Complex modes and instability of full-vectorial beam propagation methods

Huan Xie[1], Wangtao Lu[2], and Ya Yan Lu[1,*]

[1] *Department of Mathematics, City University of Hong Kong, Kowloon, Hong Kong*
[2] *Joint Advanced Research Center of University of Science and Technology of China and City University of Hong Kong, Suzhou, Jiangsu, China*
[*] *Corresponding author: mayylu@cityu.edu.hk*

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Full-vectorial beam propagation methods (FVBPMs) are widely used to model light waves propagating in high index-contrast optical waveguides. We show that the paraxial FVBPM and the wide-angle FVBPMs based on diagonal Padé approximants are unstable analytically for waveguides with complex modes. The instability cannot be removed by enlarging the computational domain, increasing the numerical resolution or using the perfectly matched layers, since the complex modes are highly confined around the waveguide core.

The beam propagation method (BPM) [1] is a popular method for simulating lightwaves in slowly varying optical waveguides. In recent years, waveguides with high index-contrast have found important applications in integrated optics. For these waveguides, the full-vectorial BPM (FVBPM) [2] is necessary, since the scalar model (based on the weakly guiding approximation) and the semi-vectorial models are no longer accurate. The simplest FVBPM is the paraxial FVBPM which can be efficiently solved by the alternating direction implicit method [3]. The paraxial FVBPM is widely used because it is efficient.

However, the paraxial FVBPM often show instabilities in numerical simulations even in straight waveguides. Yevick *et al.* [4–6] pointed out that the instability is caused by eigenmodes with complex propagation constants and it is possible to suppress the instability by special wide-angle FVBPMs [5]. In [4–6], the existence of complex propagation constants is established by numerical calculations where the transverse domain is truncated by perfect electric (or magnetic) conductor boundaries. The properties of these modes with complex propagation constants are not very clear, since some of these calculations are based on low-resolution discretizations. Furthermore, it is not clear whether the instability is numerical or analytic, whether the instability will disappear when a higher resolution discretization in a larger transverse domain is used. In recent years, the perfectly matched layer (PML) technique [7] is widely used to truncate domains for wave propagation problems, it is natural to ask whether a PML will stabilize the paraxial FVBPM.

The purpose of this Letter is to show that the instability of the paraxial FVBPM is analytic and it is caused by complex modes that are highly confined around dielectric interfaces and the waveguide core. Complex modes are true waveguide modes (not leaky modes or numerical artifacts) with complex propagation constants, and they are well-known for waveguides with closed boundaries [8]. For open waveguides, Jabłoński first showed the existence of complex modes for a waveguide with a circular core [9]. Numerically, the instability caused by a complex mode may be apparent only when the resolution (for discretizing the transverse plane) is sufficiently high, since a coarse discretization may fail to resolve the highly confined field pattern of the complex mode. The PML technique cannot stabilize the paraxial FVBPM since it should not be used very close to the waveguide core.

For a lossless dielectric waveguide with its axis in the z direction and a real refractive index profile $n(x, y)$, the frequency domain Maxwell's equations can be rigorously reduced to $\partial_z^2 \boldsymbol{u} + \boldsymbol{A}\boldsymbol{u} = 0$, where $\boldsymbol{u} = [H_y, -H_x]^T$ is the column vector of the transverse magnetic field components, $\boldsymbol{A}$ is a 2×2 matrix with entries

$$A_{11} = \varepsilon\partial_x(\varepsilon^{-1}\partial_x \cdot) + \partial_y^2 + k_0^2\varepsilon, \quad (1)$$

$$A_{12} = \varepsilon\partial_x(\varepsilon^{-1}\partial_y \cdot) - \partial_{xy}^2, \quad (2)$$

$$A_{21} = \varepsilon\partial_y(\varepsilon^{-1}\partial_x \cdot) - \partial_{yx}^2, \quad (3)$$

$$A_{22} = \varepsilon\partial_y(\varepsilon^{-1}\partial_y \cdot) + \partial_x^2 + k_0^2\varepsilon, \quad (4)$$

k_0 is the free space wavenumber and $\varepsilon = n^2$. For a waveguide mode, the z dependence can be separated, then $\boldsymbol{u} = \boldsymbol{\phi} e^{i\beta z}$ and $\boldsymbol{\phi}$ satisfies the eigenvalue problem

