VARIATIONAL TECHNIQUES INCLUDING EFFECTIVE AND WEIGHTED INDEX METHODS

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1. Introduction

1.1 Prologue

In this chapter we show mainly how to find the propagation constants $\beta$ of buried or channel waveguide structures speedily and efficiently. This might be found useful when an active device solver is needed for iterative use in the simulation of lasers, amplifiers and active couplers. We advocate the Effective Index method (EI) [1–7], the Weighted Index method (WI) [8–15] and the Variational method (direct) (VM) [16–22], which appear to have much in common. EI and WI include the variational principle in their own internal analysis, whereas VM is here called "direct" because the variational expression is minimized numerically. The formulation of method VM prior to the actual computation is similar to that of WI in many ways. However, skilful formulation is necessary in order to determine the parameters appropriate to each structure. Accordingly, the reader is referred to the many recent papers of the Waterloo University group on this topic. For EI and WI, for every case, sometimes after a brief introduction, formulae are given for computer implementation. A short proof then follows immediately.

Noting that there is no single variable variational principle available for the polarized problem, we advocate carrying out a scalar analysis, followed by a Polarization Correction (PC) [16–25]. This is equivalent to the so called perturbation technique.

An important precursor to WI and VM was the CEVAR method (Cosine Exponential Variational) [26–29] for solving the scalar wave equation. Other methods referenced later in this chapter are of considerable theoretical interest. The list is not exhaustive, and space precludes much analysis.
The structure of the chapter is as follows. The scalar and polarized effective index methods are first introduced as computing techniques. Systematic improvements to EI are then considered based upon the scalar wave equation as follows. By the weighted index method [11] or, if preferred the (direct) variational method [17], we first obtain the best separable solution from which polarized corrections [17,24] are obtained. Complex valued solutions [15,30] are also referenced. The upper/lower weighted index method [12] for the stripe waveguide in air is shown to give excellent accuracy.

1.2 Notation

In all cases only the cross-section of the waveguide will be referred to. This is taken to be the the xy-plane, namely the plane of each diagram. The refractive index \( n(x,y) \) is a function of the coordinates \( x \) and \( y \) only. The \( z \)-axis is the direction of propagation, \( \beta \) is the propagation constant and the factor \( \exp(-j\beta z) \) is suppressed. Generally we let \( n(x,y) \) denote the refractive index, \( \varepsilon = n^2 \) the dielectric constant, \( \varepsilon_0 \) the permittivity of free space, \( \omega \) the frequency, \( \mu \) the permeability, \( k_0 = \omega(\varepsilon\varepsilon_0\mu)^{1/2} \) the propagation constant of free space, and \( k = k_0 n \) the local plane wave propagation constant.

2. Scalar Effective Index Method

2.1 Introduction

Figure 1 shows some typical buried planar structures, namely the buried channel and buried rib waveguides fabricated in III-V semiconducting compounds, which might form part of a number of active devices in optoelectronics. The interface with air, which is always present, is taken to lie at such a great distance that its effect can be ignored. The internal refractive index of structures fabricated from III-V compounds may be assumed to be of low contrast. In optical fiber theory this is termed the weak guidance approximation; however, our view is that the guidance may be strong within the context of a low contrast index profile, and that in our case, weak guidance would mean that the waveguide is being run close to cut-off.
Figure 1. (a) A buried channel waveguide (b) A buried rib waveguide. The refractive indices $n$ in the various regions are shown.

2.2 Preliminary Theory

For the present, we follow earlier workers, notably Marcatili [6], in using the scalar wave equation as a good first approximation for both TE and TM modes. Then if $k = k_0 n(x, y)$
\[
\frac{\partial^2 E}{\partial x^2} + \frac{\partial^2 E}{\partial y^2} + (k^2 - \beta^2)E = 0
\]  

(1)

where \( E \) is the principal electric field component, with \( E \) and \( \partial E/\partial n \) continuous everywhere. This is a very attractive proposition, as many techniques are available for the classical wave equation. For example, it is conceptually easy to solve slowly varying continuous problems such as the trapezoidal rib waveguide of small slope shown in Figure 3. As Marcatili has emphasized, the solution is basically one in which \( k(x, y) \) in the wave equation (1) is slowly varying along the \( x \)-direction. This makes it possible to obtain an approximate solution through a function \( G(x, y) \) which satisfies vertical slab waveguide equation with a local propagation constant \( \beta_x \). Both \( G(x, y) \) and \( \beta_x \) are assumed to vary slowly with \( x \). Then as the slab waveguide equation for \( G \) is

\[
\frac{\partial^2 G}{\partial y^2} + (k^2 - \beta_x^2)G = 0
\]  

(2)

we can nearly separate the variables by writing

\[
E = F(x)G(x, y)
\]  

(3)

where \( F \) satisfies

\[
\frac{d^2 F}{dx^2} + (\beta_x^2 - \beta^2)F = 0
\]  

(4)

This finds an approximate eigenvalue for any slowly varying configuration, but it requires the solution of the problem prescribed by equation (4), which although one-dimensional has a graded index. So, in the end, some discretization method will be needed to complete the solution. From now on we therefore consider only piecewise continuous distributions in which the refractive index is uniform over rectangles such as those shown in the buried channel waveguide of Figure 1(a).
Figure 2. (a) The composition of the buried rib waveguide from two layered regions, labeled I (inner) II (outer). (b) The directions of the axes. (c) The three uniform regions are equivalent to the three layered regions in (a).
2.3 Formulae and Computational Approach for the Effective Index Method

The Effective Index method in the case when there are discontinuities was discovered by Knox and Toulios [3] and Ramaswamy [4]. It had been suspected [1,2] that there is an average value for the refractive index which would reduce a layered slab waveguide to an equivalent uniform one. The average turned out to be $\beta/k_0$ where $\beta$ is the largest propagation constant. Thus $n_{\text{mode}} = \beta/k_0$ is called the effective index or mode index of a layered slab. To apply this result, we proceed as follows.

