

# Variational analysis of buffered multilayer optical planar waveguides

V. A. POPESCU

Department of Physics, University "Politehnica" of Bucharest, Splaiul Independentei 313, 060042 Bucharest, Romania

The values of the propagation constants, which correspond to maxima of the real part of the functional derived from a variational principle, by using of the exact analytical eigenfunctions, are used as initial guesses to increase the efficiency for complex root searching of the associated dispersion equation for a multilayer planar waveguide. This variational method is used to study the effects of addition of a low-index buffer layer over a high substrate on the propagation characteristics of the waveguide.

(Received May 28, 2009 ; accepted June 15, 2009)

*Keywords:* Waveguides; Quantum mechanics, Variational analysis, Optical planar waveguides

## 1. Introduction

The propagation constants for the optical modes can be obtained by solving the dispersion transcendental equations. For many of the leaky modes and for modes of lossy waveguide, the optical propagation constants are complex numbers. It is difficult to extract a large number of the complex solutions because of the oscillatory behavior of the dispersion equation. A disadvantage of the Newton-Raphson method is the need of an initial guess value very close to the actual root for each zeros of the dispersion equation. Although the Cauchy Integration method [1] exploits the analyticity of the dispersion equation and is capable of finding all the solutions in a given region of the complex plane, however a computer implementation is not easy as it involves numerical integration along closed contour in complex plane and searching for roots of a polynomial. The perturbation approach gives better results only when there is a small difference between the refractive indices in each layer of the layered waveguide. Recently [2], an efficient and exact variational scheme was used for extraction of guided and leaky modes in layered waveguides based on a modification of the dispersion equation. The effective indices are derived from the minima of a functional dependent on the reflection coefficients and are insensitive to the choice of base layer.

In this paper we apply a variational method for exact location of each of the zeros of the dispersion equation which correspond to the leaky modes of waveguides, by using of the exact analytical eigenfunctions.

The buffered leaky planar waveguides are obtained by placing a buffer material with a lower refractive index between the waveguiding structure and the high-index low-cost silicon substrate [3]. The scalar-wave equation for a buffered leaky planar waveguide is given by

$$\frac{d^2\psi(x)}{dx^2} + k^2 n^2(x)\psi(x) = \beta^2\psi(x), \quad (1)$$

where  $\beta$  is the propagation constant,  $k$  is the free space wave number,  $n(x)$  is the refractive index profile

$$n(x) = \begin{cases} n_1, & \text{for } d_3 \leq x \leq d_1, d_3 = -d_1, d_1 > 0, \\ n_2, & \text{for } d_1 < x \leq d_2, d_2 > 0, \\ n_3, & \text{for } d_2 < x < \infty, \\ n_4, & \text{for } d_4 < x < d_3, d_4 < 0, \\ n_5, & \text{for } -\infty < x < d_4. \end{cases} \quad (2)$$

$n_1, n_2, n_3, n_4$  and  $n_5$  are the refractive indices of the core, SiO<sub>2</sub> buffer, Si substrate, SiO<sub>2</sub> by PECVD cladding and air cladding, respectively ( $n_3 > n_1 > n_4 > n_2 > n_5$ ),  $d_1 - d_3, d_2 - d_1$ , semi-infinite,  $d_3 - d_4$ , and semi-infinite are the thickness of these layers, respectively. The effective index  $\beta/k$  for the TE and TM modes can be found from the dispersion equation which is obtained by applying the boundary conditions at the interfaces between different layers.

## 2. The variational method - TE modes

In what follows we illustrate the application of the variational method to a five-layer slab waveguide that allow exact analytical solutions (the one-dimensional scalar-wave equation case). For TE modes,  $\psi = E_y$  and

$$\frac{\partial\psi}{\partial x}$$

are continuous at each interface of the waveguide.

