE NO.= 5.1 *****
***** CALCULATION OF GENERAL COMPLEX EIGEN-WAVES IN LAYERED STRUCTURES *****
*****
***** SUMMARY OF LAYERED STRUCTURE, POLARIZATION, AND BOUNDARY CONDITIONS. *****
*****
1 IMPLIED UNIT OF LENGTH YU= 1.0000E-06 METERS (NOT USED EXPLICITLY). ALL QUANTITIES NORMALIZED.
  NOMINAL WAVELENGTH MWL= 1.0000E+00 AND FREE-SPACE K0= 201.7147. K0Z= 6.28319 RADYAU.
  COMPLEX FREQUENCY FACTOR KC= ( 1.000000, .000000). EFFECTIVE K0= KC*K0= ( 6.28319, .000000).
  ALL PROPAGATION COEFFICIENTS ARE NORMALIZED TO EFFECTIVE-K0. (WAVE AND MATERIAL REFRACTIVE INDICES, IF KF= UNITY)
  (WAVE ADMITTANCE(TE) AND IMPEDANCE(TM), YX AND YZ, ARE NORMALIZED TO THAT OF FREE SPACE.
  NORMALIZED FREQUENCY KF= ( 1.000000, .000000)= FREQ/C*EFF.K0.

2 POLARIZATION: FZOL= 2. (=1 TE CASE, =2 TM CASE)
  TRANSVERSE MAGNETIC CASE. HXEY=Z0. TANGENTIAL FY=MY, FZ=EZ. TRANSVERSE FX=EX, FY=MY. LONGITUDINAL FZ=EZ.
  YX=FZYFYZ=Z0/YX, AND YZ=FXFY=EX/YX, ARE WAVE IMPEDANCES. (IN THE POS X, Z, OR WAVE DIRECTION).

LAYERED STRUCTURE. 4 LAYERS TOTAL. 3 BOUNDARIES. 2 FINITE LAYERS.

L 1 SEMI-INFINITE
  PE= ( 2.250000, .000000) PM= ( 1.000000, .000000)
  GE= ( 2.250000, .000000) YN= ( .444444, .000000)
  RE= ( 1.500000, .000000)

3 L1= 1---BOUNDARY FOR FIRST BOUNDARY CONDITION-----
  --L 1---AL= -1.000000
  PE= ( 1.000000, .000000) PM= ( .000000, .000000)
  GE= ( 1.000000, .000000) YN= ( .000000, .000000)
  RE= ( 1.000000, .000000)
  --L 2---XL= .000003
  PE= ( 2.560000, .000000) PM= ( .000000, .000000)
  GE= ( 2.560000, .000000) YN= ( .342633, .000000)
  RE= ( 1.600000, .000000)
  --L 3---AL= 2.000000
  PE= ( 1.980000, .000000) PM= ( .050000, .000000)
  GE= ( 1.980000, .000000) YN= ( .510200, .000000)
  RE= ( 1.400000, .000000)

4 L 4 SEMI-INFINITE
  PE= ( 1.980000, .000000) PM= ( .050000, .000000)
  GE= ( 1.980000, .000000) YN= ( .510200, .000000)
  RE= ( 1.400000, .000000)

FIRST BOUNDARY CONDITION. L1= 1. KBC1= 1. KBD1= 2. OPEN BOUNDARY, SEMI-INFINITE ADJACENT LAYER.
PRINCIPAL BRANCH SPECIFICATION FOR KX. ANGLE APB= .250 PI. VECTOR VPB= ( .707, .707). (MAXIMUM VPB,GE,0).
EIGEN CONDITION. OUTWARD WAVE SOLUTION ONLY. (DIRECTION OF DEAY IF 1-(MAX).GT.0. OF PHASE PROPAGATION IF RE(MAX).GT.0.)

SECOND BOUNDARY CONDITION. L2= 3. KBC2= 1. KBD2= 2. OPEN BOUNDARY, SEMI-INFINITE ADJACENT LAYER.
PRINCIPAL BRANCH SPECIFICATION FOR KX. ANGLE APB= .250 PI. VECTOR VPB= ( .707, .707). (MAXIMUM VPB,GE,0).
EIGEN CONDITION. OUTWARD WAVE SOLUTION ONLY. (DIRECTION OF DEAY IF 1-(MAX).GT.0. OF PHASE PROPAGATION IF RE(MAX).GT.0.)

END STRUCTURE DESCRIPTION.

***** SUBROUTINE SEARCH, KASE NO.= 5.1. KBCS= 1. KBCSE= 3.
SEARCHING FOR K= 7 EIGENVALUES. FOR INTERMED MODE INDICES FROM MM=MK= 0 TO MM=ML= 6.
REPRESENTATIVE VALUES OF REAL QZ AND COMPLEXPONGING PHASE INTEGRAL
QZ= .000000.
PM= 6.40000PI. 5.7610PI. 3.57027PI. 2.55600.
QZ= 1.64929. PM= 3.37226PI.

KBCSE= 3. INDIVIDUAL GUESSES FOR EACH QZ, BASED ON SIMPLE QUALITATIVE APPROXIMATION FOR REAL QZ VS PHM. KBCZ= 4
1 K= 0 QZ= ( 2.92584799, -.00010000) PM= ( 1.734PI, 3.37226PI) KME= 4
2 K= 1 QZ= ( 2.37100011, -.00010000) PM= ( 1.734PI, 3.37226PI) KME= 4
3 K= 2 QZ= ( 2.15306349, -.00010000) PM= ( 2.563PI, 2.563PI) KME= 4
4 K= 3 QZ= ( 1.87235749, -.00010000) PM= ( 3.31PI, 2.563PI) KME= 4
5 K= 4 QZ= ( 1.52742565, -.00010000) PM= ( 4.054PI, 1.945PI) KME= 4
6 K= 5 QZ= ( 1.12023946, -.00010000) PM= ( 4.754PI, .945PI) KME= 4
7 K= 6 QZ= ( .55043552, -.00010000) PM= ( 6.710PI, .00000PI) KME= 4

CALLING CZEROM FOR COMPLEX ROOT SEARCH. NN= 7 ROOTS. EPSI= 1.00E-10. IT= 15. KOUF= 3. KEIF= 1.

***** SUBROUTINE CZEROM ITERATIONS. *****
N KR 1
QZ(I)
F(Z)
F(Z)-REDUCED F=SSU
P.1 P.2

```


3	X=	1.65000	FY=	1.996292	-2.296302	FZ=	1.074736	-0.04942	PX=	1.160040E-01	-2.000000E-01	0.10
3	X=	1.80000	FY=	2.760577	-4.409742	FZ=	1.136633	-0.164706	PX=	2.315025E-00	-7.96140E-09	
3	X=	1.95000	FY=	2.491128	-3.369748	FZ=	1.571777	-0.16248	PX=	1.160040E-01	-2.000000E-01	
3	X=	2.10000	FY=	1.288842	-1.91298	FZ=	1.483340	-0.04942	PX=	4.434657E-01	-1.902564E-08	
3	X=	2.0000000Y	FY=	2.177819	-3.32245	FZ=	1.735931	-0.06606	PX=	3.011206E-00	-1.59125E-08	
4	X=	1.80000000	FY=	3.625961	-5.538187	FZ=	1.113394	-0.06606	PX=	9.468415E-09	-1.48614E-09	
4	X=	2.00000	FY=	2.177819	-3.32245	FZ=	2.694519	-0.06606	PX=	1.540190E-07	-2.781251E-00	
4	X=	2.20000	FY=	1.308038	-1.94147	FZ=	1.619579	-0.040165	PX=	9.992473E-00	-4.263710E-03	
4	X=	2.40000	FY=	1.785632	-1.16608	FZ=	1.972749	-0.024136	PX=	3.011206E-00	-1.59125E-08	
4	X=	2.60000	FY=	1.471865	-0.700037	FZ=	1.584251	-0.01886	PX=	9.468415E-09	-1.48614E-09	
4	X=	2.80000	FY=	1.283411	-0.42066	FZ=	1.350412	-0.005707	PX=	4.555819E-09	-1.003315E-00	
4	X=	3.00000	FY=	1.170222	-0.25265	FZ=	1.210764	-0.00529	PX=	1.540190E-07	-2.781251E-00	
4	X=	3.20000	FY=	1.02238	-0.15175	FZ=	1.065345	-0.003141	PX=	3.011206E-00	-1.59125E-08	
4	X=	3.40000	FY=	0.61406	-0.09114	FZ=	0.76032	-0.00186	PX=	3.011206E-00	-1.59125E-08	
4	X=	3.60000	FY=	0.36882	-0.05474	FZ=	0.45666	-0.001133	PX=	1.540190E-07	-2.781251E-00	
4	X=	3.80000	FY=	0.22152	-0.03238	FZ=	0.27428	-0.000681	PX=	1.540190E-07	-2.781251E-00	
4	X=	4.00000	FY=	0.13305	-0.01975	FZ=	0.16474	-0.00049	PX=	3.011206E-00	-1.59125E-08	
4	X=	4.20000	FY=	0.07991	-0.01186	FZ=	0.08584	-0.000245	PX=	1.540190E-07	-2.781251E-00	
4	X=	4.40000	FY=	0.00480	-0.000712	FZ=	0.05943	-0.000147	PX=	1.540190E-07	-2.781251E-00	
4	X=	4.60000	FY=	0.002843	-0.000428	FZ=	0.003569	-0.000089	PX=	1.540190E-07	-2.781251E-00	
4	X=	4.80000	FY=	0.00151	-0.000214	FZ=	0.00089	-0.0000316	PX=	1.540190E-07	-2.781251E-00	
END FIELD SOLUTIONS FOR NODE, M= 3												
TWO SOLUTIONS FOR TANGENTIAL ROY, FIELDS, INDEPENDENTLY CALC. FIL FROM ROY, COND. AT L1= 1, AND GIL FROM ROY, COND. AT L2= 3.												
NUMERICAL CHECKS, RECIPROCALITY AND EIGEN CONDITIONS, USING PYNTING CROSS PRODUCTS FOG, (F+G-DIFF) IS POSITIVE DET. J.												
EIG CHECK AT L2= 3, FY=GZ = GYFZ, (-8.0724E-01, 3.4145E-01)=(-8.0724E-01, 3.4145E-01). DIFF=(-5.3291E-14, 8.1712E-14)=0.												
EIG CHECK AT L1= 1, FY=GZ = GYFZ, (3.4145E-01, -8.0724E-01)=(-8.0724E-01, 3.4145E-01). DIFF=(-5.3291E-14, 8.1712E-14)=0.												
RECIPROCALITY CHECK, FOG-FOG=0, FOG-FOG=0, FOG-FOG=0, FOG-FOG=0, FOG-FOG=0, FOG-FOG=0, FOG-FOG=0, FOG-FOG=0, FOG-FOG=0, FOG-FOG=0, FOG-FOG=0, FOG-FOG=0.												
FIL AND GIL FIELD SETS AND WROSAIAN DETERMINANT (FY-GZ-GY-FZ) (=216 CHECK)												
L= 1	FY=	0.003708	GY=	0.003000	GY=	0.003697	GY=	0.003697	W-DET=	(-5.250698E-14, 7.709311E-14).		
L= 2	FY=	0.001024	GY=	0.000929	GY=	0.001024	GY=	0.001024	W-DET=	(-5.250698E-14, 7.709311E-14).		
L= 3	FY=	0.001024	GY=	0.000929	GY=	0.001024	GY=	0.001024	W-DET=	(-5.250698E-14, 7.709311E-14).		
L= 4	FY=	0.001024	GY=	0.000929	GY=	0.001024	GY=	0.001024	W-DET=	(-5.250698E-14, 7.709311E-14).		
SOLUTION FOR TANGENTIAL FIELDS AT THE BOUNDARIES.												
EIGEN-FUNCTION FIELD SOLUTION (AVG. OF SOLUTIONS BASED ON THE TWO ROY, COND. SEPARATELY.												
ROY, COND. CHECKS, AT L1, YX*FY-FZ = (-6.226E-12, 1.093E-11). AT L2, YX*FY-FZ = (-1.243E-14, 1.865E-14).												
TANGENTIAL BOUNDARY FIELDS AND TRANSVERSE AVG. POINTING POWER.												
1	X=	1.00000	FY=	0.003708	0.000000	FZ=	0.001024	0.000929	PX=	(-3.796282E-06, -3.396654E-07)		
2	X=	0.00000	FY=	0.003708	0.000000	FZ=	0.001024	0.000929	PX=	(1.572559E-02, 3.958035E-01)		
3	X=	2.00000	FY=	0.003708	0.000000	FZ=	0.001024	0.000929	PX=	(6.320063E-01, 2.758126E-01)		

3. PROGRAM MODEIG LISTING

```

      PROGRAM MODEIG(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
C
C      --CALCULATES SETS OF MODAL PROPAGAION EIGENVALUES FOR MULTILAYER
C      --STRUCTURE. AND FIELDS AND POWER DISTRIBUTIONS FOR EIGEN OR
C      --NON-EIGEN PROPAGATION CONSTANTS ALONG THE LAYERED STRUCTURE.
C
C      WRITTEN BY ROBERT D. SMITH, UNIVERSITY OF WASHINGTON, ELECT ENG DEPT.
C      SEATTLE, WASHINGTON. FEBRUARY, 1977.
C      --MAIN PROGRAM IS PRIMARILY A CALLING PROGRAM
C
C      200 --READ INPUT DATA, CASE PARAMETERS, AND VARIABLES.
C      --AND PRINT SUMMARY OF STRUCTURE AND MODAL CONDITIONS.
C      200 CALL PUTSIN
C
C      400 --SEARCH FOR PRESCRIBED ROOTS, AND OUTPUT SUMMARY FOR THOSE FOUND
C      400 CALL SEARCH
C
C      600 --CALCULATE FIELDS AND POWER DISTRIBUTION
C      600 CALL FIELDS
C
C      800 RETURN FOR NEXT CASE
C      800 GO TO 200
C      --NORMAL STOP OCCURS FROM PUTSIN WHEN INPUT KASE=0 OR KD00=0.
C
C      END

```

BLOCK DATA BLOKOM

```

C
C PROGRAM UNIT TO DEFINE LABELED COMMON BLOCKS, TO DESCRIBE THE VARIABLES
C AND BY DATA STATEMENTS TO PRESET VARIABLES TO A DEFAULT CASE
C NOTE. IN SUBROUTINES THE VARIABLES IN THE COMMON BOOCKS BELOW MAY
C APPEAR DIFFERENTLY. TO PERMIT THE SAME VARIABLE NAMES HERE TO BE USED
C AS LOCAL VARIABLES WITHOUT NAME CONFLICT AND BETTER EFFICIENCY
C EXAMPLES. KDOO FOR KDO1,2,3,ETC., KOUT FOR KOU1,2,3,ETC.,
C KCC FOR KC, KFC FOR KF,
C
C      --COMMON /KASETS/ CASE SPECIFICATION AND CONTROL VARIABLES
COMMON /KASETS/ KASE,KSUB,MN,MO,MK,ML,IDEN,IMAX,INFX,
$QZNR,QZNI,KGSS,PMFR,PHDM,KGCZ,UFMP,EPS1,EPS2,EPS3,IL,KMDO,
$KDOO,KDOI,KDOS,KDOM,KEIF,KDOZ,KDOF,KDOP,
$KOUT,KOUI,KOUS,KOUM,KOUE,KOUZ,KOUF,KOUP
C      MAIN,PUTS,SRCH,SYSM,EIGQ,CZRM,FLDS,PWRS
C
C      --COMMON /LAYCOM/ DIMENSIONS AND MATERIAL PROPERTIES OF LAYERED
C      --STRUCTURE. UNIT OF LENGTH AND WAVELENGTH AND FREQ FACTORS
COMMON /LAYCOM/ XU,WVL,KO,KCR,KCI,KFR,KFI,LN,KXTL,XL(10),TL(10),
$PER(10),PEI(10),PHR( 1),PHI( 1)
REAL KO,KCR,KCI,KFR,KFI
C
C      --COMMON /BDYCON/. POLARIZATION AND BOUNDARY CONDITIONS
COMMON /BDYCON/ KPOL,L1,KBC1,KBD1,APB1,VPB1,YB1,ZB1,
$L2,KBC2,KBD2,APB2,VPB2,YB2,ZB2,KBC0
COMPLEX VPB1,YB1,ZB1,VPB2,YB2,ZB2
C
C      --COMMON /STRUCT/. FOR GIVEN POLARIZATION THE CHARACTERISTIC WAVE
C      --PROPERTIES OF STRUCTURE. NUMBERS OF LAYERS, RADIAN THICKNESS,
C      --FREQ, SQD INDEX, AND PLANE-WAVE ADMIT(TE)/IMPED(TM) OF MATERIALS
COMMON /STRUCT/ LK,LL,LN,KS,KC,KF,TR(10),QN(10),KPLS,YN(10)
REAL KS
COMPLEX KC,KF,QN,YN
C
C      --COMMON /MODSET/ ARRAYS FOR SETS OF MODE PARAMETERS. PRIMARY
C      --RESULTS FROM MAIN PROGRAM MODEIGS
COMMON /MODSET/ NM,NO,NK,NL,QZN(10),PHN(10),KM(10)
COMPLEX QZN,PHN
C
C      --COMMON /MATSYS/. FOR PARTICULAR VALUE OF QZ=QZS, AND KC=KCS,
C      --THE TRANSVERSE WAVE PROPAGATION PROPERTIES, PHASE INTEGRAL,
C      --AND CHARACTERISTIC MATRICES FOR LAYERS AND OVERALL STRUCTURE
COMMON /MATSYS/ KDID,QZS,KCS,AQZ,WX(10),PH(10),PHR,PHI,YX(10),
$CL1(10),CL2(10),CL3(10),CM1,CM2,CM3,CM4,DETC(2),
$QX1,AQX1,FY1,FZ1,QX2,AQX2,FY2,FZ2,SM1,SM2,SM3,SM4,DETS,WZ,YZ(10)
COMPLEX QZS,KCS,WX,PH,PHR,PHI,YX,CL1,CL2,CL3,CM1,CM2,CM3,CM4,DETC,
$QX1,FY1,FZ1,QX2,FY2,FZ2,SM1,SM2,SM3,SM4,DETS,WZ,YZ
C
C      --COMMON /FIELDS/ COMPLEX TANGENTIAL FIELD AMPLIT AT BOUNDARIES