To simplify the explanation we use the simple case of the rib waveguide shown in Figure 2(a). After finding the slab propagation constants $\beta_I, \beta_{II}$ in the inner and outer regions of the rib waveguide of Figure 2(a), the layered regions I, and II are replaced by uniform regions I, and II with effective indices $n_I = \beta_I/k_0$ and $n_{II} = \beta_{II}/k_0$ as in Figure 2(c). Finding $\beta$ for this new symmetric slab waveguide approximates quite accurately the overall propagation constant $\beta$.

The computing method in the above paragraph does not say what to do if any of the regions I, II is neither a waveguide nor uniform. Clearly some other average is then required. If the regions were uniform, then the uniform value itself will obviously be taken as the index. Thus for the fundamental TE mode of the buried rectangle shown in Figure 4(a), we proceed as follows. In the first instance the vertical transcendental equation for symmetric modes is solved for the central region I. This gives the transcendental equation for $\beta_I$:
Figure 4. (a) The buried rectangle: a numerical example (b) reduction to a slab waveguide by means of the effective index method. The value of $n_I$ depends on the thickness $t$ and the wavelength of operation $\lambda$. For example if $\lambda = 1.15 \mu m$ and $t = 0.8 \mu m$ then $n_I = 1.47$.

$$\gamma_1 \tan(\gamma_1 t) = \gamma_2$$

where

$$\gamma_1 = (k_1^2 - \beta_I^2)^{1/2}$$

and

$$\gamma_2 = (\beta_I^2 - k_2^2)^{1/2}$$
The central slab waveguide of thickness $t$ has an effective index $n_I = \beta_I/k_0$ for region I, which depends upon its structure, see Figure 4, while the effective index of the cladding is taken to be unchanged from its uniform value of $n_{II} = 1.45$ for region II. With a slab width $w$, as in Figure 4(b) the transcendental equation for $\beta$ becomes:

$$\gamma_I \tan(\gamma_I w) = \gamma_{II}$$

where now

$$\gamma_I = (k_I^2 - \beta^2)^{1/2}$$

and

$$\gamma_{II} = (\beta^2 - k_{II}^2)^{1/2}$$

Finally, the mode index is $n_{\text{mode}} = \beta/k_0$. It should be noted that the scalar mode of a numerical slab waveguide solver (scalar is the same as TE for the uniformly plane layered slab) has been used for both transcendental equations merely as an introduction. The next section shows how to allow for polarization. An accurate measure of $\beta$ is the Kogelnik normalized form $b$ [31]. Also, a dimensionless parameter $V$ is used [32], where

$$b = \frac{\beta^2 - k_I^2}{k_2^2 - k_I^2} \quad V = w(k_1^2 - k_2^2)^{1/2} \quad (5)$$

with $k_2 = k_0n_2$ and $k_1 = k_0n_1$. Figure 5(a) shows $b$ plotted as a function of $V$ for $n_1 = 1.5$ and $n_2 = 1.45$ and aspect ratio $w/t = 2.0$ (solid) compared with scalar finite difference calculations (broken).
Figure 5. Propagation constants for buried waveguide structure with aspect ratio $w/t = 2.0$. (a) scalar effective index and finite difference calculations (b) scalar, TE and TM effective index calculations.
3. Polarized Effective Index Method

3.1 Nomenclature

The $x$-axis will be taken to be horizontal and the $y$-axis vertical as shown in Figure 2(b). We assume that there are approximate solutions corresponding to two polarizations, which may be described in terms of separate polarized wave equations. Let $E_x$ and $E_y$ denote the $x$ and $y$ components of the electric field as shown in Figure 6 and $\beta_x, \beta_y$ denote the propagation constants of the complete waveguide in either case. Designate the $x$-polarized mode as TE (Transverse Electric); then the TM (Transverse Magnetic) results will follow by interchanging $x$ and $y$.

![Diagram](image)

Figure 6. The directions of the principal electric field components for the (a) TE and (b) TM modes.

3.2 Computing Method for the Polarized Effective Index Method

The basic computing method is simple; it is the analysis of its accuracy, and the means of improving it that are less so. Thus in analyzing the buried rib waveguide in Figure 6, we use the notation of Figure 2. We solve the slab waveguide equations in the three regions II, I and II using TE mode boundary conditions, as would be correct for slabs with the electric field horizontal. This gives the same values of the slab propagation constants $\beta_I, \beta_{II}$ as before. However, after forming
the slabs of Figure 2(c) with the equivalent effective indices $n_I, n_{II}$, the electric field will now be seen to lie at right angles to the slab. Thus the TM mode boundary conditions must be used giving rise to the equation $\gamma_I \tan(\gamma_I w) = (\varepsilon_I/\varepsilon_{II}) \gamma_{II}$ for obtaining the overall value of $\beta$. This produces slightly different results from the non-polarized approach.

By way of illustration we show the TE and TM results in Figure 5(b) for the rectangular buried waveguide used there. For the TM mode overall, the procedure is the same as for the TE mode overall, but with $x$ and $y$ interchanged.

3.3 Theory of the Polarized Effective Index Method

The Effective Index methods can all be interpreted as the first terms of an important mode matching approach known as the Transverse Resonance method [5] studied from 1947 onwards [33-36] in relation to equivalent network analysis. Unfortunately, the first order terms of the modal expansion couple to the higher order terms, so that the full analysis is algebraically complicated. This has led to considerable work on improvements, notably the Generalized Transverse Resonance Technique [37] (which is identical with the first iteration of the Weighted Index method below), and the Diffractive Transverse Resonance Technique [38-40]. Since these advances replace the higher order terms in the modal expansion by a single function, we adopt a similar approach, but use a non-standard variational principle to reduce the algebra.

