X-ray waveguiding studies of ordering phenomena in confined fluids
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Chapter 2

Theory of wave propagation in planar x-ray waveguides

In this chapter we calculate the electromagnetic field amplitudes within a planar waveguide. Emphasis is put on methods applicable to waveguides having guiding layers which are homogeneous, inhomogeneous or tapered. The underlying physical principles of these methods and their numerical implementation will be discussed. Far-field diffraction patterns from the exit of the waveguide are determined from the calculated field distributions in order to compare them with experimentally obtained diffraction patterns.

2.1 Introduction

The propagation of electromagnetic (e.m.) waves through waveguides plays an important role in everyday life. For example, phone calls and television broadcasts reach us via networks of guided-wave devices such as optical fibers and integrated-optics devices. These technologies could be further developed thanks to the effort which was put into understanding their operation. As a result, a wide variety of mathematical methods exists for the calculation of e.m. field amplitudes within these, sometimes, very complex devices [7].

In general, these methods consist of solving Maxwell’s equations which describe the propagation of e.m. waves through a medium. Our aim here, is to apply some of these methods to the propagation of x rays in planar waveguides. We mainly
focus on how the amplitude and phase of the e.m. fields are affected by variations of the refractive index, i.e. the density variations, within the guiding layer of the waveguide. For the waves propagating within the waveguide, these refractive-index variations act as scattering centers. In integrated optics such variations, which are mainly caused by errors in the production process, are unwanted, since they induce power losses and cross-talk. Most of the mathematical methods were thus applied in order to quantify and reduce these scattering effects. By contrast, we aim at maximizing these effects so as to obtain the spatial distribution of the refractive-index variations.

For this purpose, we need to calculate both the amplitude and phase of the e.m. field. Often used simplifications of the mathematical treatment, which only yield the power within the waveguide [8], may not be applied since they average over the phases. However, the complication of calculating both the amplitude and the phase is largely compensated by simplifications which arise from working at x-ray wavelengths. For example, we may neglect backward scattering of waves from refractive-index variations.

We discuss methods which are applicable to the waveguiding geometries en-
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countered in our experiments (see Fig. 2.1). The planar geometries shown in Figs. 2.1a and 2.1b are invariant under translations along the z-direction (and the y-direction), whereas those corresponding to Figs. 2.1c and 2.1d are not, i.e. the refractive-index profiles depend explicitly on z.

In the former case, the e.m. field distribution within the waveguide is elegantly described in terms of modes [9]. These are special solutions of Maxwell's equations which form a complete and orthogonal set. Hence, any e.m. field distribution within these waveguides may be written as a superposition of modes. In the latter case, strictly speaking, no modes exist. However, the e.m. field may be described in terms of modes belonging to the undisturbed waveguide (Fig. 2.1a) which are coupled due to the refractive-index variations. Although the coupled mode description is convenient for understanding the effect of these variations on the propagating waves, it is less suited for the numerical calculation of the e.m. field amplitude within the waveguide. Instead, we employ the numerical Beam Propagation Method (BPM), which calculates the total e.m. field directly instead of performing a decomposition into modes.

In the following sections, we discuss the underlying physical principles of the methods in the above order, after which we consider their numerical implementation. The chapter concludes with a section dedicated to the propagation of waves emerging from the waveguide into the free space behind the waveguide.

2.2 Modes in a planar waveguide

In linear, dielectric, non-magnetic and source-less media the propagation of waves is described by the Maxwell equations (in SI units) [9],

\[ \nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t}; \quad \nabla \cdot \epsilon_0 n^2 \mathbf{E} = 0, \]

\[ \nabla \times \mathbf{H} = \epsilon_0 n^2 \frac{\partial \mathbf{E}}{\partial t}; \quad \nabla \cdot \mu_0 \mathbf{H} = 0, \] (2.1)

where \(\mathbf{E}\) is the electric field, \(\mathbf{H}\) the magnetic field, \(n\) the refractive index, \(\epsilon_0\) the free-space permittivity, \(\mu_0\) the magnetic permeability and \(t\) the time variable. If we assume the x rays to be monochromatic, so that the time dependence of the fields is \(e^{i\omega t}\), where \(\omega = 2\pi c/\lambda = k_0 c\) is the radial frequency, with \(\lambda\) the wavelength, \(k_0 = 2\pi/\lambda\) the free-space wave number and \(c = 1/\sqrt{\epsilon_0 \mu_0}\) the speed of light in
vacuum, then separation of the time and space coordinates leads to the Helmholtz equations [7],

\[ \Delta \mathbf{E} + k_0^2 n^2 \mathbf{E} = -\nabla(\nabla (\ln n^2) \cdot \mathbf{E}) \] 

