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A construction of Beam Propagation Methods for optical waveguides

Xavier Antoine*, Pierre Dreyfuss†, Karim Ramdani‡

Abstract. This paper presents a systematic method to derive Beam Propagation Models for optical waveguides. The technique is based on the use of the symbolic calculus rules for pseudodifferential operators. The cases of straight and bent optical waveguides are successively considered.

Keywords. Bent Waveguides; Beam Propagation Method; Optics

1 Introduction

Complex optical waveguides play a key role in the design of optical communications systems and integrated optical circuits [13]. In many applications, the waveguides considered are not uniform in the propagating direction, called the z -direction in this paper (inhomogeneous structures, bent waveguides e.g.). In order to simulate numerically such optical devices, one can truncate the structure in the transverse x -variable by using for example a Perfectly Matched Layer (see e.g. [11]). Since the length of the waveguide (of the order of the millimeter) is much larger than the free space wavelength λ_0 (of the order of the micrometer), a numerical simulation remains extremely costly. This is the reason why approximate efficient models like Beam Propagation Methods (BPMs) have been introduced [13]. The idea is to solve a propagation equation in the z -direction (which in some sense is considered as a time variable) with an initial condition at $z = 0$ fixed by the incident wave field. Then, all the difficulty is to built accurate BPMs for complex situations. Let us remark that similar

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problems and techniques arise in other applications (geophysics [4], acoustics [5, 8] e.g.). A widely used approach is based on a rough approximation of the Helmholtz equation resulting in the so-called Standard BPM which is a Schrödinger-type equation (also called Fresnel equation or Standard Parabolic Equation in electromagnetics [12]). However, increased accuracy is generally required for these models. To this aim, high-order BPMs have been formally proposed in the literature (see Section 2 and references herein). These models have also been numerically validated in [10] for straight waveguides, showing their importance for practical applications. Finally, bent waveguides can formally also be considered. A direction to improve the corresponding BPM is proposed in [14] but remains limited to first-order approximations. The aim of this paper is twofold: 1) we show how these models, which are often obtained formally, can be constructed systematically *via* the symbolic calculus of pseudodifferential operators for straight waveguides with variable refraction index, 2) we extend the formalism to derive high-order BPM models for arbitrary bent waveguides following similar techniques.

The outline of the paper is the following. After recalling the high-order BPMs met in the literature in Section 2, we begin by analyzing in detail the case of a straight waveguide with a smooth (z, x) -variable index. We propose a procedure for recovering these models and to possibly improve them in Section 3. In Section 4, we provide the extension to bent waveguides which are commonly used in applications [3, 15, 16]. This shows in particular the influence of the geometry in the BPM model through e.g. the curvature. This strategy provides the possibility of proposing new BPM models for the full Maxwell's equations using similar techniques for systems [1]. This is an important open problem as noticed in the recent review paper by Lu [13]: "The improved one-way models are also available for the TM case. Unfortunately, they are not available for full-vectorial cases". Finally, Section 5 draws a conclusion.

2 TM energy conserving one-way equations

Let us begin by introducing the Transverse Magnetic (TM) [13] governing equation for planar waveguides

$$n^2 \partial_z \left(\frac{1}{n^2} \partial_z u \right) + n^2 \partial_x \left(\frac{1}{n^2} \partial_x u \right) + k_0^2 n^2 u = 0, \quad (1)$$

where z denotes the propagation direction, k_0 is the reference wavenumber in vacuum and $n(x, z)$ is the refractive index. The time dependence is assumed to be $e^{-i\omega t}$, setting ω as the angular frequency. An incident wave is specified at $z = 0$. The Beam Propagation Method (BPM) approximately solves (1) by computing the solution of a one-way Helmholtz equation. Some specific difficulties arise for the TM polarization problem. In particular, it was shown by Vasallo [21] that neglecting the z -derivatives of the index n leads to the non-conservation of the optical paraxial power

$$P_{TM}(z) = \int \frac{|u|^2}{n^2} dx. \quad (2)$$

Indeed, it is shown in [21] that the resulting approximate fields are then lossy or amplifying, depending on the choice of the index n . This behavior is numerically shown for instance in [17] and a complete discussion is developed in Vasallo's paper [21]. To overcome this drawback, some solutions have been recently proposed by Ho and Lu [10]. The authors introduce formally three different models with increasing order:

- the one-way Helmholtz equation (3)

$$\partial_z u = i \tilde{L}_1(z) u, \quad (3)$$

where $\tilde{L}_1(z)$ is the square-root operator defined by

$$\tilde{L}_1(z) = \sqrt{n^2 \partial_x \left(\frac{1}{n^2} \partial_x \cdot \right) + k_0^2 n^2}, \quad (4)$$

- the energy-conserving model [7]

$$\partial_z u = i \tilde{L}_{2,1}(z) u, \quad (5)$$

setting

$$\tilde{L}_{2,1} = \tilde{L}_1 + i \tilde{L}_1^{-1/2} n \partial_z \left(\frac{1}{n} \tilde{L}_1^{1/2} \right) \quad (6)$$

- the single-scatter approximation

$$\partial_z u = i\tilde{L}_{2,2}(z)u, \quad (7)$$

with

$$\tilde{L}_{2,2} = \tilde{L}_1 + \frac{i}{2}\tilde{L}_1^{-1}n^2\partial_z\left(\frac{1}{n^2}\tilde{L}_1\right). \quad (8)$$

Let us note that models (5) and (7) coincide when L is approximated by a second-order Taylor expansion resulting in the narrow-angle BPM equation. The last two approximations yield an improved accuracy as shown in [10].

3 A construction of BPMs for TM polarization: the straight waveguide

The aim of this part is to show that alternative high-order approximate model equations can be derived *via* the techniques of pseudodifferential operator calculus. For the sake of clarity, we do not detail all the technical aspects and computational elements, but rather outline the main steps of the derivation of our strategy. Besides its systematic character, one further advantage of our technique lies in the fact that it provides the connection between the above three models.

The first step consists in developing the second order operator P involved in (1)

$$P(x, z, \partial_x, \partial_z) = \partial_z^2 + n^2\partial_z\left(\frac{1}{n^2}\right)\partial_z + \partial_x^2 + n^2\partial_x\left(\frac{1}{n^2}\right)\partial_x + k_0^2n^2. \quad (9)$$

Introducing the Fourier covariable ξ of x , the operator $A(x, \partial_x) = n^2\partial_x(n^{-2})\partial_x$ is represented for example by the symbol $a(x, z, \xi) = in^2\partial_x(n^{-2})\xi$ in the Fourier space.

We recall that given a symbol $a = a(x, z, \xi)$, we can define the pseudodifferential operator $A = Op(a)$ through the representation formula [20]

$$A(x, z, \partial_x)u(z, x) = \int a(x, z, \xi)\hat{u}(z, \xi)e^{ix\xi}d\xi, \quad (10)$$

defining $\hat{u}(z, \xi)$ as the partial Fourier transform of u with respect to x . The above formula holds for symbols a which are some \mathcal{C}^∞ -functions satisfying the following inequality

$$|\partial_x^\beta\partial_\xi^\alpha a(x, z, \xi)| \leq C_{\alpha\beta} \langle \xi \rangle^{m-\alpha}, \quad (11)$$

for $\langle \xi \rangle = (1 + |\xi|^2)^{1/2}$, $m \in \mathbb{R}$, for all α and β . Then, in this case, a is said to be in $S_{1,0}^m$ and of order m (see [20] for more details). The corresponding operator A is then of order m , belongs to the class $OPS_{1,0}^m$ and acts in suitable Sobolev spaces [20]. Following this strategy, the partial symbol of P with respect to x is given by

$$p(x, z, \xi, \partial_z) = \partial_z^2 + n^2 \partial_z \left(\frac{1}{n^2} \right) \partial_z - \xi^2 + in^2 \partial_x \left(\frac{1}{n^2} \right) \xi + k_0^2 n^2. \quad (12)$$

The next step is based on the following classical factorization formula [9, 18, 19].