$$\boldsymbol{A}\boldsymbol{\phi} = \beta^2\boldsymbol{\phi}. \quad (5)$$

A guided mode satisfies (5) for a real β and $\boldsymbol{\phi} \to \boldsymbol{0}$ exponentially as $|\boldsymbol{r}| \to \infty$, where $\boldsymbol{r} = (x, y)$. A complex mode also decays to zero exponentially as $|\boldsymbol{r}|$ goes to infinity, but the eigenvalue β^2 is complex. It is not to be confused with a leaky mode for which β^2 is also complex, but the field satisfies an outgoing radiation condition and blows up as $|\boldsymbol{r}| \to \infty$. For a closed waveguide (for example, with perfect electric conductor walls), there is an infinite sequence of eigenmodes. Since $\boldsymbol{A}$ is not self-adjoint, it is natural to have some complex eigenvalues. For open waveguides, the waveguide cross section is the entire xy plane, the number of guided modes is usually finite, since there is also a continuous spectrum for the radiation and evanescent waves. Evanescent waves with real negative β^2 (pure imaginary β) are not regarded as complex modes here, since their field patterns are standing waves at infinity. Therefore for open waveguides, the existence of complex modes is not obvious.

Complex modes for open waveguides are first found for waveguides with a circular core [9]. In the following, we show two examples. The first waveguide is shown in

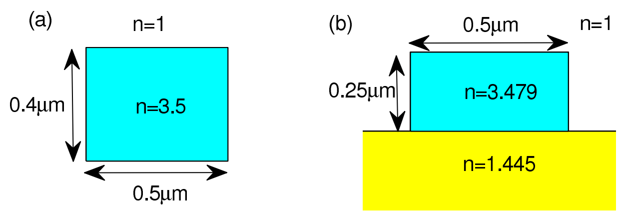

Fig. 1. Two open waveguides.

Fig. 1(a). It has a $0.5\mu\text{m}\times 0.4\mu\text{m}$ rectangular core with a refractive index $n = 3.5$ and it is surrounded by air ($n = 1$). Based on a finite difference method [10] with a non-uniform mesh and a recently developed boundary integral equation method [11], we find a complex mode with a propagation constant $\beta = 2.7114055{+}18.3497078i$ $(\mu\text{m})^{-1}$ for free space wavelength $\lambda = 1\mu\text{m}$. The transverse magnetic field patterns of the complex mode are shown in Fig. 2. Clearly, it is highly localized around

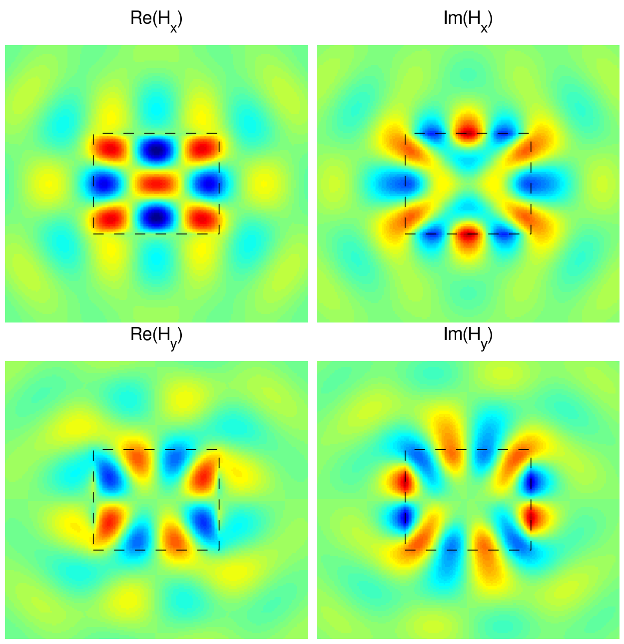

Fig. 2. Transverse magnetic field patterns of a complex mode for a waveguide (a) in Fig. 1.

the waveguide core. The second waveguide is shown in Fig. 1(b). It has a $0.5\mu\text{m}\times 0.25\mu\text{m}$ core with a refractive index $n = 3.479$, a substrate with a refractive index $n = 1.445$, and the covering medium is air. Using the same numerical methods, we obtain a complex mode with $\beta = 1.1398 + 14.0440i$ $(\mu\text{m})^{-1}$ for free space wavelength $\lambda = 1.52\mu\text{m}$. The field patterns of the complex mode are shown in Fig. 3.