(2.2a)  

\[ \Delta \mathbf{H} + k_0^2 n^2 \mathbf{H} = -\nabla(\ln n^2) \times \nabla \times \mathbf{H}. \] 

(2.2b)

Here, \( \Delta \) is the vectorial Laplace operator.

Let us first consider the propagation of waves through a planar waveguide with a homogeneous guiding layer and cladding (see Fig. 2.1a), i.e., \( \nabla n_1^2 = 0 \) and \( \nabla n_2^2 = 0 \), respectively. Then, the right-hand side of Eqs. (2.2a) and (2.2b) vanishes, i.e. the vector components of the electric and magnetic fields are decoupled. However, the step in the refractive index across the interface between the guiding layer and cladding imposes boundary conditions on the fields. Across the interface, the following components of the vector fields have to be continuous: \( E_y \), \( E_z \), \( H_x \), \( H_y \), and \( H_z \) [9]. The field component \( E_z \) has to fulfil the condition \( n_1^2 E_z^{(1)} = n_2^2 E_z^{(2)} \) at the interface, where the superscripts (1) and (2) refer to the field in the guiding layer and the cladding, respectively. These boundary conditions lead to two types of solutions to Eqs. (2.2): transverse-electric (TE) and transverse-magnetic (TM) waves. As their names indicate, both solutions consist of field components that are transverse to the propagation direction. As depicted in Fig. 2.1a, we choose our coordinate system such that the waves propagate along the \( z \)-direction. Then, for the TE waves, \( E_z = 0 \) holds everywhere and \( H_z \) is continuous across the interfaces. A TE wave consists of the following non-zero field components: \( E_y \), \( H_x \), \( H_y \). The TM waves fulfil \( H_z = 0 \) everywhere while \( E_z \) is continuous across the interfaces. For TM waves the field components \( H_y \), \( E_x \) and \( E_z \) are non-zero.

If inhomogeneities are present (\( \nabla n_1^2 \neq 0 \) or \( \nabla n_2^2 \neq 0 \)), all the field components are coupled and the solutions to Eqs. (2.2) cannot be expressed in terms of TE or TM waves only. However, if \( \Delta n / n \ll 1 \), where \( \Delta n \) is the variation of the refractive index over a distance of one wavelength, the coupling may be neglected [7]. This is the case at x-ray wavelengths, since \( \Delta n \sim 10^{-6} \) and \( n \sim 1 \). Since the x rays in our experiments are TE polarized, we focus on the TE waves only.
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For TE waves and in the absence of coupling, the Helmholtz equations (2.2) reduce to

\[
\nabla^2 E_y + k_0^2 n^2 E_y = 0, \\
H_x = -\frac{i}{\mu_0 \omega} \frac{\partial E_y}{\partial z}, \\
H_z = \frac{i}{\mu_0 \omega} \frac{\partial E_y}{\partial x},
\]

where \(\nabla^2 = \partial^2 / \partial x^2 + \partial^2 / \partial y^2 + \partial^2 / \partial z^2\). At this point, we assume that the refractive-index profile is independent of the \(z\)-coordinate and that the fields do not vary in the \(y\)-direction. Then, Eq. (2.3a) can be further simplified by separating the variables \(x\) and \(z\), while assuming a travelling-wave character of the TE waves along the \(z\)-direction:

\[
\Psi(x, z) = \phi(x) e^{-i\beta z},
\]

where \(\Psi(x, z)\) denotes \(E_y(x, z)\) for ease of notation. The so-called propagation constant \(\beta\) of the TE wave [8], is the \(z\)-component of the wave vector \(k\) with \(|k| = n_1 k_0\). Substitution of Eq. (2.4) into Eq. (2.3a) results in the differential equation:

\[
\frac{d^2 \phi}{dx^2} + (k_0^2 n^2 - \beta^2) \phi = 0.
\]

Since \(E_y\) and \(H_z\) should be continuous across the interface between the guiding layer and cladding, \(\phi(x)\) should be continuous and differentiable (see Eq. (2.3c)) at the interface. If we require that the fields vanish at infinity, then, by solving Eq. (2.5), we obtain the so-called guided modes [8] (Fig. 2.2a). If we do not apply the latter boundary condition, we obtain the so-called radiation modes [8] (Fig. 2.2b).

