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Collocation method for numerical scalar wave propagation through optical waveguiding structure

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Collocation method has been developed as a method which can treat the paraxial as well as non-paraxial wave propagation through optical waveguiding structures. The method, based on the orthogonal collocation principle, converts the Helmholtz equation into a matrix ordinary differential equation. This equation termed as the collocation equation can be solved either by using direct numerical techniques or by special techniques based on the matrix operator algebra. In the present paper, we outline the basic principle of the method and discuss its applications to the propagation of paraxial, wide-angle, bidirectional and nonlinear waves. Examples have also been included to show performance of the method.

1 Introduction

Optical fibers and integrated optical waveguides are the basic building blocks of photonic devices and systems for optical communication and information processing. In both optical fibers and integrated optical devices, the basic phenomenon is that of waveguidance, and in order to effectively analyse and design these waveguides devices, it is neceassary to understand the phenemonon of guidance through them. In the most basic form, this requires the solutions of Maxwell's equations for the boundary conditions represented by the waveguiding structure. Fortunately, in most cases of practical importance, the conditions are such that the vector nature of optical waves can be ignored, at least to a very good approximation, and then, it suffices to solve the much simpler Helmholtz equation. This *simpler* Helmholtz equation, however, is still difficult to solve particularly if the waveguides are not uniform along the direction of propagation, which is the case for most of the devices. The simulation of the field propagation through waveguides require numerical solution of the Helmholtz equation. We have developed a method for this purpose based on the principle of orthogonal collocation and during the past few years have made several advancements in this method. The method is also applicable to nonlinear pulse propagation through optical fibers which has lately assumed great importance due the possibility of repeaterless communication over several thousands of kilometer through solitons. Recently, the method has been extended to wide-angle propagation.

In this paper, we discuss some of the salient features of this method and its application to wave propagation through optical waveguides.

2 Wave Propagation through Optical Waveguides

For simplicity, we shall confine our discussions in this paper to two-dimensional waveguides; however, the methods discussed can be extended to three-dimensional structures. A 2-D waveguide structure is defined by its refractive index distribution $n^2(x, z)$ which contains all information regarding interfaces also. The electromagnetic fields that propagate through such a dielectric structure must satisfy Maxwell's equations. However, in a majority of practical waveguiding structures (we will confine our discussion to such cases), the relative variation of the refractive index is sufficiently small to allow the scalar wave approximation. It, then, suffices to consider instead a much simpler Helmholtz equation:

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial z^2} + k_0^2 n^2(x,z)\psi(x,z) = 0, \tag{1}$$

where $\psi(x,z)$ represents one of the cartesian components of the electric field (generally referred to as the scalar field). The time dependence of the field has been assumed to be $\exp(i\omega t)$ and $k_0 = \omega/c$ is the free space wave number.

The problem that is addressed in this paper is then to obtain the solutions $\psi(x,z)$ of Eq.1 given the field $\psi(x,z_0)$ at a plane $z = z_0$. Thus, we are dealing with an initial value problem with respect to the variable z (which is generally taken as the overall direction of propagation). However, the presence of the partial derivative with respect to x makes this problem much more complex and one has to devise special methods even to obtain numerical solutions. If the waveguide is uniform in the direction of propagation, the problem of wave propagation can be solved in terms of the modes of the waveguide.[1,2] These modes, which have well defined transverse field patterns and have specific phase constants, form an orthogonal set of basis functions. An incident field at z=0 can be expressed as a linear combination of these modes, which then propagate along the waveguide with their phases changing in a definite way but differently, in general, for different modes. Therefore, at any other value of z, these would combine to give a field which represents the field after propagation through the length z of the waveguide. Thus, once the modes are known for a given uniform waveguide, one can, in general, propagate a given field through any length of the waveguide. It must, however, be mentioned that these modes–the guided and the radiation–are infinite in number and, in fact, the radiation modes form a continuum of modes and, hence, the summation/integration over these modes has to be truncated leading to an inaccuracy in any propagation. The approach of total field propagation, that we discuss next, can therefore also be useful even for uniform waveguides.