We therefore now propose to establish the polarized Effective Index method as quickly as possible, but in a satisfactory way. Thus the graded index wave equation will be considered. Eventually, the gradients will be allowed to become infinite, thereby reproducing a piecewise constant planar structure. Only the TE case is considered as the TM case is somewhat similar. Suppressing the suffixes therefore, for convenience, the polarized TE mode wave equation is

$$\frac{\partial}{\partial x} \left[ \frac{1}{\varepsilon} \frac{\partial (\varepsilon E)}{\partial x} \right] + \frac{\partial^2 E}{\partial y^2} + (k^2 - \beta^2)E = 0 \quad \text{TE} \quad (6)$$

The actual details of the derivation of the wave equation (6) lie outside the scope of this chapter; however, this equation is simply the $x$-component of $\bigtriangledown \times \bigtriangledown \times E = k^2 E$ after using $\bigtriangledown \cdot (\varepsilon E) = 0$ to eliminate $E_x$ and then omitting the term which couples the equation to $E_y$. 
Adapting the slowly varying approach [15] by using a variational technique, we assume that there is a local TE mode whose vertical profile $G(x, y)$ is mainly a function of $y$ and changes only slowly with $x$. Let $G$ satisfy the slowly changing wave equation $\partial^2 G/\partial y^2 + (k^2 - \beta_x^2) G = 0$. Then we may use a non-standard variational principle known as the local potential method [71]. What this means in context is that we can take the moment of equation (6) with respect to $G$. What we sacrifice is the minimum principle. All we can say is that the value of $\beta$ obtained in the end will be accurate. We may also simplify the local slab mode by using the standard variational principle [9,32,41] in Eq. (7) below, where in all integrals throughout, the limits are $-\infty$ and $+\infty$; also $\int F^2 dx = \int G^2 dy = 1$.

$$\beta_x^2 = \int G \left( \frac{\partial^2 G}{\partial y^2} + k^2 G \right) dy$$

(7)

Writing $E = F(x)G(x, y)$ as a convenient separation of variables, then multiplying equation (6) by $G$ and integrating with respect to $y$ we obtain a slab wave equation for $F(x)$, containing an extra integral with respect to $y$.

Thus,

$$\int_{-\infty}^{+\infty} G \frac{\partial}{\partial x} \left[ \epsilon^{-1} \frac{\partial}{\partial x} (\epsilon FG) \right] dy + (\beta_x^2 - \beta^2) F = 0$$

(8)

Finally, we utilize the slow variation of $\epsilon$ with respect to $x$. Making the approximation $\epsilon \approx \epsilon_x \approx n_x^2$ in the slowly varying term, where $n_x = \beta_x / k_0$ is the local effective index and $\epsilon_x$ is the local effective dielectric constant, the integration with respect to $y$ may be performed. This gives the polarized form of the Effective Index method

$$\frac{\partial}{\partial x} \left[ \frac{1}{\epsilon_x} \frac{\partial}{\partial x} (\epsilon_x F) \right] + (\beta_x^2 - \beta^2) F = 0$$

(9)

Now, allowing the gradient of $\epsilon_x$ to become infinitely large at the horizontal discontinuity where the regions connect, it is seen that as the derivative of $\epsilon_x F$ exists, then $\epsilon_x F$ is continuous everywhere. Also, integrating equation (9) across the discontinuity shows that the jump in $\epsilon_x^{-1} \partial (\epsilon_x F)/\partial x$ is zero; therefore equation (9) leads to the boundary conditions that

$$\epsilon_x F \quad \text{and} \quad \frac{1}{\epsilon_x} \frac{\partial}{\partial x} (\epsilon_x F) \quad \text{are continuous}$$

(10)
This establishes the Effective Index method as a non-standard variational solution. Often \( \varepsilon_x \) is uniform on each side of the discontinuity, then these boundary conditions take the familiar forms that \( \varepsilon_x F \) and \( \partial F/\partial x \) are continuous.

The above argument can be taken much further and deeper, but the full details lie outside the aims of the present chapter.

4. General Implementation of the Effective Index Method

4.1 Introduction

The power of the methods considered here is that a program can readily be written to cover very general configurations such as the planar structure shown in Figure 7, where \( P \) effective indices will be needed for each vertical \( Q \)-layered slab waveguide, giving a horizontal slab waveguide consisting of \( P \) layers. Since it will help in the implementation of the other methods, we first describe how to apply the Effective Index method to these more complicated planar structures.

![Figure 7](image)

Figure 7. A general buried channel waveguide with refractive indices \( n_{pq} \) where \( p \) and \( q \) range from 1 to \( P \) and 1 to \( Q \) respectively.
Figure 8. (a) The $p$th TE slab problem yielding the local effective index $n_{xp} = \beta_{xp}/k_0$ for each section of the planar structure or staircase approximation. (b) The use of the effective indices to create a final value of $n_{mode} = \beta/k_0$. 
4.2 General Implementation of the Effective Index Method

The method below can be either a scalar problem in which the polarization is ignored, or can be made polarized by using either TE or TM boundary conditions depending on the orientation of the electric field relative to the layered slabs. There are two sweeps, one in the preferred initial direction, followed by another in the orthogonal direction. The choice of initial direction is governed by physical intuition.

(i) For the scalar modes of the slowly varying layered structure, first divide it up into straight sections, by planes \( x = \text{constant} \), using either the natural planar boundaries for a planar structure, or a staircase approximation for a structure which varies with \( x \), such as the trapezoidal buried rib of Figure 3. Then work out the value of \( \beta_x \) for each section considered as a multislab waveguide. For example in Figure 7 this would yield \( P \) values of \( \beta_x = \beta_{zp} \), \( p = 1, 2, \ldots, P \) from Fig. 8(a). Non-guiding regions must be dealt with on an ad hoc basis.

(ii) Then use the effective indices \( \frac{\beta_x}{k_0} \) for each slab shown in Figure 8(b) to create a multilayered TM slab problem in the orthogonal direction. This solution yields the final approximate value of \( \beta \). The notation \( n_{\text{mode}} = \beta/k_0 \) might be considered appropriate.