Let us now consider, as an example, the properties of the modes corresponding to a piecewise constant refractive-index profile as depicted in Fig. 2.2. A guided mode solution of Eq. (2.5) can generally be written as

\[
\phi(x) = \begin{cases} 
Ce^{-\gamma |x|} & x < 0 \\
Ae^{-ik_z x} + Be^{ik_z x} & 0 \leq x < W \\
(Ae^{-ik_z W} + Be^{ik_z W}) e^{-\gamma (x-W)} & x \geq W
\end{cases}
\]

(2.6)
where \( k_z = \sqrt{n_1^2 k_0^2 - \beta^2} \) and \( \gamma = \sqrt{\beta^2 - n_2^2 k_0^2} \). Within the guiding layer the solution is a superposition of two plane waves counter-propagating in the \( x \)-direction, whereas within the cladding it decays to zero exponentially as \( x \to \pm \infty \), provided \( \gamma \) is real and positive. Accordingly, the guided modes have a propagation constant in the range \( n_2 k_0 < |\beta| < n_1 k_0 \).

In order to obtain \( A/B, C/B \) (where \( B \) may be determined from the power of the e.m. field) and \( \beta \), we apply the requirement that \( \phi(x) \) be continuous and differentiable at \( x = 0 \) and \( x = W \) (see text below Eq. (2.5)). This leads to the following system of non-trivial equations:

\[
\begin{align*}
A + B &= C, \\
-i k_z A + i k_z B &= \gamma C, \\
-i k_z A e^{-i k_z W} + i k_z B e^{i k_z W} &= -\gamma A e^{-i k_z W} - \gamma B e^{i k_z W}.
\end{align*}
\]

Solving this set of equations, we obtain

\[
\begin{align*}
\frac{A}{B} &= \frac{i k_z - \gamma}{i k_z + \gamma}, \\
\frac{C}{B} &= \frac{2 i k_z}{i k_z + \gamma}.
\end{align*}
\]

The two ratios correspond to the complex amplitude reflection and transmission coefficients, respectively [10]. By substitution of Eq. (2.8a) into Eq. (2.7c) we
obtain the equation

\[
\frac{ik_x - \gamma}{ik_x + \gamma} = e^{ik_x W},
\]  

which determines the values of \( \beta \), given \( n_1, n_2 \) and \( k_0 \). This equation has only a finite number of solutions \( \beta = \beta_m \), where \( m = 0, 1, 2, ..., m_{\text{max}} \) is called the mode number [8]. The corresponding guided-mode profile is denoted as \( \phi_m(x) \).

For \( |\beta| \leq n_2 k_0 \), \( \gamma \) is imaginary. In this case the field profile in Eq. (2.6) would consist of a standing wave within the guiding layer and outward propagating waves within the claddings. Such a solution, however, is not normalizable. In Ref. [8] this issue is addressed in detail. Here, it suffices to note that for these values of \( \beta \), the solutions to Eq. (2.5) are called radiation modes and that they form a continuum instead of a discrete set.

In a ray-optics approach the modes are described in terms of rays instead of wave fields. Rays are the lines which cross the surfaces of constant phase of the wave field at right angles, see Fig. 2.3. In order to derive the mode properties, we consider the phase changes that a ray acquires upon propagation through a waveguide with a piece-wise constant refractive-index profile.