A straight and uniform waveguide is, however, an idealization and practical waveguides do have variations along their lengths, such as bends in optical fibers or refractive index and/or geometric variations in fibers/integrated optic (IO) waveguides. In addition and more importantly, there are devices which inherently have structures which are nonuniform. These include, *e.g.*, tapers, y-junctions, couplers, etc. Wave propagation through such guides-wave structures cannot, in general, be modelled in terms of the modes, although in some structures it can be treated via coupled mode theory (which is usually limited to very few modes).[2] This has led to the development of the approach in which the total fields or beams are propagated by numerically solving the Helmholtz equation directly and lately, a number of methods have been developed for this purpose.

There are several advantage of treating total fields, rather than individual modes; for instance, the analysis is not restricted to uniform or near uniform waveguides and one can handle, in principle, arbitrary index and/or geometry variations along the direction of propagation. Further, the radiation modes are included in the total field propagating along the waveguiding structure and it is not necessary to obtain them explicitly which is often not practical. These methods can be used to obtain the evolution of fields in a structure that are not uniform along the direction of propagation. Some of the methods are the FFT-BPM,[3–5] the FD-BPM[6–8] and the collocation method.[9–14]

The collocation method, which we have developed, is based on the collocation principle and has some unique features in comparison to other methods. The method is applicable to both guiding and non-guiding propagation problems, and it can be applied to linear and nonlinear wave propagation as well as wide angle and bidirectional propagation. In this paper, we briefly describe the method and discuss some of its recent applications.

3 Basic Collocation Method

Collocation methods have been used since the beginning of the last century for solving integral equations. These were first applied to the solution of differential equations by Frazer, Jones and Skan[15] in 1937 and independently by Lanczos[16,17] in 1938. The collocation methods belong to the family of methods used for solving differential equations which can be grouped together under the common name – the method of weighted residuals.[18,19] In the collocation method, the solution of a differential equation is sought in the form of a linear expansion as a polynomial or over a set of polynomials or functions. The coefficients of expansion are obtained by imposing the condition that the expansion satisfies the differential equation exactly at certain discrete points on the independent variable axis (or plane). These points are referred to as the collocation points. In earlier methods, these points were chosen to be equi-distant. However, Lanczos[17] showed that such a choice may lead to divergence in results and suggested the use of orthogonal polynomials as the basis functions for the expansion. Later, Villadsen and Stewart[20] developed this concept further and called it *orthogonal collocation*. Fletcher[21] has shown that the equidistant collocation yields poorer results in comparison to the othogonal collocation. Orthogonal collocation has been applied using the Radau, Tchebycheff and Legendre polynomials to solve a variety of chemical engineering problems.[19] In all these problems the range of the independent variables is finite. We have, for the first time, developed[9] the collocation method for the Helmholtz equation which is over an infinite range. We have used the Hermite-Gauss,[9] the Laguerre-Gauss[10] and the sinusoidal functions[14] as the basis functions. We have used the orthogonal collocation method (OCM) which is outlined below.

We begin with the Helmholtz equation for 2-D propagation, Eq. 1, and seek its solution for $\psi(x, z)$ as a linear combination over a set of suitable orthogonal functions, $\phi_n(x)$:

$$\psi(x,z) = \sum_{n=1}^{N} c_n(z)\phi_n(x), \tag{2}$$

where $c_n(z)$ are the expansion coefficients. The choice of $\phi_n(x)$ depends on the boundary conditions and the symmetry of the guiding structure. For a planar structure, for example, the Hermite-Gauss functions, $H_n(x)$, are suitable while for a cylindrical structure the Laguerre-Gauss functions, $L_n(x)$, would be more appropriate. For the present, we have

$$\phi_n(x) = \mathcal{N}_{n-1} H_{n-1}(\alpha x) \exp(-\alpha^2 x^2/2) \tag{3}$$