Proposition 1. *There exist two first-order pseudodifferential operators $L^\pm(x, z, \partial_x)$ with total symbols $\ell^\pm(x, z, \xi)$ such that*

$$p \sim (\partial_z - iL^-)(\partial_z - iL^+) \quad \text{mod}(OPS^{-\infty}), \quad (13)$$

where the meaning of the equivalence class \sim is detailed in [20]. The symbols ℓ^\pm admit the following asymptotic expansions

$$\ell^\pm \sim \sum_{j \geq -1}^{+\infty} \ell_{-j}^\pm \quad (14)$$

for symbols $\ell_{-j}^\pm \in S_{1,0}^{-j}$, which are uniquely determined by the condition

$$\ell_1^\pm(x, z, \xi) = \pm \sqrt{k_0^2 n^2 - \xi^2 + in^2 \partial_x (n^{-2}) \xi}. \quad (15)$$

Moreover, the zeroth-order term ℓ_0^+ is

$$\ell_0^+(x, z, \xi) = \frac{i}{2\ell_1^+} \partial_\xi \ell_1^+ \partial_x \ell_1^+ + i \frac{1}{2\ell_1^+} n^2 \partial_z (n^{-2} \ell_1^+). \quad (16)$$

The expression \sqrt{z} designates the principal determination of the square-root of a complex number z , *i.e.* $\Re(\sqrt{z}) > 0$. The pseudodifferential operator calculus assumes that n is a \mathcal{C}^∞ function. However, this assumption can be weakened to handle more general waveguides for example with \mathcal{C}^1 regularity since only first-order z derivatives of n appear in the proposed models. Even if in practical situations the BPM models are used when a (x, z) -discontinuous waveguide is concerned, we see that an adapted symbolic calculus with discontinuous symbols should lead to added contributions. This is however out of the scope of the present paper.

Proof. Let us develop the right hand side of (13)

$$p \sim \partial_z^2 - i(L^+ + L^-) \partial_z - iOp \{ \partial_z \ell^+ \} - L^- L^+ \quad \text{mod}(OPS^{-\infty}) \quad (17)$$

since the symbolic representation of operators based on (10) gives

$$\partial_z L^+ u = Op \{ \partial_z \ell^+ \} u + L^+ \partial_z u. \quad (18)$$

Identifying the operator terms appearing in front of the z -derivatives, one gets the operator system

$$\begin{cases} -i(L^+ + L^-) = n^2 \partial_z (n^{-2}), \\ -i Op \{ \partial_z \ell^+ \} - L^- L^+ = k_0^2 n^2 (1 + X), \end{cases} \quad (19)$$

with X the differential operator defined by

$$X = n^2 \partial_x (n^{-2} \partial_x \cdot) / (k_0^2 n^2), \quad (20)$$

with symbol $\sigma(X)$ given by

$$\sigma(X) = -\xi^2 / (k_0^2 n^2) + i n^2 \partial_x (n^{-2}) \xi / (k_0^2 n^2). \quad (21)$$

In order to obtain an equation for L^+ , we eliminate L^- in the second equation of (19) thanks to the first one and get

$$(L^+)^2 - i n^2 \partial_z (n^{-2}) L^+ - i Op \{ \partial_z \ell^+ \} = k_0^2 n^2 (1 + X). \quad (22)$$

Since L^+ is a first-order pseudodifferential operator, then $Q = (L^+)^2$ is a second-order operator defined as an operator product in $OPS_{1,0}^2$. Therefore, according to the Leibniz composition rule of pseudodifferential operators [20], the symbol $\sigma(Q)$ of the operator Q admits the asymptotic expansion

$$\sigma(Q) \sim \sum_{\alpha \geq 0} \frac{(-i)^\alpha}{\alpha!} \partial_\xi^\alpha \ell^+ \partial_x^\alpha \ell^+. \quad (23)$$

Then, going to the symbolic calculus and considering the symbolic terms of order two in the left hand side of (22) leads to the following calculation of ℓ_1^+

$$\ell_1^+ = \sqrt{k_0^2 n^2 - \xi^2 + i n^2 \partial_x (n^{-2}) \xi}. \quad (24)$$

This choice ensures the uniqueness of the asymptotic expansion (14). Moreover, we also have immediately : $\ell_1^- = -\ell_1^+$ using the first equation of system (19) at the symbolic level.