Propagating across the guiding layer at an angle \( \theta \), a ray picks up a phase change \( k_0 n_1 W / \sin \theta \). Upon reflection from the interfaces an additional angle-dependent phase change \( \phi \) is picked up as the complex amplitude reflection coefficient, given by Eq. (2.8a), is written as,

\[
r = e^{-i\phi},
\]  

Figure 2.3 Illustration of the ray approach to waveguiding. All rays that travel in the same direction belong to the same plane wave.
where

\[
\tan(\varphi/2) = \gamma/ik_z. \tag{2.11}
\]

Here, \(|r|^2\) is the intensity reflection coefficient. The discreteness of the guided modes follows from combining the phase changes if we take into account that the ray from A to B is not reflected whereas the one from C to D is reflected twice [8]. Because points on the same phase front must be in phase, the optical path length difference between the rays AB and CD must be a multiple of \(2\pi\), i.e.

\[
k_0n_1(s_2 - s_1) - 2\varphi = 2\pi m, \tag{2.12}
\]

where \(m\) is an integer and \(s_1\) and \(s_2\) are the distances AB and CD, respectively. Although derived from a different point of view, Eq. (2.12) is identical to Eq. (2.9). Assuming that the waves do not penetrate the cladding, i.e. \(\gamma \to \infty\), we find from Eq. (2.11) that \(\varphi = \pi\). Inserting \(s_2 - s_1 = 2W\sin \theta \approx 2W\theta\), it is possible to solve Eq. (2.12) for the angles corresponding to the guided modes,

\[
\theta_m = \frac{(m + 1)\pi}{n_1k_0W} \approx \frac{(m + 1)\pi}{k_0W}, \tag{2.13}
\]

where \(m\) is the mode number. With \(\beta_m = n_1k_0\cos \theta_m\) we obtain the solutions to Eq. (2.9).

For a guided mode, the mode angle \(\theta_m\) is smaller than the critical angle for total internal reflection \(\theta_c\). Hence, the total number of guided modes is

\[
m_{\text{max}} = k_0W\theta_c/\pi - 1. \tag{2.14}
\]

The radiation modes correspond to rays propagating at angles \(\theta > \theta_c\). Since there is no total internal reflection from the interfaces, a radiation mode is not confined to the guiding layer.

Although the modes for a waveguide with a piece-wise constant refractive-index profile may be completely different from those for a waveguide with a varying profile \(n(x)\), they have one important property in common. Since they are both solutions of Eq. (2.5), which, together with the boundary conditions, is a Sturm-Liouville type boundary-value problem, they constitute an orthogonal set [11]. By combining this property with the fact that the guided modes and the radiation modes form a complete set, we may express any field distribution within the
waveguide as a superposition of guided and radiation modes [8], i.e.

$$\Psi(x, z) = \sum_{m=0}^{m_{\text{max}}} c_m \phi_m(x)e^{-i\beta_m z} + \int_{0}^{\infty} c_\rho \phi_\rho(x)e^{-i\beta_\rho z}d\rho, \quad (2.15)$$

where $\rho$ labels the continuum of radiation modes. The coefficients $|c_m|^2$ and $|c_\rho|^2$ are proportional to the power carried by the respective modes. The value of $c_m$, and similarly that of $c_\rho$, is given by the projection of the field profile at the entrance of the waveguide onto the modes,

$$c_m = \frac{\int_{-\infty}^{\infty} \Psi(x, 0)\phi_m^*(x)dx}{\int_{-\infty}^{\infty} |\phi_m(x)|^2 dx}. \quad (2.16)$$

In most cases, the contribution of radiation modes may be neglected. Once a radiation mode is excited, it loses its power due to absorption in the cladding, so that it will not reach the end of the waveguide.

2.3 Mode coupling

Density variations within a waveguide cause its refractive index to depend on the spatial coordinates like $n = n(x)$ or $n = n(x, z)$. In the first case, the wave field within the waveguide can be described in terms of modes as discussed in the previous section. Nevertheless, it is sometimes more convenient to treat the refractive-index variation along $x$ as a perturbation of the piece-wise constant refractive-index profile corresponding to the empty waveguide and to describe the wave field in terms of the empty waveguide modes. In this way it becomes easier to understand the effect of the refractive-index variations on the wave field within the waveguide. In the second case, strictly speaking no modes exist. However, we can still write the wave field as a superposition of orthogonal modes. Usually, we take the modes belonging to the empty waveguide or the modes belonging to, e.g., $n(x, 0)$, as our basis set. The latter is more convenient for studying the influence of a $z$-dependence if $n(x, z) = f(x)g(z)$. In both cases, the modes of the 'undisturbed' waveguide are coupled to each other due to the refractive-index variations, i.e., upon propagation they exchange power continuously.