where $\mathcal{N}_{n-1}$ is the normalization constant and α is a parameter which can be chosen arbitrarily, but its choice can influence the accuracy for a given value of N.[10] Obviously, the accuracy of expansion in Eq. 2 improves as N increases. In the collocation method, it is required that the differential equation, Eq. 1, be satisfied *exactly* by the expansion in Eq. 2 at N collocation points $x_j, j = 1, 2, \ldots, N$. This implies that we can uniquely determine only N coefficients in the expansion and thus the orthogonal functions used in the expansion are $\phi_1, \phi_2, \ldots, \phi_N$. In the orthogonal collocation method, the collocation points x_j are chosen such that these are the zeroes of ϕ_{N+1}. Thus, $H_N(\alpha x_j) = 0, \quad j = 1, 2, \ldots, N$. Writing the Helmholtz equation, Eq. 1 at each of these collocation points, we obtain a set of N total differential equations, which after some algebraic manipulations can be written as a matrix ordinary differential equation (details are given elsewhere[9–11]):

$$\frac{d^2\mathbf{\Psi}}{dz^2} + \mathbf{S}(z)\mathbf{\Psi}(z) = 0, \tag{4}$$

where $\mathbf{S} = \mathbf{B}\mathbf{A}^{-1} + \mathbf{R}(z)$, with

$$\mathbf{A} = \{A_{jn} : A_{jn} = \phi_n(x_j)\} \quad \text{and} \quad \mathbf{B} = \left\{ B_{jn} : B_{jn} = \left.\frac{\partial^2 \phi_n}{\partial x^2}\right|_{x_j} \right\}$$

being constant matrices dependent on the choosen functions, $\phi_n(x)$, and

$$\Psi(z) = \text{col.}[\psi(x_1, z) \;\; \psi(x_2, z) \;\; \ldots \;\; \psi(x_N, z)], \tag{5}$$

$$\mathbf{R}(z) = k_0^2 \;.\; \text{diag.}[n^2(x_1, z) \;\; n^2(x_2, z) \;\; \ldots \;\; n^2(x_N, z)]. \tag{6}$$

Equation 4 is referred to as the collocation equation. In deriving this equation from the Helmholtz equation, Eq. 1, no approximation has been made except that N is finite and Eq. 4 is exactly equivalent to Eq. 1 as $N \to \infty$. Thus, the accuracy of the collocation method improves indefinitely as N increases.

An important feature of the collocation method is that one obtains an equation as a result which can be solved or modified in a variety of ways. It can be solved as an initial value problem using any standard method such as the Runge-Kutta method or the predictor-corrector method. In the paraxial form, it can also be solved using matrix operator methods based on the approach of symmetrized splitting of the sum of two non-commutating operators[12] (see the next Section). One could also use a suitable transformation of the independent and/or dependent variable to an advantage. Indeed, we have shown[13] that a transformation could be used to redistribute the collocation points (which are the field sampling points in the transverse cross-section) in such a way that the density of points increases in and around the guiding region, and the transverse extent, covered by the sampled field, also increases.

4 Paraxial Wave Propagation

For a majority of wave propagation problems, such as those involving waveguide tapers, y-junctions, etc., the beam can be assumed to be dominantly propagating in the z-direction and one can invoke the paraxial (or Fresnel) approximation. With this approximation, the second order collocation equation reduces a first order equation and the computation effort reduces considerably.

The field represented by $\Psi(z)$ varies rapidly on account of its phase factor. However, if one assumes that the propagation is dominantly in the z direction, one can write

$$\Psi(z) = \mathcal{X}(z)e^{-ikz}, \tag{7}$$

where $\mathcal{X}(z)$ is a slowly varying envelope of the wave and $k = k_0 n_{\text{ref}}$ with n_{ref} being the index of a reference medium. Substituting from Eq. 7 into Eq. 4, we obtain an equation satisfied by the envelope $\mathcal{X}(z)$:

$$\frac{d^2\mathcal{X}}{dz^2} - 2ik\frac{d\mathcal{X}}{dz} + (\mathbf{S} - k^2\mathbf{I})\mathcal{X}(z) = 0, \tag{8}$$

$\mathbf{I}$ being the unit matrix. Now, for a medium in which the index is not varying very rapidly along the z direction, one can make the slowly varying envelope approximation and negelct the second derivative of $\mathcal{X}(z)$ to obtain the paraxial collocation equation

$$\frac{d\mathcal{X}}{dz} = (\mathbf{S} - k^2\mathbf{I})\mathcal{X}(z)/2ik. \tag{9}$$

This approximation has been extensively used in the study of waveguides and is, in fact, an essential approximation for the FFT-BPM and the FD-BPM. In our method, on the other hand, it is optional as one could solve either of Eqs. 8 & 9. However, we have found that, in practical waveguiding problems, this approximation is extremely good except in cases where either reflections are important such as periodic structures, or where wide angled beams are involved.