The variational exact solution (Eq. (1) can be written as an eigenvalue equation) of the scalar wave Eq. (1) is found from the functional (see, for example [4])

$$J_{11} = \int_{-\infty}^{d_1} [-f_1'^2 + (kn_5f_1)^2] dx + \int_{d_1}^{d_2} [-f_2'^2 + (kn_4f_2)^2] dx + \int_{d_2}^{d_3} [-f_3'^2 + (kn_1f_3)^2] dx + \int_{d_3}^{d_4} [-f_4'^2 + (kn_2f_4)^2] dx + \int_{d_4}^{\infty} [-f_5'^2 + (kn_3f_5)^2] dx, \tag{3}$$

subject to the constraint that

$$I_{11} = \int_{-\infty}^{d_1} f_1^2 dx + \int_{d_1}^{d_2} f_2^2 dx + \int_{d_2}^{d_3} f_3^2 dx + \int_{d_3}^{d_4} f_4^2 dx + \int_{d_4}^{\infty} f_5^2 dx, \quad \beta^2 = \frac{J_{11}}{I_{11}}, \tag{4}$$

where the exact function is given by

$$\begin{aligned} f_1(x) &= A_c \frac{2\alpha_4}{\alpha_4 - \alpha_5} \exp(-d_4\alpha_4 - \alpha_5d_4 + \alpha_5x), & x < d_4, \\ f_2(x) &= A_c \left[ \frac{\alpha_4 + \alpha_5}{\alpha_4 - \alpha_5} \exp(-2d_4\alpha_4 + \alpha_4x) + \exp(-\alpha_4x) \right], & d_4 < x < d_3, \\ f_3(x) &= \cos(\alpha_1x + \frac{\phi_s - \phi_c - m\pi}{2}), & d_3 \leq x \leq d_1, m = 0,1,2,\dots, \\ f_4(x) &= A_s \left[ \frac{\alpha_2 + \alpha_3}{\alpha_2 - \alpha_3} \exp(2d_2\alpha_2 - \alpha_2x) + \exp(\alpha_2x) \right], & d_1 < x < d_2, \\ f_5(x) &= A_s \frac{2\alpha_2}{\alpha_2 - \alpha_3} \exp(d_2\alpha_2 + \alpha_3d_2 - \alpha_3x), & x > d_2, \end{aligned} \tag{5}$$

And

$$\begin{aligned} \alpha_1 &= \sqrt{(n_1k)^2 - \beta^2}, \alpha_3 = \pm \sqrt{\beta^2 - (n_3k)^2}, \alpha_2 = \sqrt{\beta^2 - (n_2k)^2}, \\ \alpha_4 &= \sqrt{\beta^2 - (n_4k)^2}, \alpha_5 = \sqrt{\beta^2 - (n_5k)^2}, \end{aligned} \tag{6}$$

$$\phi_s = \arctan \left[ \frac{\alpha_2\alpha_3 + \alpha_2^2 \tanh[\alpha_2(d_2 - d_1)]}{\alpha_1\alpha_2 + \alpha_1\alpha_3 \tanh[\alpha_2(d_2 - d_1)]} \right], \tag{7}$$

$$\phi_c = \arctan \left[ \frac{\alpha_4\alpha_5 + \alpha_4^2 \tanh[\alpha_4(d_3 - d_4)]}{\alpha_1\alpha_4 + \alpha_1\alpha_5 \tanh[\alpha_4(d_3 - d_4)]} \right], \tag{8}$$

$$A_s = \frac{(\alpha_2 - \alpha_3) \cos(\alpha_1d_1 + \frac{\phi_s - \phi_c - m\pi}{2}) \exp(-\alpha_2d_1)}{(\alpha_2 + \alpha_3) \exp(2\alpha_2(d_2 - d_1)) + (\alpha_2 - \alpha_3)}, \tag{9}$$

$$A_c = \frac{(\alpha_4 - \alpha_5) \cos(\alpha_1d_3 + \frac{\phi_s - \phi_c - m\pi}{2}) \exp(\alpha_4d_3)}{(\alpha_4 + \alpha_5) \exp(2\alpha_4(d_3 - d_4)) + (\alpha_4 - \alpha_5)}, \tag{10}$$

The minus sign for  $\alpha_3$  corresponds to the leaky modes in substrate. The integrals in equations (3-4) with the chosen exact functions are evaluated analytically to reduce the amount of numerical computation. The solutions of the equation

$$\frac{J_{11}}{I_{11}} - \beta^2 = 0 \tag{11}$$

give the propagation constants  $\beta$  and the effective index  $\beta/k$  of the waveguide. Then the field distributions can be evaluated. The values of  $\beta$  which correspond to maxima of the real part of  $J_{11}/I_{11}$  can be used as initial guesses for complex root searching. Also, we can use the Muller's method [5] to solve the equation (11), since the three initial guesses are highly sensitive to search the solution for complex roots. An alternative method that is competitive or superior (due to its insensitivity to initial guesses and high speed of convergence) to Muller's method is Davidenko's method [6]. Davidenko's method transforms a set of coupled nonlinear algebraic equations into a set of two coupled first-order ordinary differential equations in terms of the real and imaginary parts of the complex root and with a dummy variable  $t$ . The solution is reached when  $t$  is very large ( $t \rightarrow \infty$ ).