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C      --AND TRANSVERSE TIME-AVERAGED POYNTING POWERS,
C      --AND LONGITUD PROPAGATING POWER IN EACH LAYER.
COMMON /FIELDS/ FY(10),FZ(10),PX(10),PZ(10)
COMPLEX FY,FZ,PX,PZ

C
C      --COMMON /CZECOM/ FOR COMPLEX ROOT SEARCHING SUBROUTINE CZEROM
C      --SEE SUBROUTINE CZEROM(Z,NR) FOR DESCRIPTION OF VARIABLES
COMMON /CZECOM/ NN,NT,ZO(10),FM(10),IT(10),KR(10),
$EPSZ,EPST,II,KTUO
COMPLEX ZO

C
C
C      --DATA PRESET VALUES FOR DEFAULT CASE OF A FOUR LAYER STRUCTURE
DATA KASE,MN,MO,IDEN,IMAX,INFX /1,6,-1,2,15,6/
DATA QZNR,QZNI,KGSS,PMFR,PMDH,KGCZ /0.9,-1.0E-4,3,0.3,1.0,3/
DATA WFMP,EPS1,EPS2,EPS3,IL /100.0,1.0E-6,1.0E-6,1.0E-9,10/
DATA KMDO /5/
DATA KDOO,KOUT /1,1/
DATA KDOI,KOUI /1,1/
DATA KDOF,KOUS /1,3/
DATA KDOM,KOUM /0,0/
DATA KEIF,KOUE /1,0/
DATA KDOZ,KOUZ /1,3/
DATA KDOF,KOUF /1,3/
DATA KDOP,KOUP /1,1/
DATA XU,WVL /1.0E-6,1.0/
DATA LN,KXTL,XL,TL /4,0,-1.0,0.0,2.0,7*0.0,0.0,1.0,2.0,7*0.0/
DATA KCR,KCI,KFR,KFI /1.0,0.0,1.0,0.0/
DATA PER,PEI,PMR,PMI /2.25,1.00,2.56,1.96,6*1.0,10*0.0,1.0,0.0/
DATA KPOL,L1,APB1,YB1,ZB1 /1,1,0.25,(1.,0.), (1.,0.)/
DATA L2,APB2,YB2,ZB2 /3,0.25,(1.,0.), (1.,0.)/
DATA KBC1,KBD1,KBC2,KBD2 /1,2,1,2/
C      VARIABLES FOR /STRUCT/ ALL CALCULATED OR PASSED INTERNALLY
C      VARIABLES FOR /MODSET/ MOST CALCULATED OR PASSED INTERNALLY.
DATA QZM /(2.205,0.0),(2.160738,0.0),(2.030,0.0),(1.960,0.0),
$ (1.90230,0.0),(1.690,0.0),(1.481,0.0),(1.0,0.0),(0.980,0.0),(0.,0.0)/
DATA KM /10*5/
C      VARIABLES FOR /MATSYS/ ALL CALCULATED OR PASSED INTERNALLY
C      VARIABLES FOR /FIELDS/ ALL CALCULATED OR PASSED INTERNALLY
C      VARIABLES FOR /CZEROM/ ALL CALCULATED OR PASSED INTERNALLY
C
C
C      MODEIG NAMELISTS VARIABLES DESCRIPTION.  FOR INPUT.  EVERY CASE MUST
C      HAVE THREE NAMELIST INPUT LIST IN ORDER /CASE/, /LAYERS/, AND /MODCON/
C      ONLY VARIABLES CHANGED IN VALUE FROM DEFAULT CASE OR PREVIOUS CASE
C      NEED BE INCLUDED.  NORMAL STOP BY SINGLE CARD WITH $CASE KDOO=0 $END,
C      OR $CASE KASE=0 $END.  THAT IS, A LAST CARD IN A SEQUENCE OF CASES.
C      NOTES, BELOW.  WZ IS BETA, AND QZ IS BETA-SQD,  MODE PROPAGATION COEFF
C      IN Z DIRECTION.  WX IS KAPPA TRANSV PROPAGAION COEFF IN X DIRECTION

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C      BOTH NORMALIZED TO EFFECTIVE K0.
C
C  NAMELIST /KASETS/ VARIABLES DESCRIPTION. READ BY PUTSIN.
C  KASE  INTEGER CASE NUMBER, SIX DIGIT MAX. E.G. YR/MO/DY.      (1)
C        IF KASE= PREV.KASE, THEN KASE INCREMENT BY .01 INTERNALLY
C        KASE= 0  MAY BE USED FOR PROGRAM STOP.  SEE ALSO KDOO.
C  MN    NUMBER OF MODES TO BE SEARCHED FOR OR CALCULATIONS MADE(6)
C        MAXIMUM NUMBER OF MODES PRESENTLY DIMENSIONED FOR 10
C  MO    BIAS FOR MODE INDEXING OF INTENDED MODES. MM=MO+M      (-1)
C  IDEN  DENSITY OF POINTS IN X FOR FIELD CALC. PER RAD OR 1/E  (2)
C  IMAX  MAX NO. OF POINTS IN EA. LAYER FOR FIELD CALCULATIONS (15)
C  INFx  NO. OF RAD OR 1/E DIST INTO SEMI-INF LAYERS FOR FIELD CALC (6)
C  QZNR  A REAL PART OF QZ FOR GENERATION OF INITIAL GUESSES   (0.9)
C  QZNI  A IMAG PART OF QZ FOR GENERATION OF INITIAL GUESSES   (-1.0E-4)
C  KGSS  CONTROL TYPE OF INITIAL GUESSES FOR QZ ROOT SEARCH   (3)
C    =1  QZM(M) AND KM(M) FROM INPUT OR PREVIOUS CASE USED FOR GUESSES.
C    =2  ALL GUESSES THE SAME. OR MAX OF INNER LAYERS
C    =3  INDIVIDUAL GUESSES FROM SIMPLE QUADRATIC APPROX FOR REAL(QZ)
C        VS PHASE INTEGRAL= INTENDED MODE INDICES MM= MO+M.
C  PMFR  FRACTIONAL PART FOR PHASE INTEGRAL (PHASE SHIFT AT OUTER BDY)
C        ASSUMED IN GENERATING GUESSES. UNITS OF PI.           (0.3)
C  PMDM  AVG SPACING OF MODES IN PHASE INTEGRAL VS MODE INDEX. ASSUMED
C        FOR GENERATING GUESSES. UNITS OF PI PER INTEGER MM.   (1.0)
C        FOR GUESSES, INTENDED PHASE INTEGRAL PHM= PMDM*MM + PMFR
C  KGCZ  CONTROL USE OF GUESSES IN CMLPX ROOT SEARCH FOR ALL QZ (3)
C        USED TO SET KM= KGCZ FOR ALL GUESSES. (KGSS.GE.2)
C    =0  GUESSES NOT USED, INITIAL ITERATES ABOUT POINT (1.0,0.0)
C    =1,2,3  INITIAL ITERATES AT RADIUS OF 0.1*KGCZ ABOUT EACH GUESS.
C            ONLY CONVERGED AND ITERATION LIMITED ROOTS DIVIDED OUT.
C    =4,5,6,7  RADIUS OF 0.1*KGCZ, ALL OTHER GUESSES AND ROOTS DIVIDED OUT
C            WARNINGS. USE KGCZ.GE.4 IFF GUESSES ARE GOOD APPROX AND DISTINCT
C            DO NOT USE IF ALL GUESSES THE SAME (KGSS=2) OR POOR INPUT GUESS
C            IF GOOD GUESSES, KGCZ.GE.4 GREATLY SPEEDS ROOT SEARCH CONVERG.
C  WFMP  WT FUNCT MULTIPLIER USED FOR MODIFIED EIGEN EQ FUNCT (100.0)
C  EPS1  EPSILON FOR CONVERGENCE TEST ON DELTA QZ ROOT SEARCH (E-6)
C  EPS2  EPS FOR CONVERG TEST ON MAGNITUDE OF EIGEN EQ FUNCTION (E-6)
C  EPS3  NOT USED.
C  IL    ITERATION LIMIT, MAX NUMBER FOR EACH ROOT SEARCH
C        TWO SUCCESSVE ITERATION LIMITS STOPS ALL SEARCHES
C  KMDO  ONLY FOR KM.GE.KMDO MODES OUTPUT AND FIELDS CALCULATED (5)
C  QZM(M) INPUT SET OF COMPLEX QZ VALUES, M= 1,MN.LE.10.  SEE KGSS=1.
C        USED FOR GUESSES FOR ROOT SEARCH, OR FOR FIELD CALC, NO SEARCH.
C        PRESET TO SPECIAL REAL VALUES FROM DEFAULT CASE SOLUTIONS.
C  KM(M)  INDEX SHOWING QZM QUALITY OR TYPE. INPUT USED ONLY IF KGSS=1
C    =0 TO 7,  SEE KGCZ
C    =8  QZM USED AS FIXED KNOWN ROOT, NO SEARCH, DIVIDED OUT FOR OTHERS
C        (FOR OUTPUT AND PREV CASE KM= 5,6,7, SHOWS TYPE OF CONVERGENCE)
C  KDOO  A SET CONTROLLING EXTENT/TYPE OF CALC IN EACH SUBROUTINE
C  KDOO  MAIN PROGRAM, USED ONLY PROG STOP IF KDOO=0.          (1)
C  KDOI  SUBROUTINE PUTSIN (NOT USED)                          (1)

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C KDOS  SUBROUTINE SEARCH          (NOT USED)              (1)
C KDOM  SUBROUTINE SYSHAT  (INTERNAL USE ONLY, INPUT IGNORED)
C KDOE=KEIF FUNCTION SUBROUTINE EIGEQF              (1)
C KEIF  CONTROL TYPE OF EIGEN EQUATION FUNCTION USED FOR ROOT SEARCHING
C   =1  UNMODIFIED EIGEN EQUATION FUNCTION FROM SM MATRIX ELEMENT
C   =2  EIGEQF RENORMALIZED TO R.M.SQD.MAG. OF THE FOUR POSSIBLE EIGEQF
C   =3  EIGEQF MULT BY WT FUNCT TO BIAS SEARCH TOWARD INTENDED MM
C       WEIGHT FUNCTION IS WFMP TIMES SQUARED DIFFERENCE BETWEEN
C       PHASE INTEGRAL INDEX AND INTENDED MODE INDEX.
C   =2,3 WARNING. NON-ANALYTIC FUNCTIONS, CAN GREATLY SLOW ROOT SEARCH.
C KDOZ  SUBROUTINE CZEROM          (NOT USED)              (1)
C KDOF  SUBROUTINE FIELDS              (1)
C   =0  NO FIELD CALCULATIONS MADE
C   =1  TANGENTIAL FIELDS AT BOUNDARIES ONLY CALCULATED. (DEFAULT)
C   =2  FIELDS AS A FUNCTION OF X CALCULATED. IFF KOUF=4 ALSO.
C KDOP  SUBROUTINE POWERS              (1)
C KOUT  A SET CONTROLLING EXTENT OF OUTPUT FROM EACH SUBROUTINE.
C   =1,2,3,4 MIN TO MAX OUTPUT FROM EACH
C KOUT  SUBROUTINE MAIN.              (NOT USED)              (1)
C KOUI  SUBROUTINE PUTSIN.            (LITTLE USE)            (1)
C KOUS  SUBROUTINE SEARCH.              (3)
C KOUM  SUBROUTINE SYSHAT.            (NO OUTPUT)              (0)
C KOUE  FUNCTION SUBROUTINE EIGEQF.              (0)
C KOUZ  SUBROUTINE CZEROM.              (3)
C KOUF  SUBROUTINE FIELDS.              (3)
C KOUP  SUBROUTINE POWERS.              (1)
C       WARNING. USE OF OF KOUE=4 OR KOUZ=4 FOR MORE THAN A FEW MODES
C       AND LARGE IL CAN GENERATE GREAT AMMOUNTS OF OUTPUT. ALSO
C       ASKING FOR FIELD SOLN KDOF=2 FOR MORE THAN A FEW MODES AND
C       FEW LAYERS CAN GENERATE LARGE AMMOUNTS OF OUTPUT.
C
C NAMED LIST /LAYERS/ VARIABLES DISCRPTION. READ BY PUTSIN.
C XU    UNIT OF LENGTH IMPLIED FOR ALL DIMS. WVL,XL,TL. METERS (1.0E-6)
C       VALUE OF XU IS NOT USED EXPLICITLY YET.
C WVL    FREE SPACE WAVELENGTH FOR NORMALIZATION PURPOSES      (1.0)
C KO     FREE-SPACE PROPG CONST FOR NORMALIZATION PURPOSES. CALCULATED.
C       KO= 2PI/WVL USED TO NORM ALL PROPG CONSTS. SEE KC BELOW.
C       EFFECTIVE VALUES OF WVL AND KO ALTERED BY USE OF NON-UNITY KC.
C KCR,   COMPLEX FREQ FACTOR FOR NORM KO. SEPARATE REAL AND IMAG PARTS.
C KCI    KC= (KCR,KCI). EFFECTIVE KO= KO*KC.              (1.0,0.0)
C KFR,   EXPLICIT COMPLEX FREQ FACTOR, SEPARATE REAL AND IMAG PARTS
C KFI    KF= (KFR,KFI) IS NORMALIZED FREQUENCY FOR CASE.      (1.0,0.0)
C       KF= FREQ/(FREQ IMPLIED BY EFFECTIVE KO, =KC*KO*C)
C LN     TOTAL NUMBER OF MATERIAL LAYERS INCL OUTER SEMI-INF LAYERS. (4)
C       2.LE.LN.LE10. LN-1 TOTAL BDYS, LN-2 FINITE LAYERS
C KXTL   CONTROL TO SPECIFY THAT XL OR TL ARE EXPECTED AS INPUT (0)
C   .LE.0 XL EXPECTED AS INPUT, TL CALCULATED. DEFAULT
C   .GE.1 TL EXPECTED AS INPUT, XL CALCULATED. XL(1)= 0.0
C XL(L)  LOCATION IN X FOR EACH BOUNDARY. L=1,LN-1      (-1.0,0.0,+2.0)
C TL(L)  THICKNESS OF EACH FINITE LAYER. L=2,LN-1.      (0.0,1.0,2.0)

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C EACH LAYER AND ITS UPPER BDY HAVE CORRESPOND. INDEX VALUES, L.
 C TL(1) AND TL(LN) ARE NOT DEFINED (SEMI-INF LAYER) INPUT IGNORED
 C FOR INPUT TL, START WITH TL(2)= -----.
 C ALL XL(L) VALUES REORDERED FOR INCREASING X, AND TL(L) VALUES
 C ARE TAKEN AS POSITIVE. XL AND TL DIM. FOR A MAX OF 10 VALUES
 C PER(L), RELATIVE PERMITTIVITY OF EACH MATERIAL. L=1, LN.LE.10.
 C PEI(L) SEPARATE REAL AND IMAG PARTS. (2.25,1.00,2.56,1.96),(4*0.0)
 C FOR LOSSY MATERIAL PEI POS., FOR ACTIVE-GAIN MATERIAL PEI NEG.
 C PMR(1), RELATIVE PERMEABILITY, THE SAME FOR ALL LAYERS.
 C PMI(1) SEPARATE REAL AND IMAG PARTS. (1.0,0.0)
 C
 C NAMELIST /MODCON/ VARIABLES DESCRIPTION. READ BY PUTSIN.
 C KPOL POLARIZATION. TRANSV TO Z-PROPG, AND TO X-NORM DIRECT. (1)
 C .LE.1 TE, TRANSVERSE ELECTRIC CASE. FY= EY. DEFAULT
 C .GE.2 TM, TRANSVERSE MAGNETIC CASE. FY= HY
 C L1, FIRST AND LAST BOUNDARY FOR OUTER BOUNDARY CONDITIONS.
 C L2 PRESET TO L1=1,L2=LN-1 FOR EACH CASE, FOR OTHER VALUES (PARTIAL
 C STRUCTURES), L1,L2 MUST BE INPUT FOR EACH SUCCESSIVE CASE.
 C NOTE. ADJACENT LAYERS, L= L1 AND L2+1 ARE TAKEN TO BE SEMI-INF
 C FOR CLOSED BDY COND., KBC=2,3, ALL OUTER LAYERS IGNORED.
 C KBC1, CONTROL TYPE OF BOUNDARY CONDITIONS AT FIRST AND LAST BDY L1,L2
 C KBC2 OPEN-BDY SEMI-INF WAVE ADMIT/IMPED, OR FIXED SURF ADMIT/IMPED,
 C ALSO EIGEN, NON-EIGEN, CONDITIONS, AND ACCEPTABLE SOLUTIONS.
 C .LE.0 OPEN BOUNDARY CONDITION, NON-EIGEN CONDITION, NO SEARCH MADE
 C INWARD AND OUTWARD SOLN BOTH ACCEPTABLE. SEE KBD1,2.
 C FIELD SOLN EXISTS FOR EACH OF KBC1=0, OR KBC2=0, OR BOTH.
 C IF BOTH, TWO INDEPED FIELD SOLN EXIST. CALC INDEPED FROM TWO
 C BDY COND SAME AS FOR KBC=1, AND DIRECTION IMPLIED BY KBD1,2.
 C =1 OPEN BOUNDARY, EIGEN CONDITION. ONLY A SINGLE EXPONENTIAL WAVE
 C SOLUTION ACCEPTABLE IN OUTER SEMI-INF LAYER.
 C =0,1 WAVE ADMIT/IMPED FOR SEMI-INF LAYER IS FUNCT OF WX(QZ), ALWAYS
 C DEFINED FROM UX ON PRINCIPAL BRANCH. SEE KBD1,2 AND APB1,2
 C =2 CLOSED BDY, A FIXED SURF ADMIT/IMPED YB1,YB2. ZB1,ZB2 IGNORED
 C =3 CLOSED BDY, A FIXED SURF IMPED/ADMIT ZB1,ZB2. YB1,YB2 IGNORED
 C =2,3 A CLOSED BDY EIGEN COND. OUTER SEMI-INF LAYERS IGNORED.
 C KBD1, CONTROLS IMPLIED DIRECTION OF SINGLE SOLN IN SEMI-INF LAYERS
 C KBD2 INWARD/OUTWARD DIRECTION INTERPRETATION DEPENDS ON BRANCH DEF.
 C KBD1=1 POS. EXPONENT (INWARD) COMPLEX WAVE SOLUTION IN LAYER L1
 C KBD1=2 NEG. EXPONENT (OUTWARD) COMPLEX WAVE SOLUTION IN LAYER L1
 C KBD2=1 NEG. EXPONENT (INWARD) COMPLEX WAVE SOLUTION IN LAYER L2+1
 C KBD2=2 POS. EXPONENT (OUTWARD) COMPLEX WAVE SOLUTION IN LAYER L2+1
 C DEFAULT VALUES KBD1=2,KBD2=2. OUTWARD SOLN IN SEMI-INF LAYERS.
 C IFF APB= 0.5, THEN IMAG(WX) IS POS, AND DIRECTION SENSE IN/OUT
 C IS THAT OF EXP DECAY REGARDLESS OF PHASE PROPAG. INWARD= LEAKY,
 C IMPROPER OR INCOMING LOSSY WAVE. OUTWARD= BOUND, PROPER OR OUT
 C GOING LOSSY WAVE. IFF APB= 0.0, REAL(WX) IS POS. AND DIRECTION
 C IS THAT OF PHASE PROPAGATION REGARDLESS OF EXP DECAY OR GROWTH.
 C DIRECTION SENSE ALSO USED FOR NON-EIGEN CASE (KBC1,KBC2=0)
 C IN GENERATING SOLUTIONS BASED ON EACH BDY COND INDEPENDENTLY.
 C KBD. ALSO USED FOR DIRECTION SENSE FOR YB,ZB SURF ADMIT/IMPED.