One can solve the collocation equation or its paraxial form using any standard numerical method such as the Runge-Kutta method or a predictor-corrector method. These methods, however, require very small values of the numerical step, Δz in order to keep the solutions stable. We have also obtained the solution of Eq. 9 in a split-step operator form which is unconditioanlly stable for any value of Δz; of course, the error in propagation increases as Δz increases. We give here only the final propagation alogorithm and the details can be found elsewhere.[12]

Using the properties of the basis functions, Eq. 9 can be expressed in the form

$$\frac{d\mathcal{X}}{dz} = (\mathbf{D}_1 + \mathbf{R}(z) - k^2\mathbf{I} - \mathbf{A}\mathbf{D}_2\mathbf{A}^{-1})\mathcal{X}(z)/2ik, \tag{10}$$

where

$$\mathbf{D}_1 = \alpha^4 \times \text{diag.}(x_1^2 \;\; x_2^2 \ldots x_N^2) \quad \text{and} \quad \mathbf{D}_2 = \alpha^2 \times \text{diag.}[1 \;\; 3 \;\; 5 \ldots (2N-1)] \tag{11}$$

The matrix equation Eq. 10 can be solved using the spilt-step operator formalism to obtain the following algorithm[12]

$$\mathcal{X}(z + \Delta z) = \mathbf{P}\mathbf{Q}_1\mathbf{Q}_2(z)\mathbf{P}\mathcal{X}(z) + \bigcirc[(\Delta z)^3], \tag{12}$$

where

$$\mathbf{P} = \mathbf{A}e^{-\mathbf{D}_2\Delta z/4ik}\mathbf{A}^{-1}, \qquad \mathbf{Q}_1 = e^{(\mathbf{D}_1 - k^2\mathbf{I})\Delta z/2ik}, \qquad \mathbf{Q}_2(z) = e^{\mathbf{R}(z)\Delta z/2ik},$$

and the exponentials involved can be easily evaluated since the arguments are diagonal matrices (the exponential of a diagonal matrix is a diagonal matrix with the diagonal elements being simply the exponential of the corresponding diagonal elements of the argument matrix). Further, since all the matrices $\mathbf{P}, \mathbf{Q}_1$ and $\mathbf{Q}_2(z)$ are unitary for real indices, these do not blow up for any value of the arguments. Thus, this algorithm, which is termed as the split-step collocation method (SSCM), is unconditionally stable for any value of Δz.

We include a numerical example to show the performance of the collocation method. We consider the propagation of the fundamental mode through a uniform waveguide. The modal field does not undergo any change except for a phase factor; hence, any change in the amplitude of the modal field would directly reflect the error in the method of propagation. The numerical computations have been performed for a secant-hyperbolic profile:

$$n^2(x) = n_2^2 + (n_1^2 - n_2^2)\,\text{sech}^2(x/a), \tag{13}$$

with a=3μm, n_1=1.45 and n_2=1.4476. We have assumed the free space wavelength of the propagating wave to be λ_0=1.31μm so that the V-value is 1.2, where $V = k_0 a\sqrt{n_1^2 - n_2^2}$. We consider the incidence of the fundamental mode of the waveguide at z=0; thus,

$$\psi(x, z{=}\,0) = \cosh^{-W}(x/a), \tag{14}$$

where $W = a\sqrt{\beta^2 - k_0^2 n_2^2} = \frac{1}{2}[\sqrt{1+4V^2} - 1]$. As a measure of accuracy we have computed the correlation factor (CF) of the propagating field at $z{=}z_f \equiv 100\mu$m with the incident field:

$$CF = \frac{\int \psi^*(x, z=0)\; \psi(x, z=z_f)\; dz}{\sqrt{\{\int |\psi(x, z=0)|^2\, dz\}\{\int |\psi(x, z=z_f)|^2\, dz\}}} \tag{15}$$