Mehrany, Khorasani and Rashidian [2] used a different variational scheme where the functional of the form

$$J = -\frac{1}{2} + \frac{1}{2} \text{Re}(R_s R_c) = -\frac{1}{2} + \frac{1}{2} \cos [2(\phi_s + \phi_c - 2\alpha_1d_1)] \tag{12}$$

dependent on the reflection coefficients

$$R_s = \exp(2j(\phi_s - \alpha_1d_1)), R_c = \exp(2j(\phi_c + \alpha_1d_3)), d_3 = -d_1, \tag{13}$$

is based on a modification of the dispersion equation (see also [7,8])

$$2\alpha_1d_1 - \phi_s - \phi_c = m\pi, m = 0,1,2,\dots, \tag{14}$$

The effective indices are derived from the local minima of this functional and are insensitive to the choice of base layer.

Another dispersion relation of five-layer waveguide [7]

$$\alpha_3m_{22} + \alpha_5m_{11} - m_{21} - m_{12}\alpha_5\alpha_3 = 0 \tag{15}$$

is based on the transfer matrix method. Here,

$$M = M_1M_2M_3 = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}, \tag{16}$$

$$M_1 = \begin{pmatrix} \cos[\alpha_4(d_3 - d_4)] & -\frac{\sin[\alpha_4(d_3 - d_4)]}{\alpha_4} \\ \alpha_4 \sin[\alpha_4(d_3 - d_4)] & \cos[\alpha_4(d_3 - d_4)] \end{pmatrix}, \quad (17)$$

$$M_2 = \begin{pmatrix} \cos[\alpha_1(d_1 - d_3)] & -\frac{\sin[\alpha_1(d_1 - d_3)]}{\alpha_1} \\ \alpha_1 \sin[\alpha_1(d_1 - d_3)] & \cos[\alpha_1(d_1 - d_3)] \end{pmatrix}, \quad (18)$$

$$M_3 = \begin{pmatrix} \cos[\alpha_2(d_2 - d_1)] & -\frac{\sin[\alpha_2(d_2 - d_1)]}{\alpha_2} \\ \alpha_2 \sin[\alpha_2(d_2 - d_1)] & \cos[\alpha_2(d_2 - d_1)] \end{pmatrix}, \quad (19)$$

A different dispersion equation [9]

$$A_4 + \alpha_3 = 0, \quad (20)$$

where

$$A_2 = -\alpha_4 \tan \left[ \alpha_4(d_3 - d_4) - \arctan \left[ \frac{\alpha_5}{\alpha_4} \right] \right], \quad (21)$$

$$A_3 = -\alpha_1 \tan \left[ \alpha_1(d_1 - d_3) - \arctan \left[ \frac{A_2}{\alpha_1} \right] \right], \quad (22)$$

$$A_4 = -\alpha_2 \tan \left[ \alpha_2(d_2 - d_1) - \arctan \left[ \frac{A_3}{\alpha_2} \right] \right], \quad (23)$$

is based on an analytical Runge-Kutta method. It is possible to increase the efficiency for searching solutions of the propagation constants by simultaneously solving of the equations (11), (14), (15) and (20).