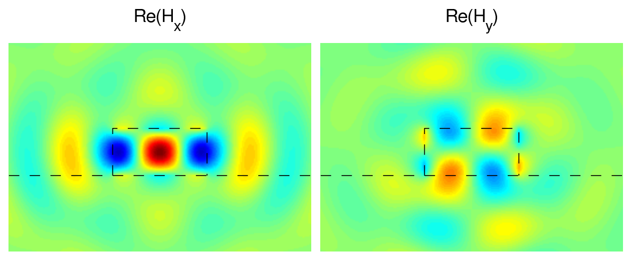

Fig. 3. Transverse magnetic field patterns of a complex mode for waveguide (b) in Fig. 1.

Since we consider lossless waveguides, complex eigenvalues of (5) show up in complex conjugate pairs: β^2 and $\overline{\beta^2}$. When β is selected from the two square roots of β^2 in the complex plane, we require that the mode with the z dependence $e^{i\beta z}$ (and time dependence $e^{-i\omega t}$ for an angular frequency ω) is valid as $z \to +\infty$. Since a physically correct mode should be bounded when z tends to infinity, we must choose a complex β such that $\text{Im}(\beta) > 0$. Let $\beta_1 = a + ib$ $(b > 0)$ be the propagation constant of a complex mode, since $\overline{\beta_1^2}$ is also an eigenvalue of (5), we have another complex mode with the propagation constant $\beta_2 = -a + ib$ for $z > 0$. The eigenfunction of the second mode is simply the complex conjugate of first mode. The complex modes decay exponentially as $z \to \infty$, but they are needed in mode expansion methods for analyzing waveguide discontinuities.

The paraxial BPM is usually derived from the slowly varying envelope approximation for slowly varying waveguides. For a reference refractive index n_*, we define the envelope $\boldsymbol{\psi}$ by $\boldsymbol{u} = \boldsymbol{\psi} e^{ik_0 n_* z}$ and a matrix operator $\boldsymbol{X}$ by $\boldsymbol{A} = k_0^2 n_*^2 (I + \boldsymbol{X})$, where $\boldsymbol{A}$ is given earlier and I is the 2×2 identity matrix. The paraxial FVBPM is the first order evolution equation

$$\partial_z \boldsymbol{\psi} = \frac{ik_0 n_*}{2} \boldsymbol{X}\, \boldsymbol{\psi}. \tag{6}$$

We consider the paraxial FVBPM for a z-invariant waveguide. If $\{\beta, \boldsymbol{\phi}\}$ is a solution of the eigenvalue problem (5), we solve Eq. (6) with the starting field $\boldsymbol{\psi}|_{z=0} = \boldsymbol{\phi}$. The solution is $\boldsymbol{\psi} = \boldsymbol{\phi}\exp(ik_0 n_* \mu z/2)$ for $\mu = \beta^2/(k_0 n_*)^2 - 1$. This leads to

$$\boldsymbol{u} = \boldsymbol{\phi} \exp\left[iz(\beta^2 + k_0^2 n_*^2)/(2k_0 n_*)\right], \quad z > 0. \tag{7}$$

The above can be written as

$$\boldsymbol{u} = \boldsymbol{\phi} e^{i\beta z} \exp\left[iz(\beta - k_0 n_*)^2/(2k_0 n_*)\right], \quad z > 0. \tag{8}$$

If $\{\beta_0, \boldsymbol{\phi}_0\}$ is a guided mode with $\beta_0 > 0$, the exact solution with $\boldsymbol{\phi}_0$ as the starting field is $\boldsymbol{u} = \boldsymbol{\phi}_0 e^{i\beta_0 z}$. If we compare it with the solution given above, we can see that the paraxial FVBPM is exactly correct if the reference refractive index satisfies $n_* = \beta_0/k_0$, and it produces a phase error that grows linearly with z if $n_* \neq \beta_0/k_0$.

Once n_* is fixed at or around β_0/k_0, Eq. (6) will not be accurate for any other modes. For the first complex mode β_1 (the corresponding eigenfunction is $\boldsymbol{\phi}_1$) where $\mathrm{Im}(\beta_1^2) > 0$, if $\boldsymbol{\phi}_1$ is used as the starting field, the paraxial FVBPM solution (7) decays exponentially as $z \to \infty$. However, solution (7) clearly blows up at infinity for the second complex mode with $\beta_2^2 = \overline{\beta_1^2}$ and $\boldsymbol{\phi}_2 = \overline{\boldsymbol{\phi}}_1$, if $\boldsymbol{\phi}_2$ is the starting field. In general, if the starting field is slightly perturbed from the guided mode $\boldsymbol{\phi}_0$ and the perturbation contains a component in $\boldsymbol{\phi}_2$, then the solution of (6) blows up as $z \to +\infty$. Therefore, when there are complex modes, the paraxial FVBPM is unstable analytically.