Now, let us compute the second asymptotic corrective term ℓ_0^+ . This is done by identifying the terms of first order in the left hand side of expression (22) using (23). This yields

$$\ell_0^+ = \frac{i}{2\ell_1^+} \partial_\xi \ell_1^+ \partial_x \ell_1^+ + i \frac{1}{2\ell_1^+} n^2 \partial_z (n^{-2} \ell_1^+) \quad (25)$$

since

$$-in^2\partial_z(n^{-2})L^+ - iOp\{\partial_z\ell^+\} = -iOp(n^2\partial_z(n^{-2}\ell^+)). \quad (26)$$

This ends the proof. \square

By using the principal symbol ℓ_1^+ of L^+ , one gets the TM Beam Propagation equation corresponding to the forward propagating part of the wavefield

$$\partial_z u = iL^+(z)u, \quad z > 0, \quad (27)$$

since it gives an $L_z^2([0; +\infty[)$ finite energy solution. The operator L^- corresponds to the backscattered part of the field. Since we only have L^+ through its asymptotic symbolic expansion (14), an approximation of the forward field can be obtained by considering the following approximate equation of (27)

$$\partial_z u_j = iL_j(z)u_j \quad \text{mod}(OPS^{1-j}), \quad (28)$$

setting L_j as the truncated one-way operator of order $j \geq 1$

$$L_j = Op\left(\sum_{-1 \leq m \leq -2+j} \ell_{-m}^+\right) = L^+ \quad \text{mod}(OPS^{1-j}). \quad (29)$$

The first-order approximation consists therefore in finding the approximate solution u_1 of the forward propagating one-way equation

$$\partial_z u_1 = iL_1(z)u_1 \quad \text{mod}(OPS^0). \quad (30)$$

Let us compare now (30) and (3)-(4). Denoting by $\sigma_m(P)$ the symbol of order m of a pseudodifferential operator P , and since we have the identification

$$\sigma(\tilde{L}_1 \tilde{L}_1) = \sigma(k_0^2 n^2 (1 + X)) = (\ell_1^+)^2, \quad (31)$$

the computation of the principal symbol of order one of \tilde{L}_1 , denoted by $\sigma_1(\tilde{L}_1)$, is equal to ℓ_1^+ by the composition rule of pseudodifferential operators. Therefore, (30) is an approximation of (3)-(4) modulo a pseudodifferential operator of OPS^0 .

A second-order one-way equation is given by

$$\partial_z u_2 = iL_2(z)u_2, \quad z > 0, \quad (32)$$

setting $L_2 = Op(\ell_1^+ + \ell_0^+)$. Let us first connect the approximation (32) to the single-scatterer equation (7). From Equation (31), the computation of the zeroth-order term $\sigma_0(\tilde{L}_1)$ of the asymptotic expansion of the operator \tilde{L}_1 gives

$$\sigma_0(\tilde{L}_1) = \frac{i}{2\ell_1^+} \partial_\xi \ell_1^+ \partial_x \ell_1^+ \quad (33)$$

by using the Leibniz composition rule for two pseudodifferential operators. This exactly corresponds to the first corrective term in (25). Moreover, a direct computation shows that

$$\sigma_0\left(-\frac{1}{2}\tilde{L}_1^{-1} n^2 \partial_z(n^{-2}\tilde{L}_1)\right) = -\frac{1}{2\ell_1^+} n^2 \partial_z(n^{-2}\ell_1^+), \quad (34)$$

meaning that the second corrective term in the right hand side of (25) is related to the principal symbol of the corrective operator in the single-scatterer improvement (7).