### 3. The variational method - TM modes

The above procedure can be extended to the TM modes where  $\psi = H_y$  and  $\frac{1}{n^2} \frac{\partial \psi}{\partial x}$  are continuous at

each interface of the waveguide. The variational exact solution for TM modes is found from the functional

$$J_{11} = \int_{-\infty}^{d_1} \left[ -\frac{1}{n_5^2} f_1'^2 + (kf_1)^2 \right] dx + \int_{d_1}^{d_2} \left[ -\frac{1}{n_4^2} f_2'^2 + (kf_2)^2 \right] dx + \int_{d_2}^{d_3} \left[ -\frac{1}{n_3^2} f_3'^2 + (kf_3)^2 \right] dx + \int_{d_3}^{d_4} \left[ -\frac{1}{n_2^2} f_4'^2 + (kf_4)^2 \right] dx + \int_{d_4}^{\infty} \left[ -\frac{1}{n_1^2} f_5'^2 + (kf_5)^2 \right] dx, \quad (24)$$

subject to the constraint that

$$I_{11} = \int_{-\infty}^{d_4} \frac{1}{n_5^2} f_1^2 dx + \int_{d_4}^{d_3} \frac{1}{n_4^2} f_2^2 dx + \int_{d_3}^{d_1} \frac{1}{n_3^2} f_3^2 dx + \int_{d_1}^{d_2} \frac{1}{n_2^2} f_4^2 dx + \int_{d_2}^{\infty} \frac{1}{n_1^2} f_5^2 dx, \quad \beta^2 = \frac{J_{11}}{I_{11}} \quad (25)$$

where the exact function is given by

$$f_1(x) = A_c \frac{2\alpha_4 n_5^2}{\alpha_4 n_5^2 - \alpha_5 n_4^2} \exp(-d_4 \alpha_4 - \alpha_5 d_4 + \alpha_5 x), \quad x < d_4, \\ f_2(x) = A_c \left[ \frac{\alpha_4 n_5^2 + \alpha_5 n_4^2}{\alpha_4 n_5^2 - \alpha_5 n_4^2} \exp(-2d_4 \alpha_4 + \alpha_4 x) + \exp(-\alpha_4 x) \right], \quad d_4 < x < d_3, \\ f_3(x) = \cos(\alpha_1 x + \frac{\phi_s - \phi_c - m\pi}{2}), \quad d_3 \leq x \leq d_1, m = 0, 1, 2, \dots, \\ f_4(x) = A_s \left[ \frac{\alpha_2 n_3^2 + \alpha_3 n_2^2}{\alpha_2 n_3^2 - \alpha_3 n_2^2} \exp(2d_2 \alpha_2 - \alpha_2 x) + \exp(\alpha_2 x) \right], \quad d_1 < x < d_2, \\ f_5(x) = A_s \frac{2\alpha_2 n_3^2}{\alpha_2 n_3^2 - \alpha_3 n_2^2} \exp(d_2 \alpha_2 + \alpha_3 d_2 - \alpha_3 x), \quad x > d_2, \quad (26)$$

and

$$\alpha_1 = \sqrt{(n_1 k)^2 - \beta^2}, \alpha_3 = \pm \sqrt{\beta^2 - (n_3 k)^2}, \alpha_2 = \sqrt{\beta^2 - (n_2 k)^2}, \\ \alpha_4 = \sqrt{\beta^2 - (n_4 k)^2}, \alpha_5 = \sqrt{\beta^2 - (n_5 k)^2}, \quad (27)$$

$$\phi_s = \arctan \left[ \frac{\alpha_2 \alpha_3 n_1^2 n_2^2 + \alpha_2^2 n_1^2 n_3^2 \tanh[\alpha_2(d_2 - d_1)]}{\alpha_1 \alpha_2 n_2^2 n_3^2 + \alpha_1 \alpha_3 n_2^2 n_2^2 \tanh[\alpha_2(d_2 - d_1)]} \right], \quad (28)$$

$$\phi_c = \arctan \left[ \frac{\alpha_4 \alpha_5 n_1^2 n_4^2 + \alpha_4^2 n_1^2 n_5^2 \tanh[\alpha_4(d_3 - d_4)]}{\alpha_1 \alpha_4 n_4^2 n_5^2 + \alpha_1 \alpha_5 n_4^2 n_4^2 \tanh[\alpha_4(d_3 - d_4)]} \right], \quad (29)$$

$$A_s = \frac{(\alpha_2 n_3^2 - \alpha_3 n_2^2) \cos(\alpha_1 d_1 + \frac{\phi_s - \phi_c - m\pi}{2}) \exp(-\alpha_2 d_1)}{(\alpha_2 n_3^2 + \alpha_3 n_2^2) \exp(2\alpha_2(d_2 - d_1)) + (\alpha_2 n_3^2 - \alpha_3 n_2^2)}, \quad (30)$$

$$A_c = \frac{(\alpha_4 n_5^2 - \alpha_5 n_4^2) \cos(\alpha_1 d_3 + \frac{\phi_s - \phi_c - m\pi}{2}) \exp(\alpha_4 d_3)}{(\alpha_4 n_5^2 + \alpha_5 n_4^2) \exp(2\alpha_4(d_3 - d_4)) + (\alpha_4 n_5^2 - \alpha_5 n_4^2)}, \quad (31)$$