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C APB1,  PRINCIPAL BRANCH SPECIFICATION FOR WX-PLANES.  ANGLE INTO WX
C APB2  HALF PLANE FOR OUTER LAYERS L1 AND L2+1.  UNITS OF PI. (0.25)
C      (DIRECTION ANGLE OF BRANCH CUTS IN QZ PLANE IS TWICE APB.)
C      +0.0.LE.APB.LE.+1.0  BRANCH INCLUDES POS IMAG AXIS OF WX-PLANE.
C      -0.5.LE.APB.LE.+0.5  BRANCH INCLUDES POS REAL AXIS OF WX-PLANE.
C      DEFAULT APB1=0.25, APB2=0.25, NOT CONVENTIONAL SPECIFICATION.
C      RATHER, IMAG(WX).GE.REAL(WX).  BOUND AND LEAKY MODE ROOTS FOR
C      LOSSLESS DIELECTRIC STRUCTURES ARE ALL ON SAME PRINCIPAL BRANCH.
C      BRANCH CUTS IN QZ PLANE ARE IN POS IMAG DIRECTION.
C      (CONVENTIONAL CHOICE OF BRANCHES, APB= 0.5, KBD=2. BOUND PROPER
C      MODE ROOTS ON PRINCIPAL BRANCH AND RIEMANN SHEET OF QZ. LEAKY
C      IMPROPER MODE ROOTS ON SECOND BRANCH AND RIEMANN SHEET.
C      BRANCH CUTS IN QZ PLANE IN NEGATIVE REAL DIRECTION.)
C YB1,  FIXED BDY SURFACE ADMIT(TE)/IMPED(TM) LOOKING OUTWARD AT L1,L2
C YB2  USED ONLY IF RESPECTIVE KBC1,KBC2 ARE EQUAL TO 2      (1.0,0.0)
C ZB1,  FIXED BDY SURFACE IMPED(TE)/ADMIT(TM) LOOKING OUTWARD AT L1,L2
C ZB2  USED ONLY RESPECTIVE IF KBC1,KBC2 ARE EQUAL TO 3.      (1.0,0.0)
C      LOOKING OUTWARD IFF KBD1,2 EQUAL 2 (DEFAULT)
C
C EXAMPLES OF NAMELIST INPUT. IMPORTANT. COL 1 BLANK(IGNORED), LEADING
C $-SIGNS AND DATA IN COL 2, ALL DATA SEPARATED BY COMMAS, SPECIFIC
C ARRAY ELEMENTS USED, AT LEAST FOR STARTING POINT. VARIABLE NAMES MAY
C APPEAR ONLY IN APPROPRIATE DEFINED NAMELISTS BETWEEN $NAME $END.
C NAMELIST GROUPS MUST BE IN THE ORDER $CASE, $LAYERS, $MODCON.
C EACH $CASE CARD BELOW MARKS THE BEGINING OF A NEW CASE.
C
C EXAMPLE1. MINIMUM INPUT NEEDED FOR DEFAULT CASE. FIRST THREE CARDS.
C FOLLOWED BY SECOND CASE. FEWER MODES, MORE ITERATIONS, SMALLER EPS,
C TM POLARIZATION, AND FULL FIELD SOLUTIONS.
C
C$CASE      $END
C$LAYERS    $END
C$MODCON    $END
C$CASE KASE=2, MN=4,
CKGCZ=4, EPS1=1.0E-8, EPS2=1.0E-8, IL= 15,
CKDOF=2, KOUF=4,
C$END
C$LAYERS    $END
C$MODCON KPOL=2 $END
C$CASE KASE=0 $END
C
C EXAMPLE 2. COMPLICATED. 7 LAYERS OPEN STRUCTURE. TWO LEAKY COUPLED
C GUIDES (L=3,5). ALL LAYERS LOSSY EXCEPT GAIN IN ONE GUIDE (L=5),
C FIRST CASE RUN FOR PARTIAL STRUCTURE AND NO FIELD SOLUTIONS.
C SECOND CASE FULL STRUCTURE, USING QZ MODE VALUES FROM FIRST CASE AS
C GUESSES. FEWER MODES AND FULL FIELD SOLUTIONS.
C
C$CASE KASE=703033,
CHN=5, QZNR=10.0,
CKGCZ=4, EPS1=1.0E-8, EPS2=1.0E-8, IL= 15,

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C$END
C$LAYERS  WVL=0.86,  LN=7,
CKXTL=2,  TL(2)= 1.0,1.4,0.3,0.4,1.0,
CPR(1)= 12.960,11.492,12.745,11.492,12.960,11.492,12.960,
CPEI(1)=2.578E-3,4.854E-4,1.021E-4,4.854E-4,-1.031E-2,4.854E-4,2.578E-3,
C$END
C$MODCON  L1=2, L2=5      $END
C$CASE  KGSS=1, MN=4,
CKDOF=2, KOUF=4,
C$END
C$LAYERS      $END
C$MODCON      $END
C$CASE KASE=0 $END
C
      END

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SUBROUTINE PUTSIN

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C
C   --DEFINES INPUT NAMELISTS, READS INPUT FOR LAYERED STRUCTURE,
C   --AND CALCULATES NECESSARY NEW PARAMETERS
C
COMMON /KASETS/ KASE,KSUB,MN,MO,MK,ML,IDEN,IMAX,INFX,
$QZNR,QZNI,KGSS,PMFR,PMDM,KGCZ,WFMP,EPS1,EPS2,EPS3,IL,KMDO,
$KDOO,KDOI,KDOS,KDOM,KEIF,KDOZ,KDOF,KDOP,
$KOUT,KOUI,KOUS,KOUM,KOUE,KOUZ,KOUF,KOUP
C   MAIN,PUTS,SRCH,SYSH,EIGQ,CZRM,FLDS,PWRS
C   --NOTE EQUIVALENCE OF VARIOUS KOUT AND KDOO WITH LAST INITIAL
C
COMMON /LAYCOM/ XU,WVL,KO,KCR,KCI,KFR,KFI,LN,KXTL,XL(10),TL(10),
$PER(10),PEI(10),PMR( 1),PHI( 1)
REAL KO,KCR,KCI,KFR,KFI
C
COMMON /BDYCON/ KPOL,L1,KBC1,KBD1,APB1,VPB1,YB1,ZB1,
$L2,KBC2,KBD2,APB2,VPB2,YB2,ZB2,KBC0
COMPLEX VPB1,YB1,ZB1,VPB2,YB2,ZB2
C
COMMON /STRUCT/ LK,LL,LM,KS,KC,KF,TR(10),QN(10),KPLS,YN(10)
REAL KS
COMPLEX KC,KF,QN,YN
C
COMMON /MODSET/ NM,NO,NK,NL,QZH(10),PHM(10),KM(10)
COMPLEX QZH,PHM
C
C   --SCRATCH VARIABLES AND CONSTANTS
COMPLEX AC,BC,CC,DC
COMPLEX CO,C1,CI
DATA CO,C1,CI/ (0.0,0.0),(1.0,0.0),(0.0,1.0)/
DATA PI,PI2,PIH/ 3.1415926535898,6.2831853071796,1.5707963267949/
C
C FOR NAMELIST INPUT VARIABLES DESCRIPTION SEE BLOKOM
C
NAMelist /CASE/ KASE,MN,MO,IDEN,IMAX,INFX,QZNR,QZNI,
$QZNR,QZNI,KGSS,PMFR,KGCZ,WFMP,EPS1,EPS2,EPS3,IL,QZH,
$KGSS,PMFR,KGCZ,WFMP,EPS1,EPS2,EPS3,IL,QZH,KM,KMDO,
$KDOO,KDOI,KDOS,KDOM,KEIF,KDOZ,KDOF,KDOP,
$KOUT,KOUI,KOUS,KOUM,KOUE,KOUZ,KOUF,KOUP
C   MAIN,PUTS,SRCH,SYSH,EIGQ,CZRM,FLDS,PWRS
C
NAMelist /LAYERS/ XU,WVL,KO,KCR,KCI,KFR,KFI,
$LN,KXTL,XL,TL,PER,PEI,PMR,PHI
C
NAMelist /MODCON/ KPOL,L1,APB1,KBC1,KBD1,YB1,ZB1,
$L2,APB2,KBC2,KBD2,YB2,ZB2
C
READ(5,CASE)
10 IF(KDOO.GE.1.AND.KASE.GE.1) GO TO 20

```

```

C
C     ELSE-10. NO MORE CASES, STOP.
      WRITE(6,1000)
1000 FORMAT(54H0*****.NO MORE CASES.*****.END PROGRAM MODEIGS.***** )
      STOP
C
C 20 THEN-10./ A NEW MODEIG CASE.
      20 WRITE(6,1020)
1020 FORMAT(1H1,9H*****.4(10H*****),20H PROGRAM MODEIG ,
1 5(10H*****),/ 2(10H * * * * ),5X,70H CALCULATION OF GENER
2AL COMPLEX EIGEN-WAVES IN LAYERED STRUCTURES ,5X,
3 2(10H* * * * ) )
C
      READ(5,LAYERS)
      L1= 1
      L2= LN-1
C
      READ(5,MODCON)
C
      IF(KASE.EQ.LAST) GO TO 40
      KSUB= 0
      LAST= KASE
      40 KSUB= KSUB+1
      WRITE(6,1040) KASE,KSUB
1040 FORMAT(34H0****SUBROUTINE PUTSIN. KASE NO.=,I6,1H.,I2, )
      KO= PI2/WVL
      KS= KO
      KC= CMPLX(KCR,KCI)
      KF= CMPLX(KFR,KFI)
      MO= MAX0(-1,MO)
      MK= MO+1
      ML= MO+MN
      MN= MAX0(1,MINO(MN,10))
      NM= MN
      NL= ML
      NK= MK
      LN= MAX0(2,MINO(LN,10))
      LM= LN
      LL= LN-1
      LK= LN-2
C
      --IF SINGLE BOUNDARY, NO FINITE THICKNESS LAYERS
      IF(LL.LE.1) GO TO 150
C
      --CALCULATE FREE-SPACE RADIAN THICKNESSES TR
      IF(KXTL.GE.1) GO TO 120
C
      --THICKNESS TL CALCULATED FROM BOUNDARY XL
C
      --CHECK AND REORDER THE XL VALUES IF NECESSARY
100 DO 105 K=1,LK
      L= K+1
      DO 105 M=L,LL
      IF(XL(K).LE.XL(M)) GO TO 105

```

```

        XA= XL(K)
        XL(K)= XL(M)
        XL(M)= XA
105 CONTINUE
110 DO 115 L= 2,LL
    TL(L)= XL(L)-XL(L-1)
    TR(L)= KO*TL(L)
115 CONTINUE
    GO TO 150
C
C    --BOUNDARY XL CALCULATED FROM THICKNESS TL
120 XL(1)= 0.0
    DO 125 L=2,LL
        TL(L)= ABS(TL(L))
        XL(L)= XL(L-1)+TL(L)
        TR(L)= KO*TL(L)
125 CONTINUE
150 CONTINUE
C    --RECORD TOTAL THICKNESS AND TOTAL RADIAN THICKNESS IN LOCATION LM
    XL(LM)= XL(LL)
    TL(LM)= XL(LL)-XL(1)
    TR(LM)= KO*TL(LM)
C
C 200 --CALCULATE SQUARED REFRACTIVE INDEX FOR EACH LAYER MATERIAL
C    --AND NORMALIZED ADMIT/IMPED FOR GIVEN POLARIZATION AND UNIT WX
C    --(POSSIBLE ENTRY POINT FOR NEW CASE WITH UNCHANGED STRUCTURE BUT
C    --NEW MODAL CONDITIONS, POLARIZATION, OR BOUNDARY CONDITIONS)
    KPLS= KPOL
    CC= KF*KF
250 IF(KPOL.GE.2) GO TO 270
C    --ELSE-250. TE, TRANSVERSE ELECTRIC CASE
260 DO 265 L=1,LM
    DC= CMPLX(PER(L),PEI(L))
    BC= CMPLX(PMR(1),PHI(1))
    QN(L)= CC*BC*DC
    YN(L)= C1/(KF*BC)
265 CONTINUE
    GO TO 280
C    --THEN-250. TM, TRANSVERSE MAGNETIC CASE
270 DO 275 L=1,LM
    DC= CMPLX(PER(L),PEI(L))
    BC= CMPLX(PMR(1),PHI(1))
    QN(L)= CC*BC*DC
    YN(L)= C1/(KF*DC)
275 CONTINUE
280 CONTINUE
C    --ENDIF-250
C
C    --INDEX PARAMETERS FOR BOUNDARIES OF FULL OR PARTIAL STRUCTURE
    LO= MIN0(L1,L2,LL)

```

```

      L2= MIN0(MAX0(1,L1,L2),LL)
      L1= MAX0(1,L0)
      L0= L1+1
C     --CONTROL PARAMETER FOR EIG, NON-EIG, COND. ONE OR BOTH BOUNDARIES
      KBC0= 0
      IF(KBC1.GE.1) KBC0= 1
      IF(KBC2.GE.1) KBC0= KBC0+2
C     --UNIT VECTORS INTO PRINCIPAL BRANCH HALF-PLANES OF WX
      VPB1= CMPLX(COS(APB1*PI),SIN(APB1*PI))
      VPB2= CMPLX(COS(APB2*PI),SIN(APB2*PI))
C
C     --CALL TO CLEAR AND INITIALIZE SYSMAT
      CALL SYSMAT(C1,C1,0,0)
C
C 300 --SUMMARY OUTPUT FOR CASE
      CC= KC*K0
      WRITE(6,1300) XU,WVL,K0,KC,CC
      WRITE(6,1301) KF
      WRITE(6,1302) KPOL
      IF(KPOL.LE.1) WRITE(6,1304)
      IF(KPOL.GE.2) WRITE(6,1306)
      WRITE(6,1308) LM,LL,LK
C     --FIRST SEMI-INFINITE LAYER.
      AC= CSQRT(QN(1))
      L= 1
      WRITE(6,1310) PER(L),PEI(L),PMR(1),PMI(1),L,QN(L),YN(L),AC
310 DO 320 L=1,LL
C     --FOR EACH FINITE LAYER.
      IF(L.LE.1) GO TO 330
      TM= TL(L)/WVL
      BC= CSQRT(QN(L))
      CC= KC*BC*TR(L)
      WRITE(6,1315) PER(L),PEI(L),PMR(1),PMI(1),L,TL(L),
      $ QN(L),YN(L),TM,BC,CC
C     --IDENTIFY OUTER BOUNDARIES, FULL OR PARTIAL STRUCTURE.
330 IF(L.EQ.L1) WRITE(6,1330) L1
C     --EACH BOUNDARY LOCATION
335 WRITE(6,1335) L,XL(L)
340 IF(L.EQ.L2) WRITE(6,1340) L2
320 CONTINUE
C     --SECOND SEMI-INFINITE LAYER.
      AC= CSQRT(QN(LM))
      L= LM
350 WRITE(6,1310) PER(L),PEI(L),PMR(1),PMI(1),L,QN(L),YN(L),AC
C
C     --DESCRIBE FIRST BOUNDARY CONDITIONS.
370 WRITE(6,1370) L1,KBC1,KBD1
      IF(KBC1.GE.2) GO TO 377
      WRITE(6,1372)
      WRITE(6,1373) APB1,VPB1