5. Weighted Index Method

5.1 Introduction

The Effective Index method [1–7] for low contrast index profiles is very accurate, and until recently was considered quite accurate enough for the design of buried laser waveguides. However, the design of more complicated structures with their reliance upon index guiding seems to demand even greater accuracy, and there has been considerable recent interest in systematic improvements. We mention three variational approaches here, in which a separable variable solution \( E = F(x)G(y) \) is used. The three are in fact equivalent to each other, and will be called the Weighted Index method (WI) [8–15], the Variational method (direct) (VM) [16–22] and the Cosine Exponential Variational method (CEVAR) [26–29]. The CEVAR method assumes a separable solution \( F(x)G(y) \) using simple forms containing arbitrary constants in each region. These are then substituted into the Rayleigh quotient of
equation (18) below and the integrals evaluated analytically for simple structures. The value of $\beta$ is then minimized directly by varying the arbitrary constants. The Weighted Index method automatically produces weighted indices for a series of successive slab problems, which converge to the best separable solution $E = F(x)G(y)$ of the problem in hand. Later, the Variational method (direct) (VM) was invented, which in principle is more general than CEVAR and WI. However, the Weighted Index method iterates to a conclusion without reference to external optimization schemes, with results very similar to those later given by VM [16–22]. Accordingly it is suggested that a self contained, straightforward way of improving on the Effective Index method is to use either WI or VM to find the best separable solution of $F(x)G(y)$ of the scalar wave equation, then use this to obtain polarized corrections along the lines of [16–22].

The (direct) variational method has been exploited further by using non-separable solutions such as $F_1(x)G_1(y) + F_2(x)G_2(y)$ or more complicated ones, along the lines of [19]. This is highly successful, but sacrifices the elegance and simplicity of the original schemes.

5.2 Formulae and Computation for the Weighted Index Method

The computing method is very similar to that of the Effective Index method discussed previously. However, only one effective index is ever calculated; the rest are all weighted indices. Moreover, as the field profile is used to form the weights which appear in the calculation, its form is supposed to be separable in the coordinates $x$ and $y$ so that $E = F(x)G(y)$, where $F$ and $G$ are the best separable functions which are generated by the computer method. The method generates $F(x)$ and $G(y)$ as the field profiles of equivalent slab waveguides, and the theory proves also that the general solution consists only of slab waveguiding solutions, which is not obvious by other means. The notation used for the slab wave guide equations is $d^2F/dx^2 + (K_x - \beta_x^2)F = 0$ and $d^2G/dy^2 + (K_y - \beta_y^2)G = 0$. Here $K_x (= k_x^2)$ and $K_y (= k_y^2)$ will be called Helmholtz constants.
Figure 9. (a) The slab problem yielding the weighted index \( n_y \) for the \( y \) direction's equivalent slab. (b) The slab problem yielding the weighted index \( n_x \) for the \( x \) direction's equivalent slab.
(1) To start the iterative process we choose any central region, such as the $p^{th}$ one shown in Figure 8(a) with its layers normal to the $y$-direction. This is the first approximation to the equivalent multilayered $y$-slab waveguide. We calculate its $\beta_y$ and store the mode profile, or any parameters needed to reproduce it simply, depending on the method being used (see next paragraph).

(2) * From these we calculate the $y$-weights $W_{yq}$ which are

$$W_{yq} = \int_{y_{q-1}}^{y_q} G^2(y)dy$$

(11)

Note that $y_0 = -\infty$ and $y_Q = +\infty$. The numerical values of the weights can be derived either by using an exact analytical form for $G$, which appears in the course of the matrix method (cascade process) or by storing $G$ as a vector using many components and a short mesh length. The latter may arguably be faster, and is certainly simpler.

(3) We then form weighted Helmholtz constants $K_{xp}$ for the orthogonal direction, namely, the $x$-direction, by a formula to be derived later:

$$K_{xp} = \sum_{q=1}^{Q} W_{yq} K_{pq}$$

(12)

This therefore has generated a new equivalent multilayered $x$-slab waveguide with the layers parallel to the $yz$-plane. (See Figure 9(b))

(4) Then we find the $\beta_x$ for this new slab waveguide and use it to calculate the $x$-direction weights. We also store the mode profile, or any parameters needed to reproduce it simply, depending on the method being used. The formula for the weights $W_{xp}$ is

$$W_{xp} = \int_{x_{p-1}}^{x_p} F^2(x)dx$$

(13)

Note that $x_0 = -\infty$ and $x_P = +\infty$.

(5) We then form the weighted Helmholtz constants $K_{yp}$ for the orthogonal direction, namely the $y$ direction, by
\[ K_{yq} = \sum_{p=1}^{P} W_{xp} K_{pq} \] (14)

This has generated a new equivalent multilayered y-slab waveguide with the layers parallel to the zx-plane. (See Figure 9(a))

(6) Now calculate the \( \beta_y \) and use the Rayleigh quotient, i.e. the variational principle to obtain an approximation to the overall propagation constant \( \beta \) from

\[ \beta^2 = \beta_z^2 + \beta_y^2 - \sum_{p=1}^{P} \sum_{q=1}^{Q} W_{xp} W_{yq} K_{pq} \] (15)

(7) Then we repeat the whole process from the point (2)* onwards until the value of \( \beta \) converges to the required accuracy. At that stage the calculation ends.