The integrals in equations (24-25) with the chosen exact functions are evaluated analytically to reduce the amount of numerical computation.

**4. Numerical results and conclusions**

An illustration of the maximum of the real part of  $J_{11}/I_{11}$  (4) in the variational method and zeros of the dispersion equation (14) for the  $TE_0$  mode of the buffered leaky planar waveguide ( $d_1 = 0.07\mu\text{m}$ ,  $d_2 = 1.07\mu\text{m}$ ,  $d_3 = -0.07\mu\text{m}$ ,  $d_4 = -1.07\mu\text{m}$ ,  $n_1 = 1.98$ ,  $n_2 = 1.45$ ,  $n_3 = 3.476$ ,  $n_4 = 1.464$ ,  $n_5 = 1$ ,  $\lambda = 1.55\mu\text{m}$ ) are shown in Fig.1. Fig. 2. shows the zeros of the dispersion equation (4) in our variational method and the variational

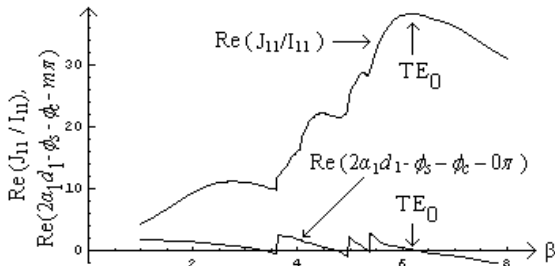


Fig. 1. Illustration of the maxima of the real part of  $J_{11}/I_{11}$  (4) in our variational method and zeros of the dispersion equation (14) for the  $TE_0$  mode of the buffered leaky waveguide.

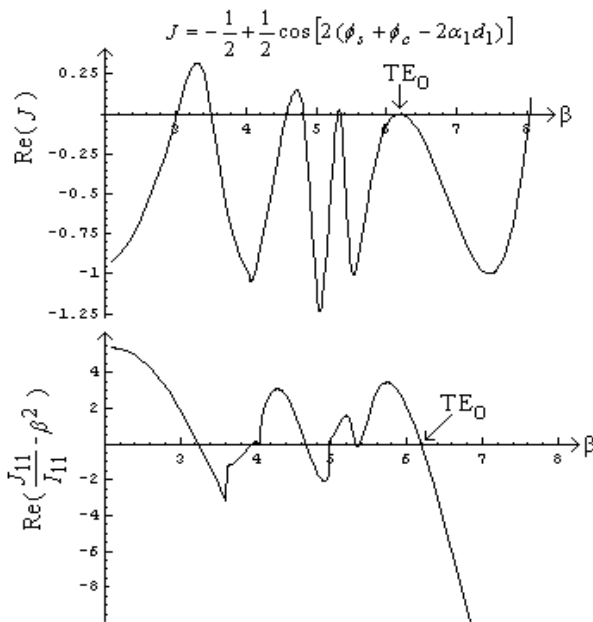


Fig. 2. Illustration of zeros of the dispersion equation (4) in our variational method and the variational functional  $J$  (12) based on reflection coefficients for the  $TE_0$  mode of the buffered leaky waveguide.

functional  $J$  (12) based on reflection coefficients for the  $TE_0$  mode of the same buffered leaky waveguide. Fig. 3. shows the zeros of the dispersion equations (20) based on an analytical Runge-Kutta method [8] and (15) based on

the transfer matrix method for the  $TE_0$  mode of the same buffered leaky waveguide. Fig.4. shows the real (-) and imaginary (-) solutions and their initial guesses in the Davidenko's method. This algorithm has exponential convergence with respect to the dummy variable  $t$  and gives very good results for the initial guesses that are very far from the exact values. Only the dispersion equation (4) in our variational method gives the same result as the Davidenko's method for initial  $\beta_0 = 100 + 0j$ . The numerical results of the propagation constant  $\beta = 6.1892610225 - 0.0031220002j$  and the effective index  $\beta/k = 1.5268298030 - 0.0007701667j$  for  $TE_0$  mode are in agreement with the previously published values [3].