In order to determine the coupling strengths between modes for the most general case, we write the field amplitude within the perturbed waveguide, with
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refractive-index profile \( n(x, z) \), as a superposition of the modes \( \phi_m \) belonging to the undisturbed waveguide having a refractive-index profile \( n_0(x) \):

\[
\Psi(x, z) = \sum_{m=0}^{\infty} c_m(z) \phi_m(x) e^{-i\beta_m z}, \tag{2.17}
\]

where the propagation constant \( \beta_m \) corresponds to the mode \( \phi_m \). The expansion coefficients \( \{c_m(z)\} \) now depend on \( z \). We have simplified the notation of Eq. (2.15) by setting the upper limit of the summation to infinity, so as to indicate the contribution of radiation modes. The linear combination is only in terms of forward propagating modes; at x-ray wavelengths there is negligible backward scattering of waves from refractive-index variations because \( \Delta n/n \ll 1 \). Substitution of Eq. (2.17) into Eq. (2.3a) results in

\[
\sum_{m=0}^{\infty} \phi_m e^{-i\beta_m z} \left( \frac{d^2c_m}{dz^2} - 2i\beta_m \frac{dc_m}{dz} - \beta_m^2 c_m \right) + c_m e^{-i\beta_m z} \left( \frac{d^2\phi_m}{dx^2} + k_0^2 n^2 \phi_m \right) = 0. \tag{2.18}
\]

If we now make use of the fact that the modes \( \phi_m \) fulfil Eq. (2.5) (with \( n = n_0(x) \)), we obtain

\[
\sum_{m=0}^{\infty} \phi_m e^{-i\beta_m z} \left( \frac{d^2c_m}{dz^2} - 2i\beta_m \frac{dc_m}{dz} \right) = -\sum_{m=0}^{\infty} c_m e^{-i\beta_m z} k_0^2 [n(x, z)^2 - n_0(x)^2] \phi_m. \tag{2.19}
\]

Multiplying both sides in Eq. (2.19) with \( \phi_k^* \) and by making use of the orthogonality of the modes, gives

\[
\frac{d^2c_k}{dz^2} - 2i\beta_k \frac{dc_k}{dz} = -\frac{k_0^2}{P_k} \sum_{m=0}^{\infty} c_m e^{i(\beta_k - \beta_m)z} \int_{-\infty}^{\infty} \phi_k^* [n(x, z)^2 - n_0(x)^2] \phi_m dx, \tag{2.20}
\]

where

\[
P_k = \int_{-\infty}^{\infty} |\phi_k(x)|^2 dx \tag{2.21}
\]

is the power in mode \( k \). Now we neglect the second-order derivative in \( z \), since [12]

\[
\frac{|d^2c_k|}{dz^2} \ll \left| 2i\beta_k \frac{dc_k}{dz} \right|. \tag{2.22}
\]
This reduces Eq. (2.20) to the following set of coupled differential equations:

\[
\frac{d c_k(z)}{d z} \approx \sum_{m=0}^{\infty} c_m(z) \Gamma_{mk}(z) e^{i(\beta_k - \beta_m)z},
\]

(2.23)

where

\[
\Gamma_{mk}(z) = \frac{k_0^2}{2i\beta_m P_k} \int_{-\infty}^{\infty} \phi_m^*(x) \left[ n(x, z)^2 - n_0(x)^2 \right] \phi_m(x) dx,
\]

\[
\approx \frac{k_0}{2i k} \int_{-\infty}^{\infty} \phi_m^*(x) \left[ n(x, z)^2 - n_0(x)^2 \right] \phi_m(x) dx,
\]

(2.24)

gives the strength of the coupling between mode \(m\) and \(k\). The initial condition \(c_m(z = 0)\) is provided by projecting the wave field which is incident onto the waveguide entrance onto mode \(m\), see Eq. (2.16).

It is seen that the \(c_m\)'s oscillate as a function of \(z\). This results in a field distribution which strongly depends on the spatial coordinates due to the interference of the modes caused by the term \(e^{i(\beta_k - \beta_m)z}\). In the case that only mode \(m\) and \(k\) are coupled, the period of the oscillations of \(|c_m(z)|^2\) is given by [12]

\[
L_c = \frac{\pi}{\sqrt{(\pi/2L_b)^2 + \Gamma_{mk}^2}},
\]

(2.25)

where \(L_b = \pi/(\beta_m - \beta_k)\) is the beating length of the modes \(m\) and \(k\). As the strength of the refractive-index variations increases, the coupling length \(L_c\) decreases and the variations in the amplitude of the field are more rapid.