5.3 Theory of the Weighted Index Method

Suppose that \( E \) is some scalar wave field satisfying equation (1). We can employ the method of moments as the equation has a variational principle: it is self adjoint [42,73]. Then write \( E = F(x)G(y) \), multiply equation (1) by \( G(y) \) and integrate, remembering that all integrals are from \(-\infty\) to \(+\infty\). Then we obtain

\[ \partial^2 F/\partial x^2 + (\int k^2 G^2 dy - \beta_z^2) F = 0 \] (16)

where \( \beta_z^2 = \beta^2 - \int GG'' dy \). Likewise multiply equation (1) by \( F(x) \) and integrate. Then

\[ \partial^2 G/\partial y^2 + (\int k^2 F^2 dx - \beta_y^2) G = 0 \] (17)

where \( \beta_y^2 = \beta^2 - \int FF'' dx \). Equations (16) and (17) constitute a pair of integro-differential equations, which couple together the two orthogonal directions. They correspond to the overall value of \( \beta \) given by the Rayleigh variational principle

\[ \beta^2 \cong \int \int E(\partial^2 E/\partial x^2 + \partial^2 E/\partial y^2 + k^2 E) dx dy \] (18)
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On substituting $E = F(x)G(y)$ using \( \int GG''dy = \beta^2 - \beta_y^2 \) and \( \int FF''dx = \beta^2 - \beta_x^2 \), it is found that

\[
\beta^2 = \beta_x^2 + \beta_y^2 - \sum_{p=1}^{P} \sum_{q=1}^{Q} W_{xp}W_{yq}K_{pq}^2
\]  \(19\)

Iteration between the two orthogonal directions until convergence is achieved minimizes \( \beta \), obtaining the best field distribution obtainable from a separable solution. Moreover the value of \( \beta \) is then an underestimate of the true value of \( \beta \).

As they stand, equations (16) and (17) constitute slab waveguide problems which may be solved alternately using a starting function \( G(y) \) and a starting value of \( \beta_y \) obtained from the solution of some central region, as in the case of the Effective Index method. Once started, the solution of (19) follows from (18) and conversely. It will be found that \( \beta_x \) and \( \beta_y \) eventually converge. The original Weighted Index approach was slightly different in practice. The above streamlined version is due to Gault, Mawsby and Towers [15].

The method was validated for buried waveguides in [13], whose results are reproduced in Figure 10. It was also applied extensively to the rib waveguide in air [8–12] under the SERC/DTI U.K. Joint Optoelectronics Research Scheme.

5.4 Variational Method (Direct)

The Variational method (direct) [16–22] in its simplest form will produce the same values of \( \beta \) as the Weighted Index method because it uses a separable solution involving a cosine or exponential separable solution in each rectangular element of the cross-section, followed by direct optimization of the overall \( \beta \) derived from the above variational principle (18). In principle, however, it is more general because non-separable trial solutions can be attempted (see earlier). The trial function used is usually \( E = F(x)G(y) \), where \( F \) and \( G \) are slab waveguides. The solution therefore consists of simple trigonometric or exponential terms in each subregion of Figure 7. Skilful choice of parameters exposes the number of degrees of freedom in the trial function. Thus, after substituting for \( E \) into the Rayleigh variational principle (18) and performing the integrals analytically, the resulting expression for \( \beta^2 \) may be minimized by varying the basic parameters. The best separable solution is obtained by means of this process, and will
therefore be the same as the Weighted Index solution.

The (direct) Variational method has extended the implementation of the earlier CEVAR method [26–29], by the addition of a Vector Correction and by its extension to a wide range of structures. Nevertheless, it operates on the same basic principles. An application to buried channel problems is shown in Figure 11 [16]. The generality of this method should not be overlooked. In principle, any number of constants can be included in the trial functions, in a much more sophisticated way than in the Weighted Index method. This is still the subject of research, but the following generalization is obviously possible, namely, \( E = A F_1(x)G_1(y) + B F_2(x)G_2(y) \). This shows that the (direct) Variational method is in principle more general than the other methods given in this chapter. In the implementation of the (non-separable) Upper/Lower Weighted Index method Robertson [12] pointed out that the pear shaped mode of the rib waveguide in air indicated a non-separable solution.

5.5 The Rib Waveguide in Air

Much work has also been done on the rib waveguide in air [8–12], which lies outside our main aim of describing the buried waveguide, and certainly does not possess a low contrast dielectric profile. However, the Upper-Lower Weighted Index method can be made to produce excellent results as shown in Figure 12. The solution is split across the base of the rib.

![Figure 10. From Roberts and Stern [13] (©1987, IEE). Scalar propagation curves for channel waveguide structure with aspect ratio \( a/d = 2.0 \). \( B \) is the dimensionless parameter \( a(k_2^2 - k_1^2)^{1/2}/\pi \).](image)
Figure 11. From Haus, Huang and Whittaker [16] (©1987, IEEE). Dispersion curves for $E_{11}$ and $E_{21}$ modes from scalar variational analysis, and comparison with the literature. For (a) and (b): effective index method (---), circular harmonic (-----), perturbation method (………), transcendental equations (Marcatili) (-----), variational principle (———).
Figure 12. From Robertson et al. [10] (©1987, IEEE). Modal refractive index at wavelength 1.15μm plotted as a function of $t_2$ for the structure shown in the inset, using the four different methods; effective index, finite difference, modified weighted index and weighted index.

6. Polarization Corrections

6.1 Introduction

In view of the speed which it achieves in modeling, there has been recent interest in obtaining polarized TE and TM results from a known scalar solution. This was first suggested in [16] in the context of planar technology, and the methodology firmly established [17–22]. The calculations start from a scalar solution $E = F(x)G(y)$. Work done
in a Sheffield-Nottingham collaboration has also dealt with the stripe waveguide [24]. In addition it has been shown that the polarized solutions are very accurate indeed [25]. These seem to be five component solutions [43]; the coupling to the sixth component has only recently been calculated numerically [44]. The basic Polarization Correction is quite simple to derive. The results are remarkably accurate and can be used as a subroutine along with the Weighted Index method, with a view to replacing much heavier numerical analyses. This is an extremely useful means of obtaining \( n_{\text{mode}} \) for polarized problems.