The absolute value of the correlation factor should be unity, since only the phase changes as the mode propagates through the waveguide. Thus, $E_R = 1 - |CF|$ gives the error in the method

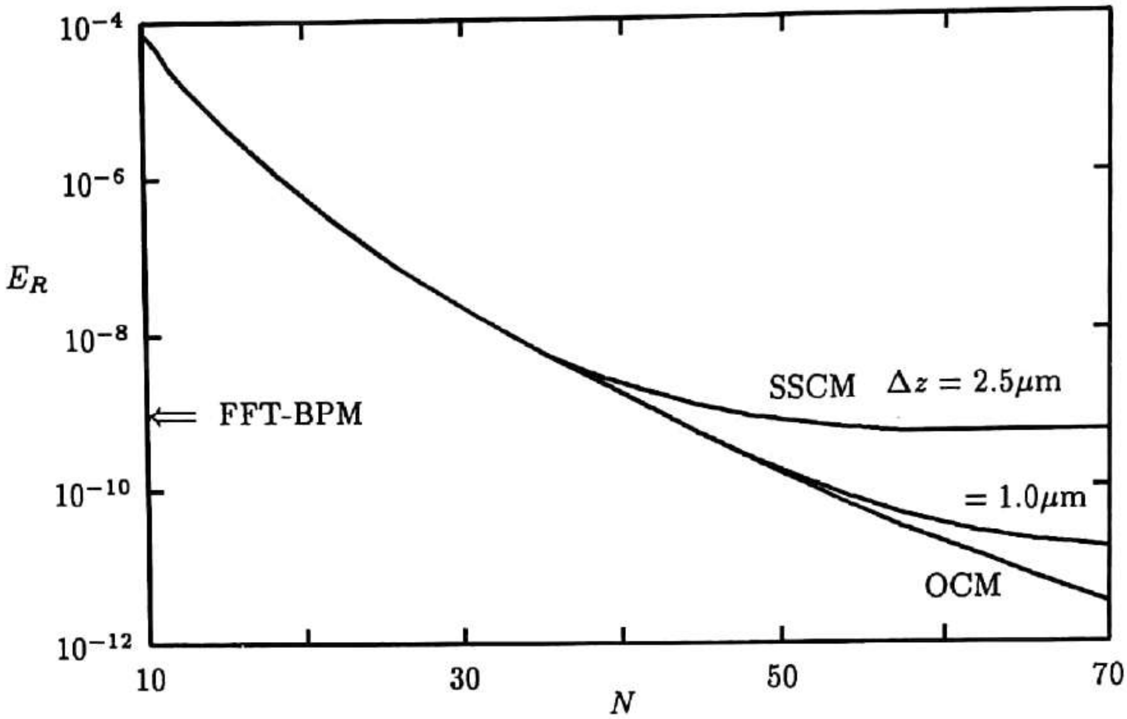

Figure 1: Error, E_R in propagation methods as a function of N.

used for computing the propagated field. This quantity is plotted in Fig. 1. For comparison, we have also included the results obtained using the FFT-BPM with a grid of 128 points in the cross-section between -50μm to 50μm. The figure shows the error E_R as a function of the number of collocation points N for the OCM for which Eq. 9 was solved using the Runge-Kutta method with the extrapolation interval $\Delta z = 2.5\mu m$, and for the SSCM for which Eq. 12 was used with $\Delta z = 2.5\mu m$ and $1.0\mu m$. The figure shows the improvement in the performance as N increases and as Δz decreases. The stability of the SSCM is demonstrated elsewhere.[12]