In order to solve the coupled-mode equations we distinguish two limits. The first is the weak-coupling limit in which the strength of the refractive-index variations is such that \(L_c\) is much larger than the length \(L\) of the waveguide. In this case, a perturbation solution to Eq. (2.23) can be found [8]. It is assumed that the amplitude of the modes do not change much over the length of the waveguide. By treating it approximately constant, we may integrate Eq. (2.23) and obtain the approximate solution to Eq. (2.23):

\[
c_k(L) \approx c_k(0) + \sum_{m=0}^{\infty} c_m(0) \int_0^L \Gamma_{mk}(z) e^{i(\beta_k - \beta_m)z} dz.
\]

(2.26)

The second limit is that of strong coupling. In this case the coupled-mode equations (2.23) are solved numerically, as will be discussed in section 2.5.2. It is in this regime that one obtains maximum sensitivity to the spatial distribution of the refractive index.
2.4 Beam propagation method

So far we have discussed methods that are based on the propagation of modes. By contrast, the beam propagation method (BPM) describes the propagation of waves in terms of total fields. This powerful numerical method was originally developed for use in underwater acoustics and seismology, before it was adapted to the simulation of wave propagation in optical devices [13]. It solves the wave equation, Eq. (2.3a), directly, given the refractive-index profile \( n(x, z) \) and the field profile incident on the waveguide entrance. In its basic form, the use of the BPM is restricted to wave propagation problems which involve scalar fields and forward propagating waves only. Alternative formulations of the BPM exist, which are able to handle vector fields [14, 15] and even back-reflections [16].

In practice, we apply the BPM whenever the refractive index is \( z \)-dependent and absorption is non-negligible. The latter is taken into account by adding a imaginary part to the refractive index, i.e. \( n = 1 - \delta + i\alpha \), where \( \alpha = \lambda\mu/4\pi \) and \( \mu \) the wavelength-dependent absorption coefficient [17]. The BPM is also used to check the consistency of results obtained with the modal techniques. It is even possible to obtain the relative strengths \( \{c_m\} \) of the modes and their propagation constants \( \{\beta_m\} \) from the BPM calculations [18].

We derive the principle of the BPM from the Helmholtz equation for TE waves:

\[
\nabla^2 \Psi + k_0^2 n^2(x, z) \Psi = 0, \quad (2.27)
\]

where \( \nabla^2 = \partial^2/\partial x^2 + \partial^2/\partial z^2 \) and \( \Psi \equiv E_y(x, z) \). First, we apply the so-called slowly varying envelope approximation [19] by substituting

\[
\Psi(x, z) = \psi(x, z) e^{-i\tilde{\beta} z}, \quad (2.28)
\]

into Eq. (2.27), which removes the rapid variations from the field. The constant \( \tilde{\beta} \) is the reference propagation constant and denotes any representative value of \( k_0 n(x, z) \) [19]. In our calculations we always used \( \tilde{\beta} = k_0 \) since \( n(x, z) \approx 1 \). Now, if we neglect the \( \partial^2 \psi/\partial z^2 \)-term, we obtain

\[
\frac{\partial \psi}{\partial z} = \frac{i}{2k_0} \left[ -\frac{\partial^2 \psi}{\partial x^2} - k_0^2 (n^2 - 1) \psi \right]. \quad (2.29)
\]

The essence of the BPM is to integrate Eq. (2.29) numerically. It calculates \( \psi(x, z + \Delta z) \), given \( \psi(x, z) \). This may be achieved in different ways [7, 19]. Section 2.5.3 presents a detailed account of the numerical implementation we have used.
By neglecting the $\partial^2 \psi/\partial z^2$-term we applied the so-called paraxial or parabolic approximation [19], which is equivalent to the approximation (2.22). This approximation is accurate if variations in the refractive index are small, i.e. $\Delta n/n \ll 1$, and if the angular spectrum of the fields is narrow, i.e. $\Delta k_x/k_0 \ll 1$ [19], where $\Delta k_x$ is the spread in $k_x$. As discussed before, the first condition is easily met for x rays. In most cases, the second condition is also easily met. If, however, $\Delta k_x$ is large, it is advisable to approximate $\partial^2 \psi/\partial z^2$ using a method of successive approximation [20].