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```

      IF(KBC1.EQ.1) GO TO 375
      WRITE(6,1374)
      GO TO 380
375  IF(KBD1.LE.1) WRITE(6,1375)
      IF(KBD1.GE.2) WRITE(6,1376)
      GO TO 380
377  WRITE(6,1377)
      IF(KBC1.EQ.2) WRITE(6,1378) YB1
      IF(KBC1.GE.3) WRITE(6,1379) ZB1
C    --DESCRIBE SECOND BOUNDARY CONDITION.
380  WRITE(6,1371) L2,KBC2,KBD2
      IF(KBC2.GE.2) GO TO 387
      WRITE(6,1372)
      WRITE(6,1373) APB2,VPB2
      IF(KBC2.EQ.1) GO TO 385
      WRITE(6,1374)
      GO TO 390
385  IF(KBD2.LE.1) WRITE(6,1375)
      IF(KBD2.GE.2) WRITE(6,1376)
      GO TO 390
387  WRITE(6,1377)
      IF(KBC2.EQ.2) WRITE(6,1378) YB2
      IF(KBC2.GE.3) WRITE(6,1379) ZB2
390  WRITE(6,1390)
C
C    FORMATS
C1300 --SUMMARY HEADING
1300  FORMAT(1H0, 9X,68HSUMMARY OF LAYERED STRUCTURE, POLARIZATION, AND
      1BOUNDARY CONDITIONS.//
      227H IMPLIED UNIT OF LENGTH XU=,E12.5,62H METERS (BUT NOT USED EXPL
      3ICITLY). ALL QUANTITIES NORMALIZED./
      424H NOMINAL WAVELENGTH WVL=,F10.5,33H XU, AND FREE-SPACE KO= 2PI/
      5WVL=,F10.5,8H RAD/XU./31H COMPLEX FREQUENCY FACTOR KC= (,F10.5,1H,
      6,F10.5,26H). EFFECTIVE-KO= KC*KO= (,F10.5,1H,,F10.5,2H).)
1301  FORMAT(115H ALL PROPAGATION COEFFICIENTS ARE NORMALIZED TO EFFECTI
      1VE-KO. (WAVE AND MATERIAL REFRACTIVE INDICES, IF KF= UNITY)//
      2 90H (WAVE ADMITTANCE(TE) AND IMPEDANCE(TM), YX AND YZ, ARE NORMAL
      3IZED TO THAT OF FREE SPACE. /27H NORMALIZED FREQUENCY KF= (,F10.5,
      41H,,F10.5,17H)= FREQ/C*EFF.KO. )
C1302 --POLARIZATION
1302  FORMAT(20H0POLARIZATION, KPOL=,I2,27H ( =1 TE CASE, =2 TM CASE) )
C1304 --TE CASE
1304  FORMAT(115H TRANSVERSE ELECTRIC CASE. EX=HY=EZ=0. TANGENTIAL FY=
      1+EY, FZ=+HZ. TRANSVERSE FX=-HX, FY=+EY. LONGITUDINAL FZ=+HZ./
      2 99H YX=FZ/FY=+HZ/EY, AND YZ=FX/FY=-HX/EY, ARE WAVE ADMITTANCES.
      3(IN THE POS X, Z, OR WAVE DIRECTION). )
C1306 --TM CASE
1306  FORMAT(115H TRANSVERSE MAGNETIC CASE. HX=EY=HZ=0. TANGENTIAL FY=
      1+HY, FZ=-EZ. TRANSVERSE FX=+EX, FY=+HY. LONGITUDINAL FZ=-EZ./
      2 99H YX=FZ/FY=-EZ/HY, AND YZ=FX/FY=+EX/HY, ARE WAVE IMPEDANCES.

```

```

3(IN THE POS X, Z, OR WAVE DIRECTION).      )
C1308 --NUMBER OF LAYERS
1308 FORMAT(21HOLAYERED STRUCTURE. ,I3,16H LAYERS TOTAL. ,I3,
1 14H BOUNDARIES. ,I3,15H FINITE LAYERS./      )
C1310 --FIRST AND LAST SEMI-INFINITE LAYERS
1310 FORMAT(25X,4H PE=,1H(,F10.5,1H,,F10.5,1H),
1 2X,4H PM=,1H(,F10.5,1H,,F10.5,1H)/
2 4H L,I3,3X,15HSEMI-INFINITE ,4H QN=,1H(,F10.5,1H,,F10.5,1H),
3 2X,4H YN=,1H(,F10.5,1H,,F10.5,1H)/
425X,4H RN=,1H(,F10.5,1H,,F10.5,1H),      )
C1315 FOR FINITE THICKNESS LAYERS
1315 FORMAT(25X,4H PE=,1H(,F10.5,1H,,F10.5,1H),
1 2X,4H PM=,1H(,F10.5,1H,,F10.5,1H)/
2 4H L,I3,3X,3HTL=,F10.5,2X, 4H QN=,1H(,F10.5,1H,,F10.5,1H),
3 2X,4H YN=,1H(,F10.5,1H,,F10.5,1H)/ 9X,1H(,F10.5,4HWVL),
4 1X,4H RN=,1H(,F10.5,1H,,F10.5,1H),
5 2X,4H PHO=,1H(,F10.5,1H,,F10.5,1H)      )
C1330 --FIRST BOUNDARY CONDITION
1330 FORMAT(4H L1=,I3,43H---BOUNDARY FOR FIRST BOUNDARY CONDITION--,
1 4(10H-----),      )
C1335 --EACH BOUNDARY
1335 FORMAT(4H --L,I3,6H---XL=,F10.5,7H-----,5(10H-----),      )
C1340 --SECOND BOUNDARY CONDITION
1340 FORMAT(4H L2=,I3,43H---BOUNDARY FOR SECOND BOUNDARY CONDITION--,
1 4(10H-----),      )
C1370 --DESCRIPTION OF BOUNDARY CONDITIONS
1370 FORMAT(34H0 FIRST BOUNDARY CONDITION. L1=,I2,
1 8H, KBC1=,I2, 8H, KBD1=,I2,1H.      )
1371 FORMAT(34H0SECOND BOUNDARY CONDITION. L2=,I2,
1 8H, KBC2=,I2, 8H, KBD2=,I2,1H.      )
1372 FORMAT(1H+,59X,44HOPEN BOUNDARY, SEMI-INFINITE ADJACENT LAYER.      )
1373 FORMAT(50H PRINCIPAL BRANCH SPECIFICATION FOR WX. ANGLE APB=,F6.3,
1 17H PI, VECTOR VPB=(,F6.3,1H,,F6.3,2H),,19H (WX*DOT*VPB.GE.0).,)
1374 FORMAT( 95H NON-EIGEN CONDITION. NO EIGEN-MODE SEARCH MADE. INWARD
1 AND OUTWARD WAVE SOLUTIONS ACCEPTABLE.      )
1375 FORMAT(119H EIGEN CONDITION. INWARD WAVE SOLUTION ONLY. (DIRECTIO
1N OF DECAY IF IM(WX).GT.0, OF PHASE PROPAGATION IF RE(WX).GT.0.)      )
1376 FORMAT(119H EIGEN CONDITION. OUTWARD WAVE SOLUTION ONLY. (DIRECTIO
1N OF DECAY IF IM(WX).GT.0, OF PHASE PROPAGATION IF RE(WX).GT.0.)      )
1377 FORMAT(55H EIGEN CONDITION. CLOSED BOUNDARY. OUTER LAYERS IGNORED)
1378 FORMAT(42H FIXED SURFACE ADMIT.(TE)/IMPED.(TM) YB=,F10.5,1H,,
1 F10.5,      )
1379 FORMAT(42H FIXED SURFACE IMPED.(TE)/ADMIT.(TM) ZB=,F10.5,1H,,
1 F10.5,      )
1390 FORMAT(27H0END STRUCTURE DESTRIPTION.,      )
C
900 RETURN
C
END

```

SUBROUTINE SEARCH

```

C
C SEARCHES FOR SETS OF EIGENVALUES (QZ,KC) IN QZ PLANE FOR FIXED KC.
C FOR GIVEN STRUCTURE AND MODAL CONDITIONS. SETS UP INITIAL GUESSES
C AND CALLS SUBROUTINE CZEROM. PRINCIPAL RESULTS TO COMMON /MODSET/.
C
COMMON /KASETS/ KASE,KSUB,MN,MO,NK,ML,IDEN,IMAX,INFX,
$QZNR,QZNI,KGSS,PHFR,PHDM,KGCZ,WFMP,EPS1,EPS2,EPS3,IL,KMDO,
$KDO1,KDO2,KDOS,KDO4,KEIF,KDOZ,KDO7,KDO8,
$KOU1,KOU2,KOUS,KOU4,KOU5,KOUZ,KOU7,KOU8
MAIN,PUTS,SRCH,SYSH,EIGQ,CZRM,FLDS,PWRS
--NOTE EQUIVQLENCE HERE OF KDOS=KDO3, AND KOUS=KOU3
C
COMMON /STRUCT/ LK,LL,LM,KS,KCC,KFC,TR(10),QN(10),KPLS,YN(10)
REAL KS
COMPLEX KCC,KFC,QN,YN
C
COMMON /BDYCON/ KPOL,L1,KBC1,KBD1,APB1,VPB1,YB1,ZB1,
$L2,KBC2,KBD2,APB2,VPB2,YB2,ZB2,KBCO
COMPLEX VPB1,YB1,ZB1,VPB2,YB2,ZB2
C
COMMON /MATSYS/ KDID,QZS,KCS,AQZ,WX(10),PH(10),PHR,PHI,YX(10),
$CL1(10),CL2(10),CL3(10),CM1,CM2,CM3,CM4,DETC(2),
$QX1,AQX1,FY1,FZ1,QX2,AQX2,FY2,FZ2,SM1,SM2,SM3,SM4,DETS,WZ,YZ(10)
COMPLEX QZS,KCS,WX,PH,PHR,PHI,YX,CL1,CL2,CL3,CM1,CM2,CM3,CM4,DETC,
$QX1,FY1,FZ1,QX2,FY2,FZ2,SM1,SM2,SM3,SM4,DETS,WZ,YZ
C
COMMON /MODSET/ NM,NO,NK,NL,QZH(10),PHM(10),KM(10)
COMPLEX QZH,PHM
C
COMMON /CZECOM/ NN,NT,ZO(10),FM(10),IT(10),KR(10),
$EPSZ,EPSE,II,KTUD
COMPLEX EIGE0F,ZO
EXTERNAL EIGE0F
C
C --LOCAL AND SCRATCH VARIABLES
COMPLEX KC,KF
COMPLEX AC,BC,CC,DC
C
DATA PI,ED/ 3.1415926535898, 2.3025850922940/
C
C
WRITE(6,1000) KASE,KSUB,KDOS,KOUS
1000 FORMAT(34H0****SUBROUTINE SEARCH. KASE NO.=,I6,1H.,I2,
1 8H, KDOS=,I2, 8H, KOUS=,I2,1H. )
IF(KBCO.GT.0) GO TO 5
WRITE(6,1002)
1002 FORMAT(1H+,T67,46HNON-EIGEN CONDITIONS. NO SEARCH MADE. RETURN. )
RETURN
C

```



```

      5 WRITE(6,1005) MN,MK,ML
1005 FORMAT(18H SEARCHING FOR MN=,I2,53H EIGENVALUES.  FOR INTENDED MOD
      $E INDICES FROM  MM=MK=,I3,10H TO MM=ML=,I3,1H.      )

```

C

```

      KC= KCC
      KF= KFC
      NM= MN
      NO= MO
      NK= MK
      NL= ML
      LO= L1+1
      LP= L2-L1

```

C

```

C 10 --SURVEY COMPLEX QZ PLANE.  FIND REPRESENTATIVE VALUES OF REAL QZ
C --AS BASIS FOR GUESSES.  SET INITIAL DEFAULT VALUES.

```

```

      QR0= 0.0
      QR1= QZNR
      QR2= 0.5
      QR3= 1.0
      PR= 0.0
      IF(LP.GE.1) GO TO 20

```

C

```

C --FOR SINGLE BOUNDARY CASE.
C IF(KBC1.LT.2.OR.KBC2.LT.2) GO TO 15
  WRITE(6,1010)

```

```

1010 FORMAT(54H ****SINGLE BOUNDARY, DOUBLY CLOSED, NO CASE, STOP.  ,)
      STOP

```

```

C --PHASE INTEGRAL NOT DEFINED, USE RECIPROCAL MEAN FOR GUESSES.

```

```

15 QR= 0.0
   PM0= 0.0
   IF(KBC1.LE.1) QR= QR+1.0/REAL(QN(L1))
   IF(KBC2.LE.1) QR= QR+1.0/REAL(QN(L2+1))
   QR3= 1.0/QR
   KGSS=2
   GO TO 80

```

C

```

C --TWO OUTER BOUNDARIES.  ONE OR MORE FINITE INNER LAYERS

```

```

C --FIND MAX QR OF INNER LAYERS, KEEP QZNR.LT.9/10 OF MIN QR.

```

```

20 DO 30 L=LO,L2
   AA= REAL(QN(L))
   QR3= AMAX1(AA,QR3)
   AA= 0.9*AA
   IF(0.0.LE.AA.AND.AA.LE.QZNR) QZNR= AA
   PR= PR+TR(L)

```

```

30 CONTINUE

```

```

      QR1= QZNR
      CC= CMPLX(QR0,0.0)
      CALL SYSMAT(CC,KC,2,0)
      PM0= REAL(PHR)/PI
      CC= CMPLX(QR1,0.0)

```

```

      CALL SYSMAT(CC,KC,2,0)
      PM1= REAL(PHR)/PI
C    --A MEAN VALUE OF QR BASED ON PHASE THICKNESS FOR QR1=QZNR.
      QR2= (QR1+QR3)/2.0
      AA= REAL(PHR*PHR)
      CC= KC*PR
      QT= REAL(CC)*REAL(CC)+AIMAG(CC)*AIMAG(CC)
      IF(AA.LT.0.001.OR.QT.LT.0.001) GO TO 40
      QR2= QR1 + AA/QT
40   QR2= (QR1+QR2+QR3)/3.0
      CC= CMPLX(QR2,0.0)
      CALL SYSMAT(CC,KC,2,0)
      PM2= REAL(PHR)/PI
      CC= CMPLX(QR3,0.0)
      CALL SYSMAT(CC,KC,2,0)
      PM3= REAL(PHR)/PI
      IF(KOUS.LE.1) GO TO 80
      WRITE(6,1030) QR0,QR1,QR2,QR3,PM0,PM1,PM2,PM3
1030 FORMAT(66H REPRESENTATIVE VALUES OF REAL QZ AND CORRESPONDING PHAS
      1E INTEGRAL, /6H QZR= ,4(F10.5,5H,    )/6H PHM= ,4(F10.5,5HPI,    ) )
C
C 80 --TEST AND REDUCE MODE SET TO ONLY PROPAGATING NON-EVANESCENT ONES
C    --REAL QZM.GT.QZNR AND PHM.LT.PHM(QZNR)
C    --FUTURE IMPLEMENTATION
80   CONTINUE
C
C    --PREPARE GUESSES AND PARAMETERS FOR CALL TO CZEROM.
90   IF(KGSS.GT.2) GO TO 300
      IF(KGSS.GT.1) GO TO 200
C
C 100 --ELSE-90. KGSS.LE.1, USE VALUES IN QZM AND KM FOR GUESSES.
C    --FROM INPUT, OR FROM JUST PREVIOUS CASE. KR=KM, NOT= KG CZ.
100  DO 110 M=1,MN
      AC= QZM(M)
      CALL SYSMAT(AC,KC,2,0)
      BC= CMPLX(REAL(PHR)/PI,AIMAG(PHI)/ED)
      ZO(M)= AC
      PHM(M)= BC
      FM(M)= -1.0
      IT(M)= 0
      KR(M)= KM(M)
110  CONTINUE
      WRITE(6,1120) KGSS,KGCZ
1120 FORMAT( 6H0KGSS=,I2,84H. INITIAL GUESSES FROM QZM OF MODSET, EITH
      1ER FROM INPUT OR RESULTS FROM PREV. CASE.,2X,5HKG CZ=,I2,    )
      GO TO 600
C
C 200 --THEN-91. KGSS.EQ.2, ALL INITIAL GUESSES THE SAME
C    -- EQUAL TO MAX QR OF INNER FINITE LAYERS.
200  AC= CMPLX(QR3,QZNI)

```

```

CALL SYSMAT(AC,KC,2,0)
BC= CMPLX(REAL(PHR)/PI,AIMAG(PHI)/ED)
KGCZ= MIN0(3,KGCZ)
DO 210 M=1,MM
  QZM(M)= AC
  PHM(M)= BC
  KM(M)= KGCZ
  ZO(M)= AC
  FM(M)= -1.0
  IT(M)= 0
  KR(M)= KGCZ
210 CONTINUE
220 WRITE(6,1220) KGSS,AC,BC,KGCZ
1220 FORMAT( 6H0KGSS=,I2,38H. ALL INITIAL GUESSES THE SAME. QZ=(,
$ F8.4,1H,,F8.4,1H),2X,5HPHM=(,F8.3,3HPI,,F8.4,4HDEC),
$ 2X,5HKGCZ=,I2,      )
GO TO 600

C
C 300 --THEN-90. KGSS.EQ.3, INDIVIDUAL GUESSES FOR QZ. SIMPLE QUADRATIC
C --APPROXIMATION FROM QZM VS PHM FOR INTENDED MODE INDICES MM.
300 D1= (QR1-QR3)/PM1
D2= (QR2-QR3)/PM2
A2= (D1-D2)/(PM1-PM2)
IF(A2.GT.0.0) A2= 0.0
A1= D1-A2*PM1

C --REVISE QUADRATIC COEFFICIENTS ON BASIS OF QR GUESS FOR AVG MM.
PM= (FLOAT(NK+NL)/2.0)+PMFR
QR2= QR3+(A1+A2*PM)*PM
BC= CMPLX(QR2,QZNI)
CALL SYSMAT(BC,KC,2,0)
PM2= REAL(PHR)/PI
WRITE(6,1305) QR2,PM2
1305 FORMAT( 6H QZR= ,F10.5,5H,      ,10X,5HPHM= ,F10.5,2HPI,      )
C --REVISE COEFFICIENTS FOR APPROXIMATING QUADRATIC
D2=(QR2-QR3)/PM2
A2= (D1-D2)/(PM1-PM2)
IF(A2.GT.0.0) A2= 0.0
A1= D1-A2*PM1

C --FORM INITIAL GUESSES
310 DO 320 M=1,MM
  PM= PMDM*FLOAT(MO+M)+PMFR
  QR= QR3+(A1+A2*PM)*PM
  AC= CMPLX(QR,QZNI)
  QZM(M)= AC
  CALL SYSMAT(AC,KC,2,0)
  PHM(M)= CMPLX(REAL(PHR)/PI,AIMAG(PHI)/ED)
  KM(M)= KGCZ
  ZO(M)= AC
  FM(M)= -1.0
  IT(M)= 0

```