### 6.2 Formulae and Implementation for the General Polarization Correction

The structure allowed for is the very general one shown in Figure 7 in which the cross section of the waveguide is divided into \( P \times Q \) regions by planes \( x = x_p \) where \( p \) runs from 1 to \( P \) and \( y = y_q \) where \( q \) runs from 1 to \( Q \). It is supposed that the polarized corrections convert the value of \( \beta = \beta_{\text{SCAL}} \) derived for the scalar wave equation to \( \beta_{\text{TE}} \) and \( \beta_{\text{TM}} \). The corrections are best calculated as part of the procedure. In general we have corrections given by equations (29) and (30) below. These have been validated extensively by comparing the scalar, TE and TM finite difference solutions [24,25] for the rib waveguide in air: a searching test. However, these expressions simplify for either the Weighted Index method or the (direct) Variational method. When these have converged to give an approximation to \( \beta_{\text{SCAL}} \), we have \( E \equiv F(x)G(y) \). Then it is easy to either pick out or calculate the values of \( F(x), dF/dx, G(y) \) and \( dG/dy \) on the boundaries. Recall also that \( \int F^2 \, dx = \int G^2 \, dy = 1 \). The following general expressions will be derived later in equations (31) and (32): for the TE mode

\[
\beta_{\text{TE}}^2 = \beta_{\text{SCAL}}^2 - \sum_{p=1}^{P-1} F_p \frac{dF_p}{dx} \int [\varepsilon]_p G^2 \, dy
\]  

(20)

Likewise, for the TM mode

\[
\beta_{\text{TM}}^2 = \beta_{\text{SCAL}}^2 - \sum_{q=1}^{Q-1} G_q \frac{dG_q}{dy} \int [\varepsilon]_q F^2 \, dx
\]  

(21)

Using the actual weighted index formulae, and quantities already calculated as part of the process, equations (20) and (21) will be later
converted to the forms (33) and (34), namely,

$$
\beta^2_{\text{TE}} = \beta^2_{\text{SCAL}} - \sum_{p=1}^{P-1} F_p \frac{dF_p}{dx} [K_{xp}]
$$  \hspace{1cm} (22)

and

$$
\beta^2_{\text{TM}} = \beta^2_{\text{SCAL}} - \sum_{q=1}^{Q-1} G_q \frac{dG_q}{dy} [K_{yq}]
$$  \hspace{1cm} (23)

where $K_x$ and $K_y$ are part of the calculation process given by equations (14) and (12), also $[K_x]_p$ and $[K_y]_q$ denote the increment in these quantities across the $p^{th} x$-interface or the $q^{th} y$-interface.

6.3 Theory of Polarization Corrections

We first deal with the quasi TE mode with the principal electric field $E$ lying horizontal, in the $x$ direction. We use a graded index approach, and when the formula has been finally produced, allow the gradients to steepen in a way which reproduces the discontinuities in refractive index, and is consistent with the electromagnetic boundary conditions. We use the displacement $D = \varepsilon_0 E$ as a convenient main variable. Then we shall eventually be seeking consistency with continuity of $D$ and $\partial E/\partial x$ when the $x$ direction is normal to a plane of discontinuity, and continuity of $E$ and $\partial E/\partial y$ when the $y$ direction is normal to a plane of discontinuity.

In general, as $\varepsilon$ is a function of both $x$ and $y$, the polarized TE wave equation (6) does not possess a variational principle involving $E$ alone because it is not self adjoint. So we must start from the scalar wave equation (1). Replacing $\beta^2$ by $\beta^2_{\text{SCAL}}$, multiplying the equation by $E$, and integrating gives

$$
\beta^2_{\text{SCAL}} = \int \int E \left( \frac{\partial^2 E}{\partial x^2} + \frac{\partial^2 E}{\partial y^2} + k^2 E \right) dx dy
$$  \hspace{1cm} (24)

where the normalization $\int \int E^2 dx dy$ is assumed. This in itself does not demonstrate that (24) is variational (but it is, see [41,63]). Then equation (24) has the property that $E$ does not have to satisfy equation (1) any longer. Moreover, any reasonable approximation to $E$ which satisfies the boundary conditions can be used in (24) as a “trial
solution”, and will give a good approximation to $\beta$ depending on the closeness of the trial solution to the actual solution. Imagine that we have solved equation (6) for the TE mode: we do not intend to actually solve it, since that defeats the purpose of a variational exercise; one hopes not to have to solve the field equations. Then $E$ now satisfies equation (6) and we would have on substituting into equation (24) and rearranging it

$$\beta_{\text{SCAL}}^2 = \beta_{\text{TE}}^2 + \iint E \left\{ \frac{\partial^2 E}{\partial x^2} - \frac{\partial}{\partial x} \left[ \frac{1}{\varepsilon} \frac{\partial (\varepsilon E)}{\partial x} \right] \right\} dxdy$$  \hspace{1cm} (25)

Integrating by parts using the fact that $E \to 0$ at infinity this becomes

$$\beta_{\text{SCAL}}^2 = \beta_{\text{TE}}^2 + \iint \frac{\partial E}{\partial x} \left( \frac{1}{\varepsilon} \frac{\partial (\varepsilon E)}{\partial x} - \frac{\partial E}{\partial x} \right) dxdy$$ \hspace{1cm} (26)

Thus, after minor simplification, we obtain the graded index form [17,24]

$$\beta_{\text{TE}}^2 = \beta_{\text{SCAL}}^2 + \iint \varepsilon E \frac{\partial E}{\partial x} \frac{\partial (e^{-1})}{\partial x} dxdy$$ \hspace{1cm} (27)

The form (27) is useful, as it immediately allows us to proceed directly to the general piecewise uniform structure of Figure 7. In fact $\partial (e^{-1})/\partial x$ is zero everywhere, except across any discontinuities of dielectric constant $\varepsilon$ in the $x$-direction. Moreover, as $\varepsilon E$ and $\partial E/\partial x$ are continuous across any such discontinuity, say $x = x_p$, then in the neighborhood of the plane $x = x_p$ we have $\partial (e^{-1})/\partial x = [e^{-1}]_p \delta(x - x_p)$, where $\delta$ is a delta function and $[e^{-1}]_p$ represents the increment in $e^{-1}$ across that plane. Thus for a general configuration we obtain from equation (27)

$$\beta_{\text{SCAL}}^2 = \beta_{\text{TE}}^2 - \sum_{p=1}^{P-1} \int \varepsilon E \frac{\partial E}{\partial x} [e^{-1}]_p dxdy $$ \hspace{1cm} (28)