5 Wide-Angle Beam Propagation

Methods that solve the paraxial equation do not give accurate results for cases which involve propagation at angles larger than few degrees. In order to treat propagation at larger angles, the so-called wide-angle propagation methods have to be used. Several schemes have recently been proposed to treat wide-angle beam propagation. In general, this would involve solving directly the wave equation, which involves a second order partial differential with (the direction of propagation) as against the first order partial differential in the paraxial wave equation. All the methods for non-paraxial propagation discussed in the literature approach this problem iteratively, in which a numerical effort equivalent to solving the paraxial equation several times is required. These methods include those based on the Taylor expansion,[22] the Padé approximants[22,23] and the Lanczos reduction.[24,25] In all these methods, the square root of the propagation operator involved in the wave equation is approximated in various ways. In the collocation method, however, one can solve the second-order equation, Eq. 4, directly and obtain wide-angle propagation which would also include evanescent waves. We have solved the equation using the Runge-Kutta method.[26]

In order to show the performance of the method, we include here an example of a Gaussian beam propagating at 45 degrees to the z-axis over a distance of 10μm. The width of the Gaussian beam intensity was 2.828μm and the wavelength 1.06μm. The computation was done with 120 collocation points and the width of the numerical window was about 80μm. The result is shown

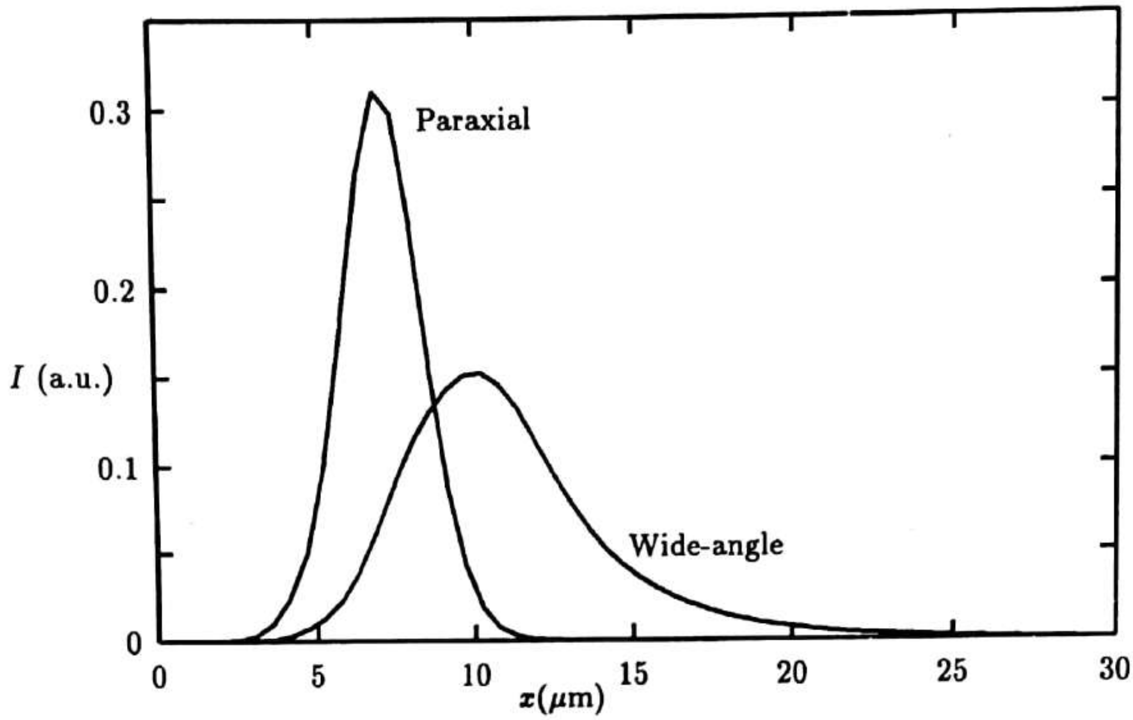

Figure 2: Intensity (arbitrary units) of a Gaussian beam after propagation at 45 degrees for a distance of $10\mu m$ using the paraxial and wide-angle collocation methods.

in Fig. 2 in which the paraxially propagated beam is also included. This result matches well with that obtained by Hadley.[23]

6 Bidirectional Wave Propagation

In the above discussions, we have considered wave propagation along the z direction and no reflections have been considered. There are, however, a number of cases where reflections are important and cannot be neglected. Bragg gratings, for example, are components which operate on the principle of reflection. These have recently attracted considerable attention because of their applications as reflector filters with narrow bandwidth and low side-lobe level in WDM systems, and for flattening of gain spectrum in erbium-doped fiber amplifiers. To model propagation through such components, one has to use methods which are bidirectional and are capabale of propagating waves in both directions ($+z$ and $-z$).