```

320 CONTINUE
C
C 350 --REFINE BY QUADRATIC INTERPOLATION BASED ON FIRST GUESSES.
C      --FUTURE IMPLEMENTATION.
380 WRITE(6,1380) KGSS,KGCZ
1380 FORMAT( 6H0KGSS=,I2,1H.,2X,92HINDIVIDUAL GUESSES FOR EACH QZ. BASE
      $D ON SIMPLE QUADRATIC APPROXIMATION FOR REAL QZ VS PHM.,
      $ 2X,5HKGCZ=,I2,      )
      GO TO 600
C
C 400 --INDIVIDUAL GUESSES FOR QZM. HIGHER ORDER POLYNOMIAL INTERPOLATE
C      --BASED ON REAL ROOT SEARCH FOR FIRST AND LAST INTENDED MODE NOS.
C      --FUTURE IMPLEMENTATION.
C
C 500 --INDIVIDUAL GUESSES EACH BASED ON REAL ROOT SEARCH OF PHM VS QZ.
C      --FUTURE IMPLEMENTATION.
C
C 600 --ENDIF-90. DISPLAY INITIAL GUESSES, CALL CZEROM FOR ROOT SEARCH
600 IF(KOUS.LE.2) GO TO 630
C 610 --OUTPUT /MODSET/ FOR INITIAL GUESSES.
610 DO 620 M=1,MN
      MM= MO+M
      WRITE(6,1710) M,MM,QZN(M),PHM(M),KM(M),IT(M)
620 CONTINUE
C
C      --SET CZEROM PARAMETERS
630 NN=MM
      EPSZ= EPS1
      EPSF= EPS2
      II= IL
      KTUO= KOUZ
      IF(KOUS.GE.1) WRITE(6,1630) NN,EPSZ,EPSF,II,KTUO,KEIF
1630 FORMAT(44H CALLING CZEROM FOR COMPLEX ROOT SEARCH. NN=,I3,
      113H ROOTS, EPSZ=,E9.2,8H, EPSF=,E9.2,6H, II=,I3,8H, KOUT=,I2,
      2 8H, KEIF=,I2,1H.)
C
C      --MAIN CALL TO CZEROM
      CALL CZEROM(EIGEQF)
C
C      --REFINE EIGENVALUES BY SECOND CALL TO CZEROM.
C      --FUTURE POSSIBILITY
C
C 700 --TRANSFER RESULTS TO /MODSET/ WITH CALCULATION OF PHM
C      --OUTPUT VARIOUS PARAMETERS FOR EACH EIGENMODE.
700 WRITE(6,1700)
      MI= 2*ML
      DO 710 M=1,MN
      MM= MO+M
      AC= ZO(M)

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QZM(M)= AC
KM(M)= KR(M)
CALL SYSMAT(AC,KC, 5,0)
BC= CMPLX(REAL(PHR)/PI,AIMAG(PHI)/ED)
PHM(M)= BC
MI= MIN0(MI,INT(REAL(BC)))
C  --OUTPUT EACH FOUND EIGENVALUE QZ AND PHM.
WRITE(6,1708)  M,M,M,M,M,M,M,M,M,M,M,M
WRITE(6,1710)  M,MM,AC,BC,KM(M),IT(M)
IF(IT(M).GT.0) GO TO 714
WRITE(6,1712)
714 IF(IL.LE.IT(M)) WRITE(6,1714)
IF(KM(M).GE.5) GO TO 718
WRITE(6,1716)
GO TO 720
718 WRITE(6,1718)
720 IF(KOUS.LE.1.OR.KM(M).LT.KMDO) GO TO 710
C
C  --ELSE-720. PROPAGATION CONSTANT, PHASE INTEGRAL, AND SM MATRIX
WRITE(6,1720) WZ,PHR,PHI,AQZ
WRITE(6,1725) SM1,SM3,DETS,SM2,SM4
IF(KOUS.LE.2) GO TO 740
C
C 730  --OUTPUT SYSTEM MATRIX AND WAVE PROPAG PARAMETERS FOR LAYERS
DC= DETC(1)-CMPLX(1.0,0.0)
WRITE(6,1730) CM1,CM3,DC,CM2,CM4,DETC(2)
740 IF(KBC1.GE.2) GO TO 750
L= L1
C  --FOR FIRST BOUNDING SEMI-INFINITE LAYER.
WRITE(6,1740) L,WX(L),YX(L),QX1,AQX1
750 IF(KOUS.LE.3.OR.LP.LE.0) GO TO 760
C  --WAVE PARAMETERS FOR EACH INNER FINITE LAYER.
DO 755 L=L0,L2
WRITE(6,1750) L,WX(L),YX(L),PH(L),CL1(L),CL2(L),CL3(L)
755 CONTINUE
C  --FOR SECOND BOUNDING SEMI-INFINITE LAYER.
760 IF(KBC2.GE.2) GO TO 710
L= L2+1
WRITE(6,1740) L,WX(L),YX(L),QX2,AQX2
C
C  --FORMAT GROUP
1708 FORMAT(1H0,12(4H ---,I2,4H ---))
1700 FORMAT(39HORESULTS FROM EIGENVALUE ROOT SEARCH. )
1710 FORMAT(1H ,I2,4H MM=,I3,2X,4HQZ=(,F13.8,1H,,F13.8,1H),2X,5HPHM=(,
1 F8.3,3HPI,,F8.3,4HDEC),2X,3HKM=,I2,13X,3HIT=,I2,15X, )
1712 FORMAT(1H+,99X,14HINITIAL GUESS.)
1714 FORMAT(1H+,99X,16HITERATION LIMIT.)
1716 FORMAT(1H+,81X,10HNOT CONVG.)
1718 FORMAT(1H+,81X,10HCONVERGED.)
1720 FORMAT(12X,4HWZ=(,F13.8,1H,,F13.8,1H),2X,5HPHR=(,F8.3,1H,,F8.3,

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1 1H),2X,5HPHI=(,F8.3,1H,,F8.3,1H), 9X,5HATQZ=,E11.4,5HP1/2.)
1725 FORMAT(12X,3HSM=, 2(2H (,E11.4,1H,,E11.4,1H)), 5X,10HDET(SM)= (,
1 E11.4,1H,,E11.4,1H) / 15X, 2(2H (,E11.4,1H,,E11.4,1H)),1H. )
1730 FORMAT(12X,3HCM=, 2(2H (,E11.4,1H,,E11.4,1H)), 5X,10HDET(CM)= (,
1 E11.4,1H,,E11.4,13H) + (1.0,0.0)/15X,2(2H (,E11.4,1H,,E11.4,1H)),
2 1H.,4X,10HDETNORM= (,E11.4,1H,,E11.4,2H). )
1740 FORMAT( 8X,2HL=,I2,3X,4HWX=(,E11.4,1H,,E11.4,6H) YX=(,E11.4,1H,,
1 E11.4,7H) QX=(,E11.4,1H,,E11.4,7H) ATQX=,F11.8,5HP1/2.)
1750 FORMAT( 8X,2HL=,I2,3X,4HWX=(,E11.4,1H,,E11.4,6H) YX=(,E11.4,1H,,
1 E11.4,7H) PH=(,E11.4,1H,,E11.4,1H),/
2 15X,3HCL=, 3(1H(,E11.4,1H,,E11.4,1H),5X),8H CL4=CL1, )
C -- END FORMATS
C
710 CONTINUE
C
800 CONTINUE
C 800 --ASSAY MODES IN /MODESET/ FOR ANY FURTHER USE BY FIELDS,POWERS
C
C --RESET INDICES TO LOWEST MODE FOUND AND MAX MM TRIED
NM= NT
NK= MINO(MI,NT)
NO= NK-1
NL= NO+NM
810 WRITE(6,1810) NM,NK
1810 FORMAT(82HORE-STATE MODE SET IN TERMS OF NUMBER TRIED AND LOWEST
$ACTUALLY FOUND. NO. TRIED=,I2,16H. LOWEST FOUND=,I2,1H., )
WRITE(6,1812) NK,NL
1812 FORMAT( 9H NOW MM= ,I3,1H,I3,80H. FOR ANY MODE WITH PHMM NOT IN
1INTENDED RANGE, VALUE OF KM IS REDUCED BY 1. )
C --FOR MODES WITH PHM NOT IN INTENDED RANGE OF MM REDUCE KM BY ONE
820 DO 825 M=1,NT
AA= REAL(PHM(M))
IF(FLOAT(MK).GT.AA+0.5) KM(M)= KM(M)-1
IF(AA-1.5.GT.FLOAT(NL)) KM(M)= KM(M)-1
825 CONTINUE
C
900 WRITE(6,1900)
1900 FORMAT(25H *****END SEARCH. RETURN.)
C
RETURN
C
END

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      COMPLEX FUNCTION EIGEQF(ZZ,NR)
C
C CALCULATES VALUE OF EIGEN EQUATION FUNCTION FROM SYSTEM CHARACTERISTIC
C MATRICES AND BOUNDARY CONDITIONS THROUGH CALL TO SUBROUTINE SYSMAT
C VALUE TO BE MADE ZERO BY ROOT SEARCHING FROM SUBROUTINE CZEROM CALLS
C
      COMMON /KASETS/ KASE,KSUB,MN,MO,MK,ML,IDEN,IMAX,INFX,
      $QZNR,QZNI,KGSS,PMFR,PMDM,KGCZ,WFMP,EPS1,EPS2,EPS3,IL,KMDO,
      $KDO1,KDO2,KDO3,KDO4,KEIF,KDO6,KDO7,KDO8,
      $KOU1,KOU2,KOU3,KOU4,KOUE,KOU6,KOU7,KOU8
C      --NOTE EQUIVALENCE HERE OF KDOO=KEIF=KDO5, AND KOUT=KOUE
C      MAIN,PUTS,SRCH,SYSM,EIGQ,CZRM,FLDS,PURS
C      --NOTE EQUIVALENCE HERE OF KDOO= KEIF=KDO5, AND KOUT=KOU5
C
      COMMON /BDYCON/ KPOL,L1,KBC1,KBD1,APB1,VPB1,YB1,ZB1,
      $L2,KBC2,KBD2,APB2,VPB2,YB2,ZB2,KBCO
      COMPLEX VPB1,YB1,ZB1,VPB2,YB2,ZB2
C
      COMMON /STRUCT/ LK,LL,LH,KS,KCC,KFC,TR(10),QN(10),KPLS,YN(10)
      REAL KS
      COMPLEX KCC,KFC,QN,YN
C
      COMMON /MATSYS/ KDID,QZS,KCS,AQZ,WX(10),PH(10),PHR,PHI,YX(10),
      $CL1(10),CL2(10),CL3(10),CH1,CH2,CH3,CH4,DETC(2),
      $QX1,AQX1,FY1,FZ1,QX2,AQX2,FY2,FZ2,      SM(2,2),      DETS,WZ,YZ(10)
      COMPLEX QZS,KCS,WX,PH,PHR,PHI,YX,CL1,CL2,CL3,CH1,CH2,CH3,CH4,DETC,
      $QX1,FY1,FZ1,QX2,FY2,FZ2,      SM,      DETS,WZ,YZ
C      --NOTE EQUIVALENCE OF SM(2,2) TO SM1,SM2,SM3,SM4 IN /MATSYS/
C
      COMPLEX AC,ZZ,QZ,KC
      DATA PI/ 3.1415926535898/
C
      QZ= ZZ
      KC= KCC
      MN= MO+NR
100 CALL SYSMAT(QZ,KC,4,0)
      PHMM= REAL(PHR)/PI
C      --SELECT EIGEN EQUATION FUNCTION FROM S MATRIX ELEMENTS
      K1= MAX0(1,MINO(2,KBD1))
      K2= MAX0(1,MINO(2,KBD2))
      EIGEQF= SM(K2,K1)
      WF= 1.0
      IF(KEIF.LE.1) GO TO 900
C
C 200 --MODIFY EIGEQF BY A RENORMALIZATION RELATIVE TO UNITY
C      --DIVIDE BY R.M.SQD.MAGNITUDES OF THE 4 ELEMENTS OF SM MATRIX
      WF= 0.0
210 DO 215 K=1,2
      DO 215 J=1,2
          AC= SM(J,K)

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      WF= WF+REAL(AC)*REAL(AC)+AIMAG(AC)*AIMAG(AC)
215  CONTINUE
      WF= SQRT(4.0/WF)
      EIGEQF= WF*EIGEQF
      IF(KEIF.LE.2) GO TO 900
C
C 300 --MODIFY EIGEQF TO BIAS SEARCH TOWARD INTENDED MODE INDEX
C      --MULTIPLY BY POS REAL WEIGHT FUNCTION, SQD DIFF BETWEEN PHASE
C      --INTEGRAL AND INTENDED MODE INDEX
      FLMM= FLOAT(MM)
C      --WEIGHT FUNCTION. NOTE IF(MM.LE.PHMM.LE.MM+1) WF= 1.0
      AA= AMAX1(PHMM-FLMM-1.0,-(PHMM-FLMM),0.0)
      WF= WFMP*AA*AA + 1.0
      EIGEQF= WF*EIGEQF
      IF(KEIF.LE.2) GO TO 900
C
C 400 --ALTERNATIVE MORE RESTRICTIVE WEIGHT FUNCTION
C      --FUTURE IMPLEMENTATION
C
C 500 --MODIFY VALUE OF QZ OR KC TO OBTAIN APPROX DESIRED PHASE INTEGRAL
C      --FUTURE IMPLEMENTATION
C
C 600 --TEST FOR APPROACH TO BRANCH CUTS DURING SEARCH,
C      --OR THAT OTHER BRANCH EIGEQF ARE SMALLER.
C      --SWITCH TO OTHER BRANCES OR REDIFINE PRINCIPAL BRANCES.
C      --FUTURE IMPLEMENTATION
C
      900 IF(KQUE.GE.4) WRITE(6,1900) NR,QZ,EIGEQF,WF,PHMM,MM,SM
1900  FORMAT(4H NR=,I2,6H QZ=(,F10.5,1H,,F10.5,10H) EIGEQF=(,E12.5,
      $ 1H,,E12.5,5H) WF=,F10.5,7H. PHR=,F10.5,7HPI MM=,I2/
      $ 8X,4HSM= , 4(3H (,E11.4,1H,,E11.4,1H),) )
C
      RETURN
C
      END

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SUBROUTINE SYSMAT(QZA,KCA,KDOO,KTUO)
C
C CALCULATES PROPAGATION VARIABLES, WAVE ADMIT/IMPED, PHASE THICKNESS
C AND INTEGRALS, CHARACTERISTIC MATRICES AND EIGEN-EQUATION FUNCTION
C FOR A SYSTEM OF LAYERS.  PRINCIPAL INPUT FROM COMMON /STRUCT/ AND
C PRINCIPAL OUTPUT TO COMMON /MATSYS/.
C
C QZ    BETA(KZ/KO)-SQUARED, PROPAGATION COEFF IN Z DIRECTION.
C KC    COMPLEX FREQUENCY NORMALIZED TO K-ZERO (NORMALLY REAL UNITY)
C KDOO  INTEGER PARAMETER CONTROLS EXTENT OF COMPUTATION
C KTUO  OUTPUT CONTROL INTEGER, =0 NO PRINTED PUTPUT
C
C      COMPLEX QZA,QZ,KCA,KC
C
C      COMMON /BDYCON/ KPOL,L1,KBC1,KBD1,APB1,VPB1,YB1,ZB1,
$      L2,KBC2,KBD2,APB2,VPB2,YB2,ZB2,KBCO
C      COMPLEX VPB1,YB1,ZB1,VPB2,YB2,ZB2
C
C      COMMON /STRUCT/ LK,LL,LN,KS,KCC,KFC,TR(10),QN(10),KPLS,YN(10)
C      REAL KS
C      COMPLEX KCC,KFC,QN,YN
C
C      COMMON /MATSYS/ KDID,QZS,KCS,AQZ,UX(10),PH(10),PHR,PHI,YX(10),
$      CL1(10),CL2(10),CL3(10),CH1,CH2,CH3,CH4,DETC(2),
$      QX1,AQX1,FY1,FZ1,QX2,AQX2,FY2,FZ2,SM1,SM2,SM3,SM4,DETS,WZ,YZ(10)
C      COMPLEX QZS,KCS,UX,PH,PHR,PHI,YX,CL1,CL2,CL3,CH1,CH2,CH3,CH4,DETC,
$      QX1,FY1,FZ1,QX2,FY2,FZ2,SM1,SM2,SM3,SM4,DETS,WZ,YZ
C
C      --SCRATCH VARIABLES AND CONSTANTS
C      COMPLEX PBV1,PBV2
C      COMPLEX AC,BC,CC,DC,UC
C      COMPLEX CO,C1,CI
C      DATA CO,C1,CI/ (0.0,0.0),(1.0,0.0),(0.0,1.0)/
C      DATA PI,PI2,PIH/ 3.1415926535898,6.2831853071796,1.5707963267949/
C      DATA EPSQ/1.0E-12/
C
C      --STATEMENT FUNCTION FOR MAGNITUDE SQUARED
C      ABSQ(CC)= REAL(CC)*REAL(CC)+AIMAG(CC)*AIMAG(CC)
C      --STATEMENT FUNCTION FOR ARCTAN QUADRANT INDICATOR
C      AQ(CC)= ATAN2(AIMAG(CC),REAL(CC))/PIH
C      --COEFFICIENTS OF POWER SERIES FOR SINC(Z) FUNCTION
C      DATA A0,A2,A4,A6,A8,A10 /1.0, 16.6666666666667E-2,
$      83.333333333333E-4,      198.412698413E-6,
$      275.5731922E-8,      250.52108E-10      /
C
C      --SET LOCAL VARIABLES FROM CALLING ARGUMENTS AND COMMON VARIABLES
C      QZ= QZA
C      KC= KCA
C      QZS= QZ
C      KCS= KC