where $E$ is a trial function for the TE mode. However, although $\varepsilon$ is discontinuous, its profile is nearly uniform. Thus we may use the approximation that $\varepsilon[e^{-1}]_p \approx -[\varepsilon]_p$. Therefore, as we are dealing with small corrections, we may now obtain $E$ from the scalar wave equation (1). In general therefore for the low contrast profile piecewise uniform case,
\[ \beta_{TE}^2 = \beta_{SCAL}^2 - \sum_{p=1}^{P-1} \int E \frac{\partial E}{\partial x} [\varepsilon]_p dy \]  \hspace{1cm} (29)

and by interchange of the direction of polarization

\[ \beta_{TM}^2 = \beta_{SCAL}^2 - \sum_{q=1}^{Q-1} \int E \frac{\partial E}{\partial y} [\varepsilon]_q dx \]  \hspace{1cm} (30)

However, simpler expressions may be used for particular cases. Using the approximation \( E = F(x)G(y) \) already derived in Section 5 of this chapter by the Weighted Index method gives

\[ \beta_{TE}^2 = \beta_{SCAL}^2 - \sum_{p=1}^{P-1} F_p \frac{dF_p}{dx} \int [\varepsilon]_p G^2 dy \]  \hspace{1cm} (31)

and by interchange of the direction of polarization

\[ \beta_{TM}^2 = \beta_{SCAL}^2 - \sum_{q=1}^{Q-1} G_q \frac{dG_q}{dy} \int [\varepsilon]_q F^2 dx \]  \hspace{1cm} (32)

Finally, we observe that over the \( q^{th} \) interval, \( \int \varepsilon G^2 dy \) is simply \( W_{yq}\varepsilon_{pq} \), namely, the local dielectric constant weighted by \( W_{yq} \) as given by equation (11). Thus

\[ \beta_{TE}^2 = \beta_{SCAL}^2 - \sum_{p=1}^{P-1} F_p \frac{dF_p}{dx} \sum_{q=1}^{Q-1} W_{yq}(\varepsilon_{p+1,q} - \varepsilon_{pq}) \]  \hspace{1cm} (33)

and by interchange of the direction of polarization, if \( W_{xp} \) is given by equation (13), we have

\[ \beta_{TM}^2 = \beta_{SCAL}^2 - \sum_{q=1}^{Q-1} G_q \frac{dG_q}{dy} \sum_{p=1}^{P-1} W_{xp}(\varepsilon_{p,q+1} - \varepsilon_{pq}) \]  \hspace{1cm} (34)

These formulae explicitly give both general and weighted index type polarized correction formulae for use with either (direct) Variational solutions, or Weighted Index solutions. They are quoted earlier as equations (22) and (23) in a suitable form for computation.
7. Connections Between Various Theories

7.1 The Nature of Separable Solutions

Early analytic work [45,46] on the rectangular dielectric waveguide dates from 1982. Since 1984 various papers have appeared [47,55] which shed some light on why the Effective Index method sometimes gives too high an answer, and put forward intended improvements on its accuracy.

In deriving this mathematically complete version of the argument we have taken advantage of a private communication [56]. Let \( \hat{E} = F(x)G(y) \) be a separable trial solution of the scalar wave equation giving rise to a value \( \hat{\beta} \) of the propagation constant such that

\[
\frac{\partial^2 \hat{E}}{\partial x^2} + \frac{\partial^2 \hat{E}}{\partial y^2} + (\hat{k}^2 - \hat{\beta}^2) \hat{E} = 0
\]  

(35)

where

\[
d^2 F/dx^2 + (k_x^2 - \beta_x^2) F = 0
\]  

(36)

and

\[
d^2 G/dy^2 + (k_y^2 - \beta_y^2) G = 0
\]  

(37)

Also

\[
\hat{k}^2 = k_x^2 + k_y^2 \quad \text{and} \quad \hat{\beta}^2 = \beta_x^2 + \beta_y^2
\]  

(38)

where \( k_x \) and \( k_y \) are the equivalent slab distributions of local plane wave propagation constant, and \( \beta_x \) and \( \beta_y \) are the \( x \) and \( y \)-slab propagation constants. Then it is easy to derive the so called perturbation formula

\[
\beta_T^2 = \hat{\beta}^2 + \iint (k^2 - \hat{k}^2) \hat{E}^2 dx dy / \iint \hat{E}^2 dx dy
\]  

(39)

In [52] it was pointed out that the fictitious distribution of \( \hat{k} \) which gives rise to to the Effective Index value of \( \hat{\beta} \) is greater in some regions than in others, and this shows that for the buried channel this causes \( \hat{\beta} \) to be greater than the trial result \( \beta_T \). This enables improvements to be made to the accuracy of \( \hat{\beta} \). On the other hand, in [54], in effect, \( \beta_T^2 - \hat{\beta}^2 \) is minimized formally, where
\[ \beta_T^2 - \hat{\beta}^2 = \iint (k^2 - k_x^2 - k_y^2) F^2 G^2 \, dx \, dy / \iint F^2 G^2 \, dx \, dy \]  

(40)

This does not lead to new principles, but is convenient for some purposes. In fact, since \( F \) and \( G \) already satisfy their respective slab waveguide equations, \( \hat{\beta} \) is guaranteed always to lie at a minimum value. Even though the value of \( \hat{\beta} \) can vary, it always does so in such a way that it lies at a minimum. What this means is that minimizing the left hand side of equation (40) is equivalent to minimizing \( \beta_T \), as in the Weighted Index or (direct) Variational methods. Since it proves necessary to correct the solution iteratively in a very similar way to the Weighted Index method it is concluded that in the scalar case, the two solutions would be the same. In the polarized cases, the respective wave equations are not self adjoint, and therefore possess no true variational principle. This leaves open some basic questions which we have answered in this chapter by first working out a mathematically rigorous solution for the scalar wave equation, followed by a clear mathematical approximation to the polarized correction.