Another way of writing ℓ_0^+ is

$$\ell_0^+ = \frac{i}{2\ell_1^+} \partial_\xi \ell_1^+ \partial_x \ell_1^+ + i \frac{1}{(\ell_1^+)^{1/2}} n \partial_z(n^{-1}(\ell_1^+)^{1/2}). \quad (35)$$

This gives an approximation of the energy-conserving equation by considering the principal symbol of the corrective operator. These approximations of the models can be summarized as follows

$$L_1 = Op\left(\sigma_1(\tilde{L}_1)\right) \quad \text{mod}(OPS^0) \quad (36)$$

and

$$L_2 = Op\left(\sum_{m=1}^2 \sigma_{2-m}(\tilde{L}_{2,q})\right) \quad \text{mod}(OPS^{-1}), \quad q = 1, 2. \quad (37)$$

Remark 1. *In optics, the BPM model is often written accordingly to a reference background index n^r . This formulation can be easily deduced from our analysis by setting $u = \phi e^{-ikn^r z}$, rewriting the Helmholtz equation with respect to the unknown ϕ and finally applying the proposed approach.*

Remark 2. *More terms can be used to build higher-order TM BPMs. Furthermore, the extension to higher dimensions can be considered by using a similar derivation.*

Remark 3. *The previous derivation has been developed in terms of pseudodifferential operators but requires the following precision. Using the classical symbolic calculus leads to consider a symbol having a singularity. Rigorously speaking, the factorization theorem 1*

holds for frequencies (k_0, ξ) such that $\ell_1^+(x, z, \xi) \neq 0$. This means that the definition of the operators involved in the BPMs must be understood in the sense of microlocal analysis and not pseudodifferential analysis. However, for the sake of simplicity, we will use the term of pseudodifferential operators.

Remark 4. Finally, let us remark that the first application of pseudodifferential operators and factorization techniques was in the background of Absorbing Boundary Conditions for variable coefficients systems by Engquist and Majda [6]. They have next led to many developments and in particular when the fictitious boundary is supposed to be convex, smooth but arbitrarily shaped [1, 2].

4 TM bent waveguides: geometry corrections

In many applications, practitioners have to deal with arbitrarily bent waveguides like S -guides e.g. [3, 15, 16]. In [3], Baets and Lagasse derived a BPM for general waveguides. A new model, similar to the one-way model (3)-(4), has been proposed in [14] to take into account the curvature effects. We show below that our approach can be adapted to derive TM BPMs for general waveguides.

The main difference with the previous derivation of Section 3 is that we have to deal with a generalized system of coordinates. For the sake of clarity, we use the notation of [14]. More precisely, the waveguide axis is described by a curve with arclength parameter s

$$\begin{cases} z(s) = f(s) \\ x(s) = g(s) \end{cases} \quad (38)$$

where f, g are smooth functions (namely $f, g \in \mathcal{C}^1(\mathbb{R})$) satisfying

$$f'^2(s) + g'^2(s) = 1, \quad \forall s \in \mathbb{R}.$$

The unit normal vector to the waveguide is then $(-g'(s), f'(s))$. For $s < 0$ and $s > L$, we assume that the waveguide is straight (see Figure 1), denoting by L the length of the curved waveguide.

The expression of a point $M(z, x)$ of the waveguide is given in the system of coordinates (s, r) by

$$\begin{cases} z(r, s) = f(s) - rg'(s) \\ x(r, s) = g(s) + rf'(s) \end{cases} \quad (39)$$

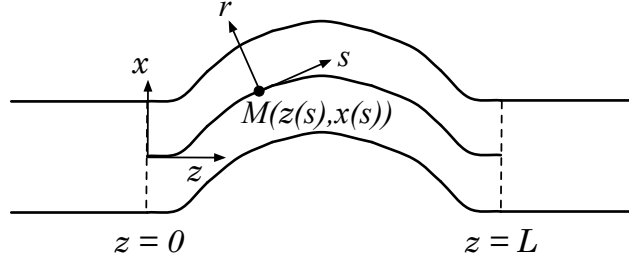


Figure 1: A bent waveguide: notations.

where r denotes the distance of M to the waveguide axis. Let us introduce

$$N(r, s) = n(x, z)$$

the refractive index in the generalized system of coordinates (r, s) , and the parameter $\gamma(r, s) = 1 - r\kappa(s)$, where $\kappa(s) = (f'(s)g''(s) - f''(s)g'(s))^{-1}$ is the curvature of the waveguide along the principal axis. A straightforward computation shows that, using the above notations, the TM Helmholtz equation can be rewritten in the coordinates system (s, r) as

$$\partial_s \left(\frac{1}{N^2 \gamma} \partial_s \tilde{u} \right) + \partial_r \left(\frac{\gamma}{N^2} \partial_r \tilde{u} \right) + k^2 \gamma \tilde{u} = 0, \quad (40)$$