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      KDID= KDOO
      KOUT= KTUO
      IF(KDID.GT.0) GO TO 100
C
C      --IMPORTANT. AN INITIAL CALL WITH KDOO=0 IS REQUIRED.
C      --CLEAR, INITIALIZE, AND SET LOCAL VARIABLES
10  LO= L1+1
      LP= L2-L1
      AQZ= -0.0
      PHR= C0
      PHI= C0
      CM1= C1
      CM2= C0
      CM3= C0
      CM4= C1
      DETC(1)= -C0
      DETC(2)= -C0
      QX1= C1
      QX2= C1
      AQX1= -0.0
      AQX2= -0.0
      PBV1= VPB1
      PBV2= VPB2
      SM1= -C0
      SM2= -C0
      SM3= -C0
      SM4= -C0
      DETS= C0
20  DO 30 L=1,10
      WX(L)= C0
      PH(L)= C0
      YX(L)= C1
      CL1(L)= C1
      CL2(L)= C0
      CL3(L)= C0
      YZ(L)= C1
30  CONTINUE
      GO TO 900
C
C      --IF NO FINITE LAYERS, LP.LE.0, SKIP CALC AND SET CM TO UNIT MATR.
100 IF(LP.LE.0) GO TO 300
C      --CALC VARIABLES FOR FINITE LAYERS LO THROUGH L2
110 DO 120 L= LO,L2
C      --TRANSV PROPAGATION COEFF, WX, FOR INNER LAYERS, POS REAL PART.
      WC= CSQRT(QN(L)-QZ)
      WX(L)= WC
C      --TRANSVERSE WAVE ADMIT(TE)/IMPED(TM) YX
      YX(L)= WC*YN(L)
120 CONTINUE
      IF(KDID.LE.1) GO TO 900

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C
C 200 --PHASE THICKNESS FOR EACH LAYER AND ACCUMULATE PHASE INTEGRALS
C      --WITH ALL POS REAL PARTS (PHR) AND WITH ALL POS IMAG PARTS (PHI)
C      --(POSSIBLE ENTRY POINT FOR RECALC WITH OLD QZ AND NEW KC)
      PHR= C0
      PHI= C0
210 DO 220 L= L0,L2
      AC= WX(L)*KC*TR(L)
      PH(L)= AC
      PHR= PHR+AC
      IF(AIMAG(AC).LT.0.0) AC= -AC
      PHI= PHI+AC
220 CONTINUE
      IF(KDID.LE.2) GO TO 900
C
C 300 --CALCULATE LAYER MATRICES AND SYSTEM CHARACTERISTIC MATRIX
300 CM1= C1
      CM2= C0
      CM3= C0
      CM4= C1
      IF(LP.LE.0) GO TO 400
C      --MATRIX FOR EACH LAYER (CL1,CL2,CL3,CL4=CL1)
310 DO 320 L=L0,L2
C      --CALL LAYMAT(TR(L),WX(L),KC,YN(L),CL1(L),CL2(L),CL3(L))
C      --A CALL TO LAYMAT MAY REPLACE FOLLOWING CARDS THROUGH 350
C      --MORE EFFICIENT TO DO IN-LINE LOCALLY.
      AC= PH(L)
      CL1(L)= CCOS(AC)
      BC= CSIN(AC)
      CL2(L)= CMPLX(-AIMAG(BC*YX(L)),+REAL(BC*YX(L)))
      IF(ABSQ(AC).GE.0.1) GO TO 340
C 330 --FOR TOO SMALL A PHASE THICKNESS USE PWR SERIES SINC FUNCTION
      DC= AC*AC
      CC= A0-DC*(A2-DC*(A4-DC*(A6-DC*(A8-DC*A10))))
      AC= KC*TR(L)*CC/YN(L)
      CL3(L)= CMPLX(-AIMAG(AC),+REAL(AC))
      GO TO 350
C      --FOR LARGE ENOUGH PH THICKNESS USE LIBRARY CSIN(PH)/YX
340 CL3(L)= CMPLX(-AIMAG(BC/YX(L)),+REAL(BC/YX(L)))
350 CONTINUE
C
C      --ACCUMULATE SYSTEM MATRIX
C      --MULTIPLY BY EACH LAYER MATRIX, FROM THE LEFT
      AC = CL1(L)*CM1 + CL3(L)*CM2
      CM2= CL2(L)*CM1 + CL1(L)*CM2
      CM1= AC
      BC = CL1(L)*CM3 + CL3(L)*CM4
      CM4= CL2(L)*CM3 + CL1(L)*CM4
      CM3= BC
320 CONTINUE

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C      --DETERMINANT AND ANTIDETERMINANT
      CC= CM1*CM4
      DC= CM2*CM3
      DETC(1)= CC-DC
      DETC(2)= CC+DC
C      --LAYER AND SYSTEM CHARACTERISTIC MATRICES COMPLETED
      IF(KDID.LE.3) GO TO 900
C
C      --IMPOSE BOUNDARY CONDITIONS AT OUTER BOUNDARIES
C 400 --BOUNDARY CONDITIONS AT FIRST BOUNDARY L1
      400 IF(KBC1.GE.2) GO TO 420
C      --TRANSVERSE PROPAGATION COEFFICIENT, WX, POSITIVE REAL PART.
      410 AC= C1
          QX1= QN(L1)-QZ
          WC= CSQRT(QX1)
C      --FOR PRINCIPAL BRANCH HALF-PLANE OF WX, CHANGE SIGN IF NECESSARY.
          IF(REAL(WC*CONJG(PBV1)).LT.0.0) WC= -WC
          WX(L1)= WC
C      --TRANSVERSE WAVE ADMIT/IMPED, YX, FOR OUTER LAYER MATERIAL.
          BC= WC*YN(L1)
          YX(L1)= BC
          GO TO 440
C
C 420 IF(KBC1.GE.3) GO TO 430
C      --A FIXED BOUNDARY SURFACE ADMIT(TE)/IMPED(TM) YB1
          AC= C1
          BC= YB1
          QX1= C1
          GO TO 440
C      --A FIXED BOUNDARY SURFACE IMPED(TE)/ADMIT(TM) ZB1
      430 AC= ZB1
          BC= C1
          QX1= C1
C
C      --SAVE BOUNDARY FIELD VALUES AT L1
      440 FY1= +AC
          FZ1= -BC
          IF(KBD1.LE.1) FZ1= -FZ1
C
C      --PARTIAL MATRIX PRODUCT, FROM THE RIGHT BY BOUNDARY MATRIX
          CC = CM1*AC
          DC = CM3*BC
          SM1= CC+DC
          SM3= CC-DC
          CC = CM2*AC
          DC = CM4*BC
          SM2= CC+DC
          SM4= CC-DC
C
C 450 --BOUNDARY CONDITION AT SECOND BOUNDARY, L2

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450 IF(KBC2.GE.2) GO TO 470
C  --TRANSVERSE PROPAGATION COEFFICIENT, WX, POSITIVE REAL PART.
460 QX2= QN(L2+1)-QZ
    WC= CSQRT(QX2)
C  --FOR PRINCIPAL BRANCH HALF-PLANE OF WX, CHANGE SIGN IF NECESSARY.
    IF(REAL(WC*CONJG(PBV2)).LT.0.0) WC= -WC
    WX(L2+1)= WC
C  --TRANSVERSE WAVE ADMIT/IMPED, YX, FOR OUTER LAYER MATERIAL.
    AC= WC*YN(L2+1)
    YX(L2+1)= AC
    BC= C1
    GO TO 490
C
470 IF(KBC2.GE.3) GO TO 480
C  --A FIXED BOUNDARY SURFACE ADMIT(TE)/IMPED(TM) YB2
    AC= YB2
    BC= C1
    QX2= C1
    GO TO 490
C  --A FIXED BOUNDARY SURFACE IMPED(TE)/ADMIT(TM) ZB2
480 AC= C1
    BC= ZB2
    QX2= C1
C  --SAVE BOUNDARY FIELD VALUES AT L2
490 FY2= +BC
    FZ2= +AC
    IF(KBD2.LE.1) FZ2= -FZ2
C
C  --COMPLETE THE MATRIX PRODUCT, FROM THE LEFT BY INV BDY MATRIX
    CC = AC*SM1
    DC = BC*SM2
    SM1= CC+DC
    SM2= CC-DC
    CC = AC*SM3
    DC = BC*SM4
    SM3= CC+DC
    SM4= CC-DC
    DETS= SM1*SM4 - SM2*SM3
C  --MATRIX OF EIGENEQUATION FUNCTIONS COMPLETED
    IF(KDID.LE.4) GO TO 900
C
C 500 --CALCULATE LONGITUDINAL PROPAGAT VARIABLES, WAVE ADMIT/IMPED,
C  --AND QUADRANT INDICATORS FOR QZ AND QX PLANES.
500 WZ= CSQRT(QZ)
    DO 510 L=1,LH
        YZ(L)= WZ*YN(L)
510 CONTINUE
C  --PROTECT FROM INDETERMINANT FORM ATAN2(0,0), (FATAL ERROR)
520 AQZ= -0.0
    IF(ABS(REAL(QZ)) + ABS(AIMAG(QZ)).LT.EPSQ) GO TO 522

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      AQZ= AQ(QZ)
522 AQX1= -0.0
      IF(ABS(REAL(QX1))+ABS(AIMAG(QX1)).LT.EPSQ) GO TO 524
      AQX1= AQ(QX1)
524 AQX2= -0.0
      IF(ABS(REAL(QX2))+ABS(AIMAG(QX2)).LT.EPSQ) GO TO 526
      AQX2= AQ(QX2)
526 CONTINUE
C
900 RETURN
C
      END
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SUBROUTINE FIELDS

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C
C  --CALCULATES BOUNDARY FIELDS AND FIELD DISTRIBUTION IN LAYERS
C  --FOR EACH OF MODAL CONDITIONS LISTED IN COMMON /MODSET/
C
COMMON /KASETS/ KASE, KSUB, MN, MO, MK, ML, IDEN, IMAX, INFX,
$QZNR, QZNI, KGSS, PMFR, PMDM, KGCZ, WFMP, EPS1, EPS2, EPS3, IL, KMDO,
$KDO1, KDO2, KDO3, KDO4, KEIF, KDO6, KDOF, KDO8,
$KOU1, KOU2, KOU3, KOU4, KOU5, KOU6, KOUF, KOU8
C  MAIN, PUTS, SRCH, SYSH, EIGQ, CZRM, FLDS, PWRS
C  --NOTE EQUIVALENCE HERE OF KDOF=KDO7, AND KOUF= KOU7
C
COMMON /LAYCOM/ XU, WVL, KO, KCR, KCI, KFR, KFI, LN, KXTL, XL(10), TL(10),
$PER(10), PEI(10), PMR( 1), PHI( 1)
REAL KO, KCR, KCI, KFR, KFI
C
COMMON /BDYCON/ KPOL, L1, KBC1, KBD1, APB1, VPB1, YB1, ZB1,
$L2, KBC2, KBD2, APB2, VPB2, YB2, ZB2, KBCO
COMPLEX VPB1, YB1, ZB1, VPB2, YB2, ZB2
C
COMMON /STRUCT/ LK, LL, LM, KS, KC, KF, TR(10), QN(10), KPLS, YN(10)
REAL KS
COMPLEX KC, KF, QN, YN
C
COMMON /MATSYS/ KDIS, QZS, KCS, AQZ, WX(10), PH(10), PHR, PHI, YX(10),
$CL1(10), CL2(10), CL3(10), CM1, CM2, CM3, CM4, DETC(2),
$QX1, AQX1, FY1, FZ1, QX2, AQX2, FY2, FZ2, SM1, SM2, SM3, SM4, DETS, WZ, YZ(10)
COMPLEX QZS, KCS, WX, PH, PHR, PHI, YX, CL1, CL2, CL3, CM1, CM2, CM3, CM4, DETC,
$QX1, FY1, FZ1, QX2, FY2, FZ2, SM1, SM2, SM3, SM4, DETS, WZ, YZ
C
COMMON /MODSET/ NM, NO, NK, NL, QZM(10), PHM(10), KM(10)
COMPLEX QZM, PHM
C
COMMON /FIELDS/ FY(10), FZ(10), PX(10), PZ(10)
COMPLEX FY, FZ, PX, PZ
C
COMPLEX GY(10), GZ(10), FYX, FZX, FXX
COMPLEX KCO, QZ, FG1, FG2, GF1, GF2, PZX, PXX
COMPLEX AC, BC, CC, DC, TM1, TM2, TM3
C
C  --STATEMENT FUNCTION FOR ABSOLUTE MAGNITUDE SQUARED
C  ABSQ(CC)=REAL(CC)*REAL(CC) + AIMAG(CC)*AIMAG(CC)
C
DATA PI, ED /3.1415926535898, 2.3025850922940/
DATA DELX, DELW /1.01E-04, 1.0E-04/
C
WRITE(6,1000) KASE, KSUB, KDOF, KOUF
1000 FORMAT(34H0***SUBROUTINE FIELDS. KASE NO.=, I6, 1H., I2,
1 8H, KDOF=, I2, 8H, KOUF=, I2, 1H. )
IF(KDOF.GE.1) GO TO 40

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      WRITE(6,1110) L,WX(L),YX(L),PH(L)
1110 FORMAT( 8X,2HL=,I2,3X,4HWX=(,E11.4,1H,,E11.4,1H),
      1 5H YX=(,E11.4,1H,,E11.4,1H),6H PH=(,E11.4,1H,,E11.4,1H),
      112 CONTINUE
114 IF(KBC2.GE.2) GO TO 116
      WRITE(6,1108) L3,WX(L3),YX(L3)
116 CONTINUE
C
C 120 --SET UP TWO PROVISIONAL SETS OF TANGENTIAL BOUNDARY FIELDS
C      --FROM OUTER BDY FIELDS AND LAYER MATRICES SAVED IN /MATSYS/
C      --FY,FZ FROM FIRST BDY L1 TRANSFORM FORWARD TO SECOND BDY L2
C      --GY,GZ FROM SECOND BDY L2 TRANSFORM BACKWARD TO FIRST BDY L1
C
C 120 --THENDIF-106,108. SET OUTER BOUNDARY FIELDS
120 FY(L1)= FY1
      FZ(L1)= FZ1
      GY(L2)= FY2
      GZ(L2)= FZ2
C      --ACCUMULATE NORMALIZATION
      FN= ABSQ(FY1)+ABSQ(FZ1)
      GN= ABSQ(FY2)+ABSQ(FZ2)
C      --IF SINGLE BOUNDARY CASE NO FINITE LAYER TRANSFORMATIONS
125 IF(LP.LE.0) GO TO 136
C      --MATRIX TRANSFORMATION ACROSS FINITE LAYERS. BOTH DIRECTIONS
130 DO 135 L=1,LP
      K1= L1+L
      J1= K1-1
      J2= L2-L
      K2= J2+1
      FY(K1)= +CL1(K1)*FY(J1) +CL3(K1)*FZ(J1)
      FZ(K1)= +CL2(K1)*FY(J1) +CL1(K1)*FZ(J1)
      GY(J2)= +CL1(K2)*GY(K2) -CL3(K2)*GZ(K2)
      GZ(J2)= -CL2(K2)*GY(K2) +CL1(K2)*GZ(K2)
C      --ACCUMULATE NORMALIZATION
      FN= FN + ABSQ(FY(K1)) + ABSQ(FZ(K1))
      GN= GN + ABSQ(GY(J2)) + ABSQ(GZ(J2))
C      --ENDDO-130, THENDIF-125.
135 CONTINUE
136 CONTINUE
C      --RENORMALIZE FIELDS, UNITY R.M.SQD.MAGNITUDES OF BOUNDARY VALUES
C      --SIMPLE ARBITRARY CHOICE. OTHER NORMALIZATIONS POSSIBLE
      GN= SQRT(2.0*FLOAT(LP+1)/GN)
      FN= SQRT(2.0*FLOAT(LP+1)/FN)
140 DO 145 L=L1,L2
      FY(L)= FN*FY(L)
      FZ(L)= FN*FZ(L)
      GY(L)= GN*GY(L)
      GZ(L)= GN*GZ(L)
145 CONTINUE
      KBF6= 1

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C      --TANGENTIAL BOUNDARY FIELD SETS COMPLETED
C
C      --F*G CROSS PRODUCTS FOR RECIPROCITY AND EIGEN CHECKS
      FG1= FY(L1)*GZ(L1)
      FG2= FY(L2)*GZ(L2)
      GF1= GY(L1)*FZ(L1)
      GF2= GY(L2)*FZ(L2)
190  IF(KOUF.LT.2) GO TO 300
C 200  --ELSE-190./OUTPUT SUMMARY OF PROVISIONAL FIELD SETS F AND G
C      --RECIPROCITY AND EIGEN CHECKS USING POYNTING CROSS PRODUCTS F*G
      WRITE(6,1200) L1,L2
1200  FORMAT(39H TWO SOLN. FOR TANGENTIAL BDY. FIELDS, ,
1      1 49H INDEPENDENTLY CALC., F(L) FROM BDY. COND. AT L1=, I2,
2      2 34H, AND G(L) FROM BDY. COND. AT L2=, I2, 1H. )
      IF(KOUF.LT.3) GO TO 300
      WRITE(6,1210)
1210  FORMAT(116H NUMERICAL CHECKS, RECIPROCITY AND EIGEN CONDITIONS. US
      $ING POYNTING CROSS PRODUCTS F*G. (F*G-DIFF IS WRONSKIAN DET.) )
      DC= FG2-GF2
      WRITE(6,1212) L2
1212  FORMAT(17H EIG CHECK AT L2=, I3, 18H, FY*GZ = GY*FZ , )
      WRITE(6,1218) FG2,GF2,DC
      DC= FG1-GF1
      WRITE(6,1214) L1
1214  FORMAT(17H EIG CHECK AT L1=, I3, 18H, FY*GZ = GY*FZ , )
      WRITE(6,1218) FG1,GF1,DC
      AC= FG2-FG1
      BC= GF2-GF1
      CC= AC - BC
      WRITE(6,1216)
1216  FORMAT(38H RECIPROCITY CHECK. FG2-FG1=GF2-GF1, )
      WRITE(6,1218) AC,BC,CC
1218  FORMAT(1H+, 40X, 1H(,E11.4,1H,,E11.4,3H)=(,E11.4,
1      11H,,E11.4,9H). DIFF=(,E11.4,1H,,E11.4,4H)=0. )
C      --RECIPROCAL TRANSMISSION AND REFLECTION COEFFICIENTS AND
C      --NOT YET IMPLEMENTED