In summary, the methods of [52] and [54] have proved valuable as an alternative interpretation of the Effective Index method, but when taken to a logical conclusion seem to be equivalent to using the standard variational method of equation (18). In a sense, all stem from the insight originally obtained by Sharma [26–29].

7.2 Averaging Effective and Weighted Index Results

It will be obvious that the methods given in this chapter are the subject of current research. Since they are variational methods using the minimum principle they produce a value of \( \beta \) which is lower than the true value. This always holds good, and may be found useful near cut off for low contrast index profiles.

We conclude this section by quoting the suggestion of a good "rule of thumb": an extremely accurate result may be obtained for \( n_{\text{mode}} \) by using the Effective Index method followed by the Weighted Index method, then averaging the two [15, 56]. Figure 13 shows the results of this calculation [9] for the difficult case of the rib waveguide in air using the parameters [57].
Figure 13. Modal refractive index at wavelength 1.15\(\mu m\) plotted as a function of \(t_2\) for the structure shown in the inset, using the four different methods: effective index, weighted index, "rule of thumb" average, and a variational method (WAVE [72]).

8. Use of Complex Variables in Variational Methods

In view of its usefulness in studying loss, gain and radiation in waveguides, lasers and traveling wave amplifiers [7,15,30,58–62] it is appropriate to comment on the validity of the complex dispersion equation. This chapter has repeatedly used the variational principle in the form of ref. [63], namely,

\[
\beta^2 \approx \frac{\iint (k^2 E^2 - \nabla_T \cdot E \cdot \nabla_T E) dx dy}{\iint E^2 dx dy} \tag{41}
\]

Another expression is often quoted, namely,

\[
\beta^2 \approx \frac{\iint (k^2 EE^* - \nabla_T \cdot E \cdot \nabla_T E^*) dx dy}{\iint EE^* dx dy} \tag{42}
\]

and this should be used when an extra complex variable has been introduced, for example, as part of a complex Fourier analysis. The
complex conjugates shown explicitly in equation (42) then apply only to the extra complex variable.

It is allowable in most circumstances to use the above Rayleigh variational principles when the indices are complex, that is, when the system is lossy or has gain. This has been analyzed in [41] where references [60,61] are quoted; see also reference [62], which uses dyadics. Provided that the expression of the right hand side of equation (18) is analytic in a region surrounding the true value of $\beta$ in the complex plane, then this will be a stationary value. This will usually be the case, and may be restated thus: both the real and imaginary part of $\beta$ will be stationary simultaneously. Some detailed applications are to be found in reference [64].

When seeking the stationary values of a variational expression such as the right hand side of equation (24) with complex $k$, the curvature of the search surfaces in terms of the real and imaginary parts of $\beta = \beta_r + j\beta_i$ often varies rapidly along the imaginary axis. Complex searches can easily jump onto the wrong solution. This behavior can be improved by making the imaginary part of $k$, or any other parameter vary slowly in small steps, as in the classical method of embedding. This can be made to apply to any structure, especially systems with loss or gain [65], and there seems to be no reason why leaky modes with a propagating region which extends to infinity should not be treated in this elementary way. The process would be initiated by starting from the non-radiative case and gradually extending the propagating region inward from infinity. In practice, all complex values of $\beta$ seem to have a large real part, and a smaller complex part, and this disparity in magnitude helps to avoid a general search over the complex plane. If a starting problem can be found, whose solution gives a real value of $\beta$, and a physical parameter whose increase from zero at the start converts the problem to the complex one in a gradual way, then under most circumstances the complex root can be approached continuously.

9. Summary

In conclusion, we have shown that the Effective Index Method and its generalizations are extremely powerful, and may be applied to quite general configurations.
Variational techniques including effective and index methods

We have shown that the accuracy and theory of the Effective Index method (EI) [3,4] can be improved. Although accurate enough for many purposes [66] the $\beta$ values obtained using EI tend to be too large, and there are laser and coupler structures which seem to produce inaccurate results [15,67,68]. There are also cases where a waveguide section is layered, but is neither uniform nor propagating. We conclude therefore that the Effective Index method is mainly applicable to a planar waveguiding structure with a common guiding region throughout. Even in this case improvement is possible, at the expense of using a saddle point variational principle [69,70]. The Effective Index method can be looked upon as the first term of a modal expansion in each subregion, and might be called a perturbation problem. In this connection the Transverse Resonance method [5,33–36], Generalized TRM [37] and Diffractive TRM are referenced [38–40]. However, here we use a different variational approach which suppresses the extra terms and displays the slowly varying nature of the apparently abrupt discontinuities in dielectric constant.

Recent progress has been shown to arise from the use of variational methods and was heralded by the CEVAR method [26–29]. There followed the Waterloo University group's extensive development of the Variational (direct) method (VM) [16–2] with Polarization Correction (PC), which makes the Rayleigh principle [41,63] of equations (41) or (42) stationary. A Sheffield-Nottingham University collaboration [23–25] has also studied the PC, and shown that the solution of the polarized wave equation is extremely accurate, giving rise to only a very small correction [25].

The "work horse" presented here is the Weighted Index method (WI) [8–15] together with the polarized corrections (PC) already mentioned. This solves the scalar wave equation by finding the best separable solution $F(x)G(y)$. The method iterates between orthogonal directions, converging rapidly to the solution. Then a PC is applied. Perturbation methods have been shown to result in the same solution.

Which of the two main methods considered here, namely VM or WI is the more general is an open question because (i) in VM, trial functions of the non-separable form $A F_1(x)G_1(y)+B F_2(x)G_2(y)$, can be used, as in reference [19], but (ii) in WI the variables can be separated differently as $F_1(x)G_1(y)$ or $F_2(x)G_2(y)$ in different regions as in [12]. Both generalizations are highly successful.
Finally it is pointed out that these methods work for complex parameters, and recent work [15,30,60–62,64,65] and its theoretical background is briefly summarized. Moreover, the best values obtained to date have been obtained by averaging the Effective and Weighted Index Methods [15].

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References