The instability of the FVBPM is actually used to calculate the complex modes for the two examples above. Based on a starting field with a Gaussian profile, we propagate the field by solving Eq. (6) with the Crank-Nicolson method. The transverse plane and the operator $\boldsymbol{X}$ are discretized by a finite difference method with a non-uniform mesh [10]. After propagating some distance in z, the complex mode $\boldsymbol{\phi}_2$ dominates the field. A rough approximation for $\boldsymbol{\phi}_2$ is obtained by rescaling the field. Using this as the first iteration, more accurate solutions are obtained by solving the discretized version of (5) with the Rayleigh quotient iteration scheme and by the boundary integral equation method [11].

Wide-angle BPMs [12] have been developed to extend the capability of the paraxial BPM. The starting point of existing wide-angle FVBPMs [4, 5, 13, 14] is the ideal one-way equation

$$\partial_z \boldsymbol{\psi} = ik_0 n_* (\sqrt{I + \boldsymbol{X}} - I)\boldsymbol{\psi}, \tag{9}$$

where the square root operator $\sqrt{I + \boldsymbol{X}}$ must be defined such that Eq. (9) gives only outgoing or exponentially decaying solutions as $z \to +\infty$. The first family of wide-angle FVBPMs can be written as

$$\partial_z \boldsymbol{\psi} = ik_0 n_* [R(\boldsymbol{X}) - I]\, \boldsymbol{\psi}, \tag{10}$$

where $R(\xi)$ is a rational approximation of $\sqrt{1+\xi}$. If $\{\beta, \boldsymbol{\phi}\}$ is a waveguide mode and if the starting field is $\boldsymbol{\phi}$, then Eq. (10) gives $\boldsymbol{\psi} = \boldsymbol{\phi}\ \exp\{ik_0 n_*[R(\mu) - 1]z\}$, for $\mu = \beta^2/(k_0 n_*)^2 - 1$. In particular, $R(\xi)$ may be a diagonal Padé approximant of $\sqrt{1+\xi}$, where the numerator and the denominator of $R(\xi)$ are polynomials of ξ with the same degree. In that case, $R(\xi)$ is real for any real ξ. This implies that (10) will not be able to suppress the evanescent waves corresponding to $\beta^2 < 0$ or $\mu < -1$. More importantly, for the complex mode $\{\beta_2, \boldsymbol{\phi}_2\}$ with $\mathrm{Im}(\beta_2^2) < 0$, we have $\mathrm{Im}\, R(\mu_2) < 0$ (μ_2 is related to β_2^2 as before), then Eq. (10) is unstable since it blows up as $z \to +\infty$ if the starting field is $\boldsymbol{\phi}_2$.

The second family of wide-angle FVBPMs first discretizes (9) as $\boldsymbol{\psi}_{j+1} = \exp[is(\sqrt{I+\boldsymbol{X}} - I)]\boldsymbol{\psi}_j$, where $\boldsymbol{\psi}_j$ and $\boldsymbol{\psi}_{j+1}$ denote $\boldsymbol{\psi}$ at z_j and $z_{j+1} = z_j + \Delta z$ respectively, and $s = k_0 n_* \Delta z$, then approximates the exponential of the square root operator such that

$$\boldsymbol{\psi}_{j+1} = Q(\boldsymbol{X}, s)\, \boldsymbol{\psi}_j. \tag{11}$$

Here, $Q(\xi, s)$ is a rational function of ξ that approximates $\exp[is(\sqrt{1+\xi} - 1)]$. As before, if $Q(\xi, s)$ is a diagonal Padé approximant, then $|Q(\mu, s)| = 1$ for all real μ and $|Q(\mu_2, s)| > 1$ if $\mathrm{Im}(\mu_2) < 0$. Therefore, Eq. (11) incorrectly propagates the evanescent waves and is unstable for the complex mode $\{\beta_2, \boldsymbol{\phi}_2\}$. Stable wide-angle FVBPMs of both families are discussed in [5, 13, 14].

In summary, we show complex modes for two high index-contrast dielectric waveguides, and explain that the paraxial FVBPM and the wide-angle FVBPMs based on diagonal Padé approximants are unstable analytically due to the complex modes which are highly confined near the waveguide core. The instability cannot be cured by a higher resolution numerical discretization, a larger computational domain or the use of a PML. Stable FVBPM can be developed for the wide-angle version using special rational approximants to suppress the complex modes. However, these wide-angle FVBPMs are more expensive to implement.

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