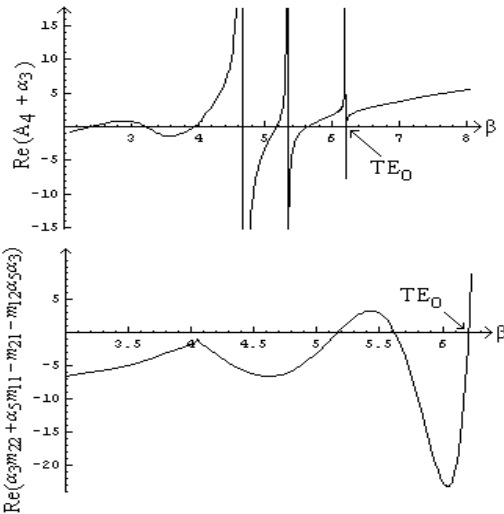


Fig. 3. Illustration of zeros of the dispersion equations (20) based on an analytical Runge-Kutta method and (15) based on the transfer matrix method for the  $TE_0$  mode of the buffered leaky waveguide.

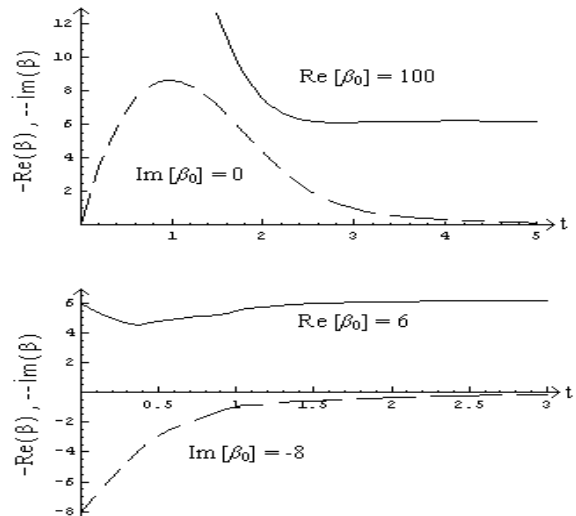


Fig.4. The real (-) and imaginary (-) solutions and their initial guesses in the Davidenko's method.

We can see a distinct oscillatory behavior for the dispersion equations in the region of their roots and thus a different optimum initial guess for each of their zeros. The values of  $\beta$  which correspond to maxima of the real part of  $J_{11}/I_{11}$  are very good initial guesses for complex root searching of the associated dispersion equation (11).

This variational method can be used for a better understanding of the effects of addition of a low-index buffer layer over a high substrate on the propagation characteristics of the waveguide.

### References

- [1] C. Chen, P. Berini, D. Feng, S. Tanev, V. P. Tzolov, *Optics Express* **7**, 260 (2000)
- [2] K. Mehrany, S. Khorasani, B. Rashidian, *J. Opt. Soc. Am. B* **19**, 1978 (2002)
- [3] H. P. Uranus, H. J. W. M. Hoekstra, E. van Groesen, *Optics Commun.* **253**, 99 (2005)
- [4] R. A. Sammut and C. Pask, *J. Opt. Soc. Am. B* **8**, 395 (1991)
- [5] C-C. Chou and N-H. Sun, *J. Opt. Soc. Am. B* **25**, 545 (2008)
- [6] S. H. Talisa, *IEEE Trans. Microwave Theory Tech.* **MTT-33**, 967 (1985)
- [7] T. Tamir (Ed.), *Guided-wave Optoelectronics*, Springer Verlag, Berlin, 1990
- [8] C. L. Bonner, T. Bhutta, D. D. Shepherd, A. C. Tropper, *IEEE J. Quantum Electron.* **36**, 236 (2000)
- [9] V. A. Popescu, *Optics Commun.* **271**, 96 (2007)

\*Corresponding author: [cripoco@physics.pub.ro](mailto:cripoco@physics.pub.ro)