260  IF(KOUF.LT.4) GO TO 300
C 265  --ELSE-260. OUTPUT BOTH F AND G SETS OF TANGENTIAL BOUNDARY FIELDS
265  WRITE(6,1265)
1265  FORMAT(80H F(L) AND G(L) FIELD SETS AND WRONSKIAN DETERMINANT (FY*
1      1GZ-GY*FZ) (=EIG CHECK) )
270  DO 275 L= L1,L2
      DC= FY(L)*GZ(L)-GY(L)*FZ(L)
      WRITE(6,1270) L,FY(L),GY(L),FZ(L),GZ(L),DC
275  CONTINUE
1270  FORMAT(3H L=, I3, 3X, 4HFY=(,F13.6,1H,,F13.6,8H) GY=(,F13.6,1H,,
1      1F13.6,1H)/9X, 4HFZ=(,F13.6,1H,,F13.6,8H) GZ=(,F13.6,1H,,F13.6,
2      212H) W-DET= (,E13.6,1H,,E13.6,2H). )
C      --ENDELSE-260, THEN DIF-260

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C
C 300 --USE BOTH, ONE OR OTHER, OR AVG OF THE TWO FIELD SOLUTIONS
C    --ALSO CALCULATE TIME-AVG TRANSVERSE POYNTING POWER
      300 IF(KBCO.GE.3) GO TO 350
      310 IF(KBCO.EQ.2) GO TO 340
C
C    --ELSE-300,310.
C 320 --KBCO.LE.1, USE FIRST FIELD SET FY,FZ. ONLY SET IF KBCO.EQ.1
      320 DO 325 L=L1,L2
            PX(L)= FY(L)*CONJG(FZ(L))
      325 CONTINUE
C    --PROCEDE WITH FIRST FIELD SET F
      GO TO 380
C
C 340 --THEN-310.
C 340 --EXCHANGE F AND G SETS, FOR USE OF SECOND FIELD SET GY,GZ
C    --A RETURN ENTRY POINT FOR USING G SET AFTER USING F SET, KBCO=0
      340 DO 345 L=L1,L2
            AC= GY(L)
            BC= GZ(L)
            GY(L)= FY(L)
            GZ(L)= FZ(L)
            FY(L)= AC
            FZ(L)= BC
            PX(L)= AC*CONJG(BC)
      345 CONTINUE
      KBFG= 2
C    ENDTHEN-310/ PROCEDE WITH SECOND FIELD SET G, NOW IN F ARRAY
      GO TO 380
C
C 350 THEN-300./ A TRUE EIGEN-MODE CASE, F AND G SOLUTIONS EQUIVALENT
C    --FORM AVERAGE OF F AND G SETS AS EIGEN-FUNCTION SOLUTIONS
C    --STANDARDIZE GY SOLN TO BE SAME AS FY AT L1. COMPLEX PHASE MULT.
      350 CC= FY(L1)/GY(L1)
      360 DO 365 L=L1,L2
            FY(L)= 0.5*(FY(L)+CC*GY(L))
            FZ(L)= 0.5*(FZ(L)+CC*GZ(L))
            PX(L)= FY(L)*CONJG(FZ(L))
      365 CONTINUE
      KBFG= 3
C    --ENDTHEN-300/ PROCEDE WITH AVG FIELD SET, NOW IN F-ARRAY
      GO TO 380
C
C    --ENDIF-300,310.
      380 CONTINUE
C
C 400 --SUMMARY OUTPUT DESCRIPTION OF TYPE OF FIELD SOLUTION
C    --AND LISTING OF TANGENTIAL FIELDS AT BOUNDARIES
      400 WRITE(6,1400)
      1400 FORMAT( 50HOSOLUTION FOR TANGENTIAL FIELDS AT THE BOUNDARIES.)

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        IF(KBFG.EQ.3) GO TO 430
        IF(KBFG.EQ.2) GO TO 420
    410 WRITE(6,1410)
    1410 FORMAT( 54H FIELD SOLUTION BASED ON BOUNDARY CONDITION AT L1. (F))
        GO TO 440
    420 WRITE(6,1420)
    1420 FORMAT( 54H FIELD SOLUTION BASED ON BOUNDARY CONDITION AT L2. (G))
        GO TO 440
    430 WRITE(6,1430)
    1430 FORMAT( 90H EIGEN-FUNCTION FIELD SOLUTION (AVG. OF SOLUTIONS BASE
        $D ON THE TWO BDY. COND. SEPARATELY.      )
        CC= FZ1*FY(L1)-FZ(L1)*FY1
        DC= FZ2*FY(L2)-FZ(L2)*FY2
        WRITE(6,1432) CC,DC
    1432 FORMAT( 39H BDY. COND. CHECKS. AT L1, YX*FY-FZ= (,E10.3,1H,,E10.3
        $,22H). AT L2, YX*FY-FZ= (,E10.3,1H,,E10.3,2H).      )
C      --ENDIFS-400.
    440 CONTINUE
        IF(KOUF.LT.2) GO TO 500
C 440 --OUTPUT TANGENTIAL BOUNDARY FIELDS AND TRANSV POYNT AVG POWER
        WRITE(6,1440)
    1440 FORMAT( 65H TANGENTIAL BOUNDARY FIELDS AND TRANSVERSE AVG. POYNTIN
        $G POWER.      )
        DO 445 L=L1,L2
            WRITE(6,1700) L,XL(L),FY(L),FZ(L),PX(L)
    445 CONTINUE
C 450 --TIME-AVG NET POYNTING POWER INTO STRUCTURE FROM THE OUTSIDE
        DC= PX(L1) - PX(L2)
        WRITE(6,1450) DC
    1450 FORMAT(72H NET TIME-AVG POYNT. PWR. INTO STRUCTURE FROM OUTSIDE,
        $PX(L1)-PX(L2)= (,E13.6,1H,,E13.6,2H).      )
C
C 460 --OUTPUT WAVE AMPLITUDES AT OUTER BOUNDARIES, TRANS AND REFL COEFF
C      --NOT YET IMPLEMENTED
C
C 500 --CALCULATE POWER AND ENERGY RELATIONS FOR FIELD SOLUTION
    500 CALL POWERS
C
    600 IF(KDOF.LE.1.OR.KOUF.LE.1) GO TO 800
C      --ELSE-600./ CALCULATE AND OUTPUT FIELDS AS A FUNCTION OF X
        WRITE(6,1600)
    1600 FORMAT( 36H0FIELD SOLUTIONS AS A FUNCTION OF X.      )
C      --START DO-LOOP OVER ALL LAYERS
        DO 605 L=L1,L3
C          --DO FOR EACH LAYER
    610 IF(L.GT.L1) GO TO 630
    620 IF(KBC1.GE.2) GO TO 790
C          --ELSE-610,620/ FOR FIRST SEMI INFINITE LAYER IF PRESENT
C          --SET UP AN INITIAL BOUNDARY AND FIELDS AT INFX
C          --FACTORS OF E OR RADIAN INTO SEMI-INF LAYER

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TX= FLOAT(INFX)/(CABS(WX(L)*KCO)+DELW)
X1= XL(L)-TX
CALL LAYMAT(KO*TX,WX(L),KC,YN(L),TM1,TM2,TM3)
FYX= +TM1*FY(L) -TM3*FZ(L)
FZX= -TM2*FY(L) +TM1*FZ(L)
GO TO 640
C 630  --THEN-610.  SET INITIAL X AND FIELDS FOR EACH OF OTHER LAYERS
630  LI= L-1
      X1= XL(LI)
      FYX= FY(LI)
      FZX= FZ(LI)
C      --ENDIF-610.
640  IF(L.GT.L2)  GO TO 650
C      --ELSE-640/  SET UP FINAL X AS XL(L), EXCEPT 2ND SEMI-INF LAYER
      X2= XL(L)
      GO TO 660
C 650  --THEN-640.  FOR SECOND SEMI-INF LAYER IF PRESENT
650  IF(KBC2.GE.2)  GO TO 790
C      --SET UP A FINAL BOUNDARY AT INFX FACTORS
C      --OF E OR RADIAN INTO SEMI-INF LAYER
      TX= FLOAT(INFX)/(CABS(WX(L)*KCO)+DELW)
      X2= XL(L2)+TX
660  CONTINUE
C 660  --ENDIF-640/  CALCULATE INCREMENT DX AND TRANSFORM MATRIX
C
      TX= X2-X1
      DX= 1.0/(FLOAT(IDEN)*(CABS(WX(L)*KCO)+DELW))
      DX= AMAX1(DX,TX/FLOAT(IMAX),DELX)
C      --ROUND OFF DX TO A TWO DIGIT FACTOR TIMES A POWER OF TEN
C      --ROUNDED VALUES OF 1.0,1.5,2.0,2.5,4.0,5.0,7.5,10.0.
C      --OF EACH RANGE, ABOUT 1/3 ROUNDS UP AND 2/3 ROUNDS DOWN
C      --LOG10 OF DX.  INTEGER AND FRACTIONAL PART
      DL= ALOG10(DX)
      JL= INT(DL)
      DL= DL-FLOAT(JL)
C      --CHECK THAT FRACTIONAL PART IS POSITIVE
      IF(DL.GT.0.0)  GO TO 665
      DL= DL+1.0
      JL= JL+1
C      --PWR OF 10 FACTOR, AND ROUND THE FRACTIONAL PART
665  DP= 10.0**JL
      DX= 1.0
      IF(DL.LT.0.11)  GO TO 670
      DX= 1.5
      IF(DL.LT.0.26)  GO TO 670
      DX= 2.0
      IF(DL.LT.0.36)  GO TO 670
      DX= 2.5
      IF(DL.LT.0.53)  GO TO 670
      DX= 4.0

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        IF(DL.LT.0.67) GO TO 670
        DX= 5.0
        IF(DL.LT.0.81) GO TO 670
        DX= 7.5
        IF(DL.LT.0.96) GO TO 670
        DX= 10.0
670    DX= DX*DP
C
C 680    --ROUND DOWN INITIAL X1 TO INTEGER NO. OF DX, AND SET UP FIELDS
        TX= X1
        X1= DX*AIN(TX/DX)
        IF(TX.LE.X1) X1= X1-DX
        TX= X1-TX
        CALL LAYMAT(KO*TX,UX(L),KC,YN(L),TM1,TM2,TM3)
        DC= +TM1*FYX +TM3*FZX
        FZX= +TM2*FYX +TM1*FZX
        FYX= DC
C
C        --TRANSFORMATION MATRIX FOR DX THICKNESS IN LAYER L
        CALL LAYMAT(KO*DX,UX(L),KC,YN(L),TM1,TM2,TM3)
C
C 700    --CALCULATE AND OUTPUT FIELDS FROM X1 TO X2, INCREMENTS OF DX
        IX= INT((X2-X1)/DX+1.5)
        PXX= FYX*CONJG(FZX)
        WRITE(6,1700) L,X1,FYX,FZX,PXX
        WRITE(6,1702)
        IF(KOUF.LT.3) GO TO 700
        FXX= YZ(L)*FYX
        PZX= CONJG(FXX)*FYX
        WRITE(6,1720) FXX,PZX
C        --START DO-LOOP INCREMENTING DX THROUGH EACH LAYER
        DO 710 I=1,IX
            XX= X1+FLOAT(I)*DX
            DC= +TM1*FYX +TM3*FZX
            FZX= +TM2*FYX +TM1*FZX
            FYX= DC
            PXX= FYX*CONJG(FZX)
            WRITE(6,1700) L,XX,FYX,FZX,PXX
1700    FORMAT(1X,I3,3H X=,F11.5,3X,3X,4H FY=(,F13.6,1H,,F13.6,1H),4X,
             1 4HFZ=(,F13.6,1H,,F13.6,1H),3X,4HPX=(,E13.6,1H,,E13.6,1H) )
1702    FORMAT(1H+,17X,3H***)
1704    FORMAT(1H+,17X,3HBDY)
        720    IF(KOUF.LT.3) GO TO 730
C        --ELSE-720.
C        --CALCULATE AND OUTPUT FX AND PZ
        FXX= YZ(L)*FYX
        PZX= CONJG(FXX)*FYX
        WRITE(6,1720) FXX,PZX
1720    FORMAT(24X,32X,3X,4H FX=(,F13.6,1H,,F13.6,1H),3X,
             1 4HPZ=(E13.6,1H,,E13.6, 2H). )

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C 730      --THENDIF-720.
730      IF(XX.LE.X2) GO TO 710
C          --ELSE-730/  END OF LAYER L, OUTPUT FIELDS AT BOUNDARY
          WRITE(6,1702)
740      IF(L.GE.L3) GO TO 710
          WRITE(6,1700) L,X2,FY(L),FZ(L),PX(L)
          WRITE(6,1704)
          GO TO 605
C 710      --ENDDO-700, THENDIF-730,740./END EACH DX INCREMENT
710      CONTINUE
C 790      --THENDIF-610,650.  END SKIPPING OF SEMI-INF LAYERS
790      CONTINUE
C
C 605 -ENDDO-600.  FINISHED WITH EACH LAYER L
605 CONTINUE
C          --FINISHED WITH THE FIELD SOLUTION OVER ALL THE LAYERS
800 CONTINUE
C
C          --FOR EIGEN CONDITIONS AT NEITHER BDY RETURN FOR SECOND SOLUTION
          IF(KBCO.LE.0.AND.KBFG.EQ.1) GO TO 340
C
810 WRITE(6,1810) M
1810 FORMAT(33H END FIELD SOLUTIONS FOR MODE, M=,I3,      )
C
C 101 --ENDDO-100.  FINISHED WITH EACH MODE VALUE OF QZ
101 CONTINUE
C
900 WRITE(6,1900) KASE,KSUB
1900 FORMAT(26H ***END FIELDS. KASE NO.=,I6,1H.,I2,9H RETURN.      )
      RETURN
C
      END

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SUBROUTINE LAYMAT(TR,WX,KC,YN,TH1,TH2,TH3)
C
C  --CALCULATE FIELD TRANSFORMATION MATRIX FOR ANY LAYER
C  --TR= NORMALIZED RADIAN THICKNESS, TR= K0*(X2-X1)
C  --WX= PROPAG COEFF IN X, NORMALIZED TO K0, KX= K0*WX
C  --KC= COMPLEX FREQUENCY FACTOR, A MULTIPLIER OF K0,
C  --YN= TRANSV WAVE ADMIT/IMPED FACTOR, YX= WX*YN
C  --TH1,TH2,TH3, MATRIX ELEMENTS, TH4= TH1.
C
C  COMPLEX WX,KC,YN,TH1,TH2,TH3
C  COMPLEX ZZ,TH,SN,QH,SC
C
C  --STATEMENT FUNCTION FOR SQUARED MAGNITUDE
C  ABSQ(ZZ)= REAL(ZZ)*REAL(ZZ) + AIMAG(ZZ)*AIMAG(ZZ)
C
C  --COEFFICIENTS OF POWER SERIES FOR SINC(Z) FUNCTION
C  DATA A0,A2,A4,A6,A8,A10 /1.0, 16.6666666666667E-2,
$      83.333333333333E-4,      198.412698413E-6,
$      275.5731922E-8,          250.52108E-10 /
C
C  --COMPLEX PHASE THICKNESS, COSINE, AND SINE
C  TH= WX*KC*TR
C  TH1= CCOS(TH)
C  SN= CSIN(TH)
C  ZZ= WX*YN*SN
C  TH2= CMPLX(-AIMAG(ZZ),+REAL(ZZ))
100 IF(ABSQ(TH).GT.0.1) GO TO 120
C  --ELSE-100. FOR TOO SMALL TH USE POWER SERIES FOR SIN(TH)/TH
110 QH= TH*TH
C  SC= A0-QH*(A2-QH*(A4-QH*(A6-QH*(A8-QH*A10))))
C  ZZ= KC*TR*SC/YN
C  TH3= CMPLX(-AIMAG(ZZ),+REAL(ZZ))
C  GO TO 130
C  --THEN-100. FOR LARGE ENOUGH TH USE LIBRARY CSIN(TH)/YX
120 ZZ= SN/(WX*YN)
C  TH3= CMPLX(-AIMAG(ZZ),+REAL(ZZ))
C  --ENDIF-100. FINISHED, RETURN
C
130 RETURN
END

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SUBROUTINE POWERS

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C
C  --CALCULATES POYNTING POWER FLOWS AND ENERGY DENSITIES FOR
C  --TANGENTIAL AND TRANSVERSE FIELDS
C
COMMON /KASETS/ KASE,KSUB,MN,MO,MK,ML,IDEN,IMAX,INFX,
$QZNR,QZNI,K6SS,PMFR,PMDM,KGCZ,WFMP,EPS1,EPS2,EPS3,IL,KHDO,
$KDO1,KDO2,KDO3,KDO4,KEIF,KDO6,KDO7,KDOP,
$KOU1,KOU2,KOU3,KOU4,KOU5,KOU6,KOU7,KOUP
C  MAIN,PUTS,SRCH,SYSH,EIGQ,CZRN,FLDS,PURS
C  --NOTE EQUIVALENCE HERE OF KDOP=KD08, AND KOUP=KOUB
C
COMMON /LAYCOM/ XU,WVL,K0,KCR,KCI,KFR,KFI,LN,KXTL,XL(10),TL(10),
$PER(10),PEI(10),PMR( 1),PMI( 1)
REAL K0,KCR,KCI,KFR,KFI
C
COMMON /BDYCON/ KPDL,L1,KBC1,KBD1,APB1,VPB1,YB1,ZB1,
$L2,KBC2,KBD2,APB2,VPB2,YB2,ZB2,KBC0
COMPLEX VPB1,YB1,ZB1,VPB2,YB2,ZB2
C
COMMON /STRUCT/ LK,LL,LH,KS,KC,KF,TR(10),QN(10),KPLS,YN(10)
REAL KS
COMPLEX KC,KF,QN,YN
C
COMMON /MATSYS/ KDID,QZS,KCS,AQZ,WX(10),PH(10),PHR,PHI,YX(10),

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$CL1(10),CL2(10),CL3(10),CM1,CM2,CM3,CM4,DETC(2),
$QX1,AQX1,FY1,FZ1,QX2,AQX2,FY2,FZ2,SM1,SM2,SM3,SM4,DETS,WZ,YZ(10)
  COMPLEX QZS,KCS,WX,PH,PHR,PHI,YX,CL1,CL2,CL3,CM1,CM2,CM3,CM4,DETC,
$QX1,FY1,FZ1,QX2,FY2,FZ2,SM1,SM2,SM3,SM4,DETS,WZ,YZ