where we have set $\tilde{u}(s, r) = u(z, x)$. Compared with Section 3, the direction of propagation z is now s while the transverse direction x is r . A similar statement to the one of Proposition 1 can be obtained by setting

$$\ell_1^+(r, s, \xi) = \sqrt{k^2 \gamma^2 N^2 - \gamma^2 \xi^2 + i \gamma N^2 \partial_r (\gamma N^{-2}) \xi}, \quad (41)$$

where ξ is the Fourier variable according to r . A computation of the zeroth-order term yields

$$\ell_0^+(r, s, \xi) = \frac{1}{2\ell_1^+} i \partial_r \ell_1^+ \partial_\xi \ell_1^+ + \frac{1}{2\ell_1^+} i \gamma N^2 \partial_s \left(\frac{1}{\gamma N^2} \right) \ell_1^+ + \frac{1}{2\ell_1^+} i \partial_s \ell_1^+. \quad (42)$$

Let us introduce the new square-root operator \tilde{L}_1 as

$$\tilde{L}_1 = \sqrt{\gamma N^2 \partial_r \left(\frac{\gamma}{N^2} \partial_r \cdot \right) + k^2 \gamma^2 N^2}. \quad (43)$$

Then, using the first symbol ℓ_1^+ given by (41) leads to the following approximate TM BPM

$$\partial_s u_1 = i L_1(s) u_1, \quad s > 0, \quad (44)$$

with $L_1 = Op(\ell_1^+)$, which is an approximation of

$$\partial_s u = i\tilde{L}_1(s)u, \quad s > 0, \quad (45)$$

with \tilde{L}_1 given by (43). Equation (43)-(45) was first given in [14] and is recovered here by using its first symbol since

$$L_1 = Op\left(\sigma_1(\tilde{L}_1)\right) \quad \text{mod}(OPS^0). \quad (46)$$

If we now consider the second corrective term ℓ_0^+ given by (42), then one obtains the approximate BPM

$$\partial_s u_2 = iL_2(s)u_2, \quad s > 0, \quad (47)$$

which can be considered as an approximation of an energy-conserving

$$\tilde{L}_{2,1} = \tilde{L}_1 + i\gamma^{1/2}N\tilde{L}_1^{-1/2}\partial_s\left(\frac{1}{\gamma^{1/2}N}\tilde{L}_1^{1/2}\right) \quad (48)$$

or single-scatter

$$\tilde{L}_{2,2} = \tilde{L}_1 + \frac{i}{2}\gamma N^2\tilde{L}_1^{-1}\partial_s\left(\frac{1}{\gamma N^2}\tilde{L}_1\right). \quad (49)$$

BPM for a curved waveguide since we now have

$$L_2 = Op\left(\sum_{m=1}^2 \sigma_{2-m}(\tilde{L}_{2,m})\right) \quad \text{mod}(OPS^{-1}), \quad m = 1, 2. \quad (50)$$

These last equations provide extended versions of the improved TM BPMs derived in the previous section since the case of a straight waveguide is obtained by setting $\kappa(s) = 0$. We can also remark that the TE case developed in [14] can be recovered by taking $N = 1$ in (45).

Remark 5. *We did not prove here that the new approximate BPMs are energy conserving for bent waveguides. However, their symmetrical forms suggest that it should be the case. Computational simulations could be helpful for analyzing this problem. A mathematical proof based on estimates for pseudodifferential operators should therefore be possible.*

From a numerical point of view, the algorithms proposed in [10] and [14] can be used to approximate the models proposed in this paper.

5 Conclusion

This paper provides a rigorous and systematic construction of TM Beam Propagation Models for a straight waveguide. The technique is based on the asymptotic expansion of the total symbol of the propagating operator related to the BPM. We also provide the extensions to bent waveguides of the single-scatter and energy-conserving models which are corrections to the one-way TM BPM. The construction can be extended to the three-dimensional full Maxwell's equations by using microlocal diagonalization techniques [1] which represent the extension of the factorization theorem used in Proposition 1 to hyperbolic systems.

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