Generally, periodic media such as gratings have been analyzed using the coupled mode theory.[27–29] However due to various assumptions involved, there is always an uncertainty of the accuracy of this approach. On the other hand numerical methods such as the FFT-BPM and FD-BPM, which use Fresnel approximation, cannot take reflected waves into account. As we have seen in Sec. 5, in the collocation method, we can directly solve the wave equation without the Fresnel approximation, and hence, it can be used for modelling reflections from a periodic structure. We have implemented the collocation method for wave propagation through periodic waveguides[11,30] and have used it to model Bragg gratings and grating sensors.[31] Here, we briefly discuss the method of implementation and some of the results.

In the case of periodic waveguides, $\mathbf{R}(z)$ and, hence, $\mathbf{S}$ in Eq. 4, vary periodically with z. We look for analytical solutions of Eq. 4 by writing it in the following form

$$\frac{d\mathbf{\Phi}}{dz} = \mathcal{H}(z)\mathbf{\Phi}(z), \quad \mathbf{\Phi} = \begin{bmatrix} \mathbf{\Psi} \\ d\mathbf{\Psi}/dz \end{bmatrix}, \quad \mathcal{H}(z) = \begin{bmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{S} & \mathbf{0} \end{bmatrix}, \tag{16}$$

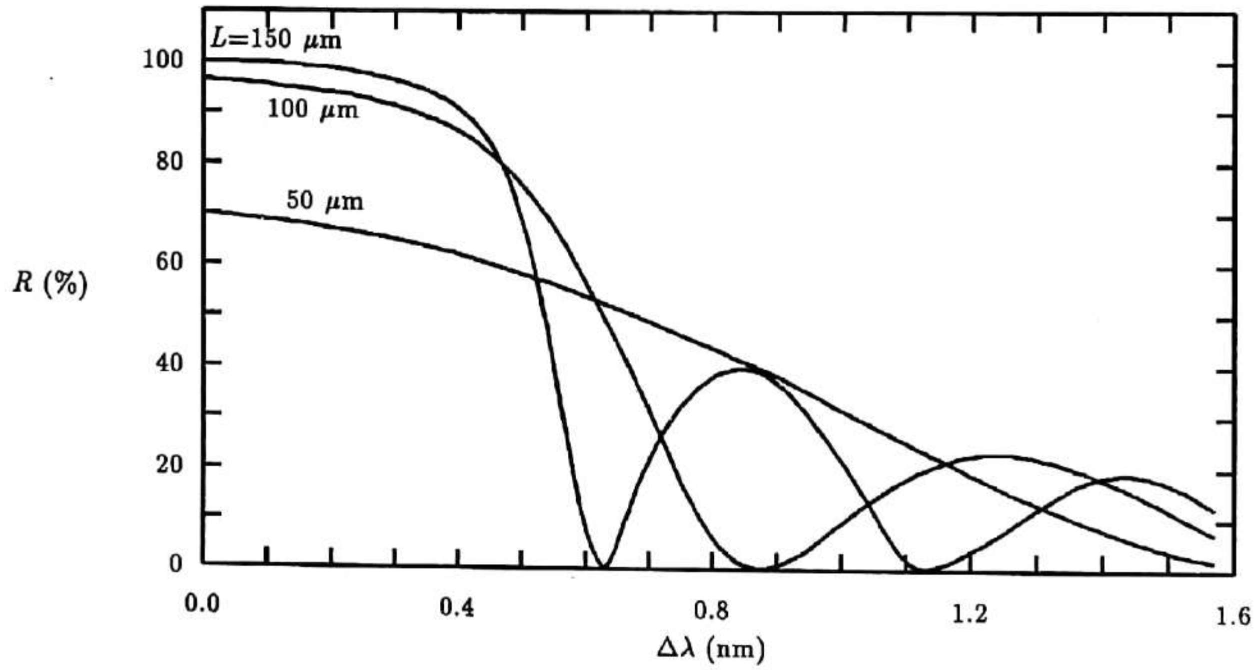

Figure 3: Variation of modal reflection coefficient, R, as a function of the change in wavelength from the Bragg wavelength, λ_B for different values of the length, L, of the periodic section.