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```

C
  COMMON /MODSET/ NM,NO,NK,NL,QZH(10),PHM(10),KM(10)
  COMPLEX QZH,PHM

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C
  COMMON /FIELDS/ FY(10),FZ(10),PX(10),PZ(10)
  COMPLEX FY,FZ,PX,PZ

```

```

C
  COMPLEX CO,C1,CI
  DATA CO,C1,CI/ (0.0,0.0),(1.0,0.0),(0.0,1.0)/
  DATA PI,PI2,PIH/ 3.1415926535898,6.2831853071796,1.5707963267949/
  WRITE(6,1000) KASE,KSUB,KDOP,KOUP
1000 FORMAT(34H0***SUBROUTINE POWERS. KASE NO.=,I6,1H.,I2,
1 8H, KDOP=,I2, 8H, KOUP=,I2,1H. )
  IF(KDOP.GE.1) GO TO 100
  WRITE(6,1010)
1010 FORMAT(1H+,T67, 40HNO POWERS CALCULATED. KDOP=0. RETURN. , )
  GO TO 900
  100 CONTINUE
  WRITE(6,1100)
1100 FORMAT(42H NO CALCULATION OF POWERS YET IMPLEMENTED.)
C
  --NOT YET IMPLEMENTED

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C
  900 RETURN

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C
  END

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```

      SUBROUTINE CZEROM(CFCN)
C
C FINDS COMPLEX ROOTS OF COMPLEX FUNCTION CFCN(Z,N). USING MULLER-TRAUB
C METHOD. QUADRATIC FIT TO LAST THREE ITERATES PREDICTS NEXT ONE.
C COMPLEX FUNCTION CFCN(Z,N) MUST BE PROVIDED. OTHER NAME MAY BE USED
C IN CALLING PROGRAM. NAME USED MUST BE DECLARED AS EXTERNAL.
C
C WRITTEN BY ROBERT B. SMITH, UNIVERSITY OF WASHINGTON, ELECT ENG DEPT.
C SEATTLE, WASHINGTON. FEBRUARY, 1977.
C
C
C
C CFCN COMPLEX FUNCTION CFCN(Z,N) WHOSE ROOTS ARE TO BE SEARCHED FOR
C
C COMMON /CZECON/ BELOW MUST BE PROVIDED ALSO IN CALLING PROGRAM FOR
C COMMUNICATION OF VARIABLES, PARAMETERS, AND RESULTS BETWEEN PROGRAMS.
C IN MAIN PROGRAM COMMON OTHER VARIABLE NAMES MAY BE USED, BUT LIST MUST
C AGREE IN TYPE, DIMENSIONS, AND NUMBER OF VARIABLES.
C
      COMMON /CZECON/ NN,NT,ZO(10),FM(10),IT(10),KR(10),
      $EPSZ,EPSF,II,KTOU
      COMPLEX CFCN, ZO
C NN      NUMBER OF ROOTS TO BE SEARCHED FOR. TEN MAX. INPUT.
C NK      NUMBER OF ROOT LAST TRIED. IF NK=NN ALL ROOTS TRIED. OUTPUT.
C ZO      INPUT, USED FOR GUESSES. OUTPUT, COMPLEX ROOTS FOUND
C FM      ABS MAGNITUDE OF TRUE FUNCTION AT ROOTS. SHOULD BE ZERO.
C IT      NUMBER OF ITERATIONS COMPLETED FOR EACH ROOT. OUTPUT.
C KR      ROOT STATUS AND QUALITY INDEX. CONTROLS USE OF GUESSES ON INPUT
C          SHOWS TYPE OF CONVERGENCE ON OUTPUT. INPUT/OUTPUT.
C KR= .LT.0 ROOT IGNORED, NO ACTION./ =0, NO GUESS, USE 1.0 AND UNIT RA-
C      DIUS./ =1,2,3, POOR,GOOD,VG GUESSES, USE ZO AND RADIUS= 0.1,0.01,
C      0.001/ =4, EXCELLENT GUESS, USE ZO AND RADIUS E-4. ZO DIVIDED OUT
C      FOR OTHER ROOTS. ON OUTPUT KR=4 MEANS ITERATION LIMIT./ =5 CONVERG
C      OF REDUCED FUNCTION ONLY. MAY BE USED FOR INPUT ALSO, GUESS RADIUS
C      =E-5./ =6, CONVERG OF TRUE FUNCTION./ =7, CONVERG OF DZ./ =8, A
C      FIXED ROOT OR POLE TO BE DIVIDED OUT, NO SEARCH./
C      ROOT SEARCH FOR ZO(N) MADE ONLY FOR KR(N), 0.LE.KR.LE.7
C      ZO(N) DIVIDED OUT FOR ALL OTHER ROOTS OR GUESSES IFF KR(N).GE.4
C      RADIUS FOR INITIAL ITERATES= 1.0E-KR, USING INPUT VALUE FOR KR
C      (RADII NOT ABOUT ZO BUT ABOUT AN ORIGIN. SUBSEQUENT MOBIUS
C      TRANSFORMATION TO A NON-CENTERED CIRCLE ABOUT ZO)
C      OUTPUT. ITERATION LIMIT IF KR= 4. CONVERGENCE IF 5.LE.KR.LE.7.
C
C EPSZ EPSILON FOR CONVERGENCE TEST OF DELTA Z. INPUT.
C EPSF EPSILON FOR CONVERGENCE TEST OF FUNCTION MAGNITUDE. INPUT.
C II   ITERATION LIMIT FOR EACH ROOT SEARCH. INPUT.
C KTOU CONTROLS AMOUNT OF OUTPUT. INPUT. LOCALLY KOUT=KTOU.
C      /=0, NO OUTPUT. /=1, ONE LINE EACH CALL. /=2, TWO LINE SUMMARY.
C      /=3, SUMMARY OF ROOTS FOUND. /=4, EACH ITERATION.
C      /=5 TO 8, DEBUG, ADDITIONAL VARIABLES.

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C
C  --ARRAY OF ITERATES AND EQUIVALENCE
COMPLEX ZI(4),ZA,ZB,ZC,ZZ,ZG,FI(4),FA,FB,FC,FCZ,FZ
DIMENSION FQ(4)
EQUIVALENCE (ZI(1),ZA),(ZI(2),ZB),(ZI(3),ZC),(ZI(4),ZZ),
$(FQ(4),FQR),(FI(1),FA),(FI(2),FB),(FI(3),FC),(FI(4),FZ)
C
C  --SCRATCH VARIABLES AND CONSTANTS
COMPLEX CA,CB,CC,CD,CZ,DFAB,DFBC,DDFC,DFDZ,DZ,CO,C1,CG,ROTC
DATA CO,C1,ROTC / (0.0,0.0), (1.0,0.0), (-0.6,+0.8) /
C  --MACHINE CONSTANT. FLOATING PT. RESOLUTION
DATA AM / 1.0E-14 /
C
C  --STATEMENT FUNCTION FOR SQUARED MAGNITUDE
ABSQ(CA)= REAL(CA)*REAL(CA) + AIMAG(CA)*AIMAG(CA)
C
C  NAMELIST /DEBUG1/ ZA,FQ(1),ZB,FQ(2),ZC,FQ(3)
C  NAMELIST /DEBUG2/ DFDZ,DZ,ZZ,FQR
C
C  --INITIALIZE AND SET LOCAL VARIABLES.
NN= MINO(NN,10)
NT= 0
IF(NN.LE.0) GO TO 900
NL= NN
C  --A LOWER LIMIT ON THE EPSILONS
AA= 100.0*AM
IF(EPSZ.LT.AA) EPSZ= AA
IF(EPSF.LT.AA) EPSF= AA
C  --SQUARED EPSILONS. FORM USED IN CONVERGENCE TESTS.
EPQZ= EPSZ*EPSZ
EPQF= EPSF*EPSF
CG= ROTC
KOUT= KTUD
KANT= 0
IF(KOUT.GE.1) WRITE(6,1090)
1090 FORMAT(30HOSUBROUTINE CZEROM ITERATIONS.)
IF(KOUT.GE.3) WRITE(6,1091)
1091 FORMAT(3X,1HN,2X,2HKR,3X,1HI,T23,5HDZ(I),T49,4HZ(I),T74,4HF(Z),
$T95,12HF(Z)-REDUCED,T115,5HF-SQD )
C
C  --MAIN LOOP SEARCHING FOR NN ROOTS
100 DO 110 N= 1,NL
NT= N
NR= N
KS= KR(N)
ZZ= ZO(N)
C
112 IF(0.LE.KS.AND.KS.LE.7) GO TO 115
C  --NO SEARCH FOR IGNORED OR FIXED ROOTS. SET PARAMETERS FOR THEM.

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      IT(N)=0
      DZ= C0
      FCZ= CFCN(ZZ,NR)
      FZ= -C0
      FQR=-0.0
      GO TO 590
C      --ENDELSE-112.  BYPASS ROOT SEARCH
C      --THEN-112.  PROCEED WITH EACH ROOT SEARCH
115  CONTINUE
C      --SET UP GUESSES.  THREE ON A CIRCLE ABOUT Z0, AND ONE NEAR Z0
      I= 0
      IF(KS.EQ.0) ZZ= C1
      CC= CONJG(ZZ)
C      --SET A MAX RADIUS FOR CIRCLE OF GUESSES ABOUT AN ORIGIN.
      RR= CABS(ZZ)
      RR= 0.5/(RR+0.5)
C      --USE A FRACTION OF MAX RADIUS, POWERS OF (0.1)**KR
      FF= 1.0
      IF(KS.GT.1) FF= 0.1**KS
C      --SET RADIUS VECTOR FOR FIRST GUESS.
      CZ= FF*RR*CG
C      --GENERATE THE FOUR GUESSES
120  DO 130 K=1,4
C      --UNITARY MOBIUS TRANSFORMATION TO POINTS ABOUT Z0
      ZG= (ZZ+CZ)/(C1-CC*CZ)
      ZI(K)= ZG
      FCZ= CFCN(ZG,NR)
C      --FACTOR OUT KNOWN AND FIXED ROOTS.  FORM DENOMINATOR POLYNOMIAL
      CD= C1
140  DO 150 L=1,NL
C      --BUT NOT OTHER GUESSES, POORLY KNOWN, OR CURRENT ROOT
      IF(KR(L).LE.3.OR.L.EQ.N) GO TO 150
      CA= ZG-Z0(L)
C      --IF TOO NEAR A KNOWN ROOT ACCEPT AS A MULTIPLE ROOT
C      --AVOIDS INFLATING REDUCED FUNCT OR NUMERICAL INDETERMINACY
C      --CHORDAL METRIC ON RIEMANN SPHERE FOR Z-PLANE
      BB= (1.0+ABSQ(ZG))*(1.0+ABSQ(Z0(L)))
      IF(ABSQ(CA).GT.EPQZ*BB) GO TO 160
      ZZ= ZG
      FZ= FCZ
      FQR= FQ(K)
      KS= KR(L)
      IT(N)= 0
      GO TO 500
160  CD= CD*CA
150  CONTINUE
C      --DIVIDE OUT POLYNOMIAL OF KNOWN ROOTS
      CD= FCZ/CD
      FI(K)= CD
      FQ(K)= ABSQ(CD)

```

```

C
C      --ROTATE RADIUS VECTOR FOR NEXT GUESS. FOR LAST GUESS USE SMALL
C      --RADIUS FOR APPROX ZERO AVG OF THE FOUR GUESSES.
      CZ= CZ*ROTC
      IF(K.GE.3) CZ= (-.019,+.064)*CZ
C      --OUTPUT EACH INITIAL GUESS ITERATE
      IF(KOUT.GE.4) WRITE(6,1470) N,KS,I,C0,ZI(K),FCZ,FI(K),FQ(K)
130 CONTINUE
C      --SET RADIUS VECTOR START FOR NEXT(NTH+1) SET OF GUESSES.
      CG= -CG*ROTC
C      --GUESSES COMPLETED
C
C      --REORDER GUESSES IN DECREASING ABSQD OF REDUCED FUNCTION
C      --FQ1.GE.FQ2.GE.FQ3.GE.FQ4
180 DO 185 I=1,3
      J= I+1
      DO 185 K= J,4
        IF(FQ(K).LT.FQ(I)) GO TO 185
        CA= ZI(I)
        CB= FI(I)
        AA= FQ(I)
        ZI(I)= ZI(K)
        FI(I)= FI(K)
        FQ(I)= FQ(K)
        ZI(K)= CA
        FI(K)= CB
        FQ(K)= AA
185 CONTINUE
C      --DUMP GUESS FOR LARGEST FQ, PUSH UP THE REST.
190 DO 195 I=1,3
      J= I+1
      ZI(I)= ZI(J)
      FI(I)= FI(J)
      FQ(I)= FQ(J)
195 CONTINUE
C      --GUESSES ORDERED, USED AS INITIAL ITERATES
C
C      --MAIN MULLER ITERATION LOOP
      KS= 4
      KR(N)= KS
200 DO 210 I= 1,II
C
C      --CALCULATE NEXT MULLER ITERATE.  TRAUB FORMULAS
C      --ITERATIONS BASED ON REDUCED FUNCTION
C      IF(KOUT.GE.5) WRITE(6,DEBUG1)
      DFAB= (FA-FB)/(ZA-ZB)
      DFBC= (FB-FC)/(ZB-ZC)
      DDFC= (DFAB-DFBC)/(ZA-ZC)
      CB= DFBC+(ZC-ZB)*DDFC
      CA= CSQRT(CB*CB-4.0*FC*DDFC)

```

```

      CC= CB+CA
      CD= CB-CA
C    --SELECT LARGEST DENOMINATOR
      IF(ABSQ(CC).LT.ABSQ(CD)) CC= CD
      DFDZ= 0.5*CC
C    --INCREMENT FOR ITERATE
      DZ= -FC/DFDZ
C    --NEW ITERATE APPROXIMATION FOR ROOT
      ZZ= ZC+DZ
C
C    --EVALUATE FUNCTION AT NEW ITERATE
300  FCZ= CFCN(ZZ,NR)
      FZ= FCZ
      FQZ= ABSQ(FCZ)
C
C    --FACTOR OUT KNOWN ROOTS. FORM DENOMINATOR POLYNOMIAL.
      CD= C1
310  DO 320 L= 1,NL
C    --BUT NOT GUESSES, POORLY KNOWN, OR CURRENT ROOT
      IF(KR(L).LE.3.OR.L.EQ.N) GO TO 320
      CA= ZZ-ZO(L)
C    --IF TOO NEAR A KNOWN ROOT ACCEPT AS A MULTIPLE ROOT
C    --AVOIDS INFLATING REDUCED FUNCT OR NUMERICAL INDETERMINACY
C    --CHORDAL METRIC ON RIEMANN SPHERE FOR Z-PLANE
      IF(KR(L).LE.4) GO TO 330
      BB= (1.0+ABSQ(ZZ))*(1.0+ABSQ(ZO(L)))
      IF(ABSQ(CA).GT.EPQZ*BB) GO TO 330
      KS= KR(L)
      IT(N)= I
      GO TO 500
330  CD= CD*CA
320  CONTINUE
C    --DIVIDE OUT POLYNOMIAL OF KNOWN ROOTS
      FZ= FZ/CD
      FQR= ABSQ(FZ)
C    IF(KOUT.GE.5) WRITE(6,DEBUG2)
C
C 400 --TESTS FOR CONVERGENCE.
C    --CONVERGENCE TEST ON MAGNITUDE OF REDUCED FUNCTION
      IF(FQR.LT.EPQF) KS= 5
C    --CONVERGENCE TEST ON MAGNITUDE OF ACTUAL FUNCTION
      IF(FQZ.LT.EPQF) KS= 6
C    --CONVERGENCE TEST ON ITERATE INCREMENT DZ
C    --CHORDAL METRIC ON RIEMANN SPHERE FOR Z-PLANE
      IF(ABSQ(DZ).LE.EPQZ*(1.0+ABSQ(ZZ)**2)) KS= 7
      IF(KS.LT.5) GO TO 440
      IT(N)= I
      GO TO 500
C
C    --NOT CONVERGED. COMPLETE ITERATION, UPDATE ARRAY OF ITERATES

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```

C      --DUMP BIGGEST OLD ITERATE, INSERT NEW ITERATE IN ORDER
440  DO 450 J= 1,2
      K= J+1
      IF(FQR.GT.FQ(K)) GO TO 460
      ZI(J)= ZI(K)
      FI(J)= FI(K)
      FQ(J)= FQ(K)
450  CONTINUE
      J=3
460  ZI(J)= ZZ
      FI(J)= FZ
      FQ(J)= FQR
C
C      --OUTPUT EACH ITERATION
470  IF(KOUT.GE.4) WRITE(6,1470) N,KS,I,DZ,ZZ,FCZ,FZ,FQR
1470  FORMAT(1X,I3,I4,I4, 3(2H (,E10.3,1H,,E10.3,2H) ),
      $ 2H (,E10.3,1H,,E10.3,2H) ,G10.3 )
C
C      --EACH ITERATION COMPLETED
210  CONTINUE
C
C      --ITERATION LIMIT
      IT(N)= II
      KANT= KANT+1
C
C      --ACCEPT ITERATE AS A CONVERGED ROOT OR AS LAST ITERATE.
500  ZO(N)= ZZ
      FM(N)= SQRT(FQZ)
      KR(N)= KS
      IF(KS.GE.5) KANT= 0
C      --OUTPUT CONVERGED ROOT, LAST ITERATE, OR FIXED ZO.
590  IF(KOUT.GE.3) WRITE(6,1470) N,KR(N),IT(N),DZ,ZO(N),FCZ,FZ,FQR
C      --IF TWO SUCCESSIVE ITERATION LIMITS GIVE UP ON REMAINING ROOTS.
      IF(KANT.GE.2) GO TO 900
C
C      --END LOOP FOR NTH ROOT
110  CONTINUE
C
C      --NN ROOTS COMPLETED, OR GIVE UP.  END CZEROM
C
900  RETURN
C
      END

```


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