where $\mathbf{\Phi}$ is a vector of dimension $2N \times 1$, and $\mathcal{H}(z)$, a $2N \times 2N$ square matrix, is a periodic function of z $[\mathcal{H}(z+\Lambda) = \mathcal{H}(z)$, Λ being the period along $z]$. We have to solve Eq. 16 with a given initial condition, say $\mathbf{\Phi}(0) = \mathbf{\Phi_0}$. One begins by solving an auxiliary equation

$$d\mathcal{F}/dz = \mathcal{H}(z)\mathcal{F}(z) \tag{17}$$

where $\mathcal{F}(z)$ is a square matrix such that $\mathcal{F}(0) = \mathbf{I}$. The solution of Eq. 16 then is: $\mathbf{\Phi}(z) = \mathcal{F}(z)\mathbf{\Phi_0}$. The solution of Eq.17 is obtained by using the collocation method over one period and by using the Floquet's theorem to construct the solution of the entire length of the periodic waveguide. The details are given elsewhere.[11,30,31]

We now consider an example of a sech^2 waveguide with a periodic section of length L created due to the variation of the half-width of the waveguide. Thus, the refractive index distribution is given by Eq. 13 with the half-width in the periodic section varying as

$$a(z) = a_0 + b_0 \cos(2\pi z/\Lambda). \tag{18}$$

We have chosen the following parameters: $n_1 = 1.45, n_2 = 1.444, a_0 = 2.5\mu\text{m}$, $b_0 = 0.5\mu\text{m}$ and $\Lambda = 0.536\mu\text{m}$. These parameters corresponds to peak reflectivity at λ_B=1.55126 μm, the Bragg wavelength. We obtained the typical variation of the reflection coefficient as a function of $\Delta\lambda = \lambda - \lambda_B$ shown in Fig.3 for different values of the length L. The curves are very similar to those obtained using coupled mode theory.[29] Examples on modelling of grating sensors can be found elsewhere.[31]

7 Nonlinear Pulse Propagation

The nonlinear evolution of short pulses in an optical fiber is usually described by the nonlinear Schrödinger equation (NLS) which has been analytically solved.[32,33] The NLS equation holds good for pulses of picosecond duration. However, some assumptions implicit in the equation are no longer valid for pulses of smaller duration. Hence, the NLS equation has to be modified to include a host of other phenomena, such as higher order dispersion, higher order nonlinearities, attenuation and self-steepening. Thus, in presence of Kerr-like nonlinearity, pulse propagation can be described by the Generalised Nonlinear Schrödinger Equation (GNLSE),[34] which has to be solved numerically. The numerical method often used to solve the GNLSE is the split-step Fourier method (SSFM),[34] which is in fact a form of the FFT-BPM. This type of procedure has some inherent drawbacks. One has to use numerical differentiation in evaluating terms containing derivatives of the pulse envelope. Further, the effects of nonlinearity and dispersion are assumed to be separated in space, whereas in reality both act simultaneously. The collocation method does not suffer from these drawbacks and numerical examples show that the collocation method is considerably more efficient even for solving GNLSE. The details of the implementation of the collocation method and some examples are given elsewhere.[11,35] Recently, a comparison[36] has been made of the numerical efficiencies of the collocation method and the SSFM for propagation of a fundamental soliton to about 200 km for a pulse of 20 ps width in a standard single mode fiber. This result shows that the collocation method is about 10...100 times more accurate for a given computation time and is 2...20 times faster for a given accuracy.

8 Summary

We have discussed the collocation method which is, in several cases of importance, numerically more efficient than the conventionally used methods for beam propagation. The method can used to obtain paraxial, wide-angle, bidirectional and nonlinear wave propagation through waveguiding structures. Examples in each case have been included, which show the effectiveness and performance of the method.

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