2.5 Numerical methods

2.5.1 Finite difference mode solver (FD-MS)

Only for very few refractive-index profiles $n = n(x)$ can the modes be solved analytically, i.e. for stepped refractive-index profiles and parabolic refractive-index profiles [7]. In the other cases they are found by numerically solving:

$$\frac{d^2 \phi}{dx^2} + \left[k_0^2 n(x)^2 - \beta^2\right] \phi = 0. \quad (2.30)$$

The $x$-coordinate is discretized such that $\phi(x_0 + i \Delta x) = \phi(x_i) \equiv \phi_i$, where $i = 0, ..., N - 1$, $x_0$ the lower limit of $x$ and $\Delta x$ the step size. The derivatives are approximated by difference expressions [21], which changes Eq. (2.30) into

$$\frac{\phi_{i-1} + \phi_{i+1} - 2\phi_i}{(\Delta x)^2} + k_0^2 n(x_i)^2 \phi_i = \beta^2 \phi_i. \quad (2.31)$$

Now we group the $\phi_i$'s into a column vector $\phi = (\phi_0, \phi_1, \ldots, \phi_{N-2}, \phi_{N-1})$ and write Eq. (2.31) as a matrix eigenvalue equation

$$\mathbf{M} \cdot \phi = \beta^2 \phi, \quad (2.32)$$

where $\mathbf{M}$ is a $N \times N$ tri-diagonal matrix with the following non-zero elements:

$$M_{i,i} = -\frac{2}{(\Delta x)^2} + k_0^2 n(x_i)^2, \quad (2.33a)$$

$$M_{i,i-1} = M_{i,i+1} = \frac{1}{(\Delta x)^2}. \quad (2.33b)$$

Many numerical procedures are available for finding the eigenvalues and eigenvectors of the matrix $\mathbf{M}$. In this thesis, we applied the powerful QR-algorithm after
transforming $M$ to a Hessenberg form [22]. Once the eigenvectors and eigenvalues, i.e. the modes and propagation constants, are known, the field distribution within the waveguide is calculated using Eq. (2.15).

The matrix $M$, with the matrix elements (2.33), includes the assumption $\phi_{-1} = 0$ and $\phi_N = 0$. The boundaries of the computational window must therefore be sufficiently far away from the guiding layer so that the amplitudes of the guided modes have decayed to zero. The obtained radiation modes are those of the continuous spectrum that fulfill these boundary conditions. Therefore, it is advisable to use the FD-MS only for calculations which do not require an accurate description of radiation phenomena.

The step size $\Delta x$ should be much smaller than the oscillation period of the mode:

$$\Delta x \ll \frac{1}{\sqrt{n_1^2 k_0^2 - \beta_m^2}},$$

where $n_1$ is the refractive index of the guiding layer and $\beta_m$ the propagation constant corresponding to the mode $\phi_m$. The convergence of the numerical method was checked for a waveguide with a stepped refractive-index profile. The calculated mode profiles $\phi_m(x)$ are shown in Fig. 2.4 for a few step sizes. The lowest mode $\phi_0$ is found to converge already for $\Delta x = 24$ nm, whereas for $\phi_6$ a step size of $\Delta x \ll 24$ nm is needed. However, more stringent is a convergence test of the propagation constants $\{\beta_m\}$, see Fig. 2.5. The relative error $(\beta_m - \beta_m^c)/\beta_m^c$ in the propagation constants, with $\beta_m^c$ the value to which $\beta_m$ converges, decreases with step size as shown in Fig. 2.5b. It is seen that the difference in relative errors for $m = 0$ and $m = 13$ reduces to only one order of magnitude for $\Delta x < 3$ nm. In conclusion, the higher modes and corresponding propagation constants should be calculated with much smaller step size than the lower ones.

The finite-difference mode solver has been used to calculate field distributions within the waveguide. An example of such a calculation is shown in Fig. 2.6. The x-ray beam entered the waveguide from the left and the field profile at the entrance $\Psi(x,0)$ was chosen to excite both the TE$_2$ and TE$_3$ modes. The strong intensity variations along the $x$ and $z$ directions are the result of interference between modes due to the difference in their propagation constants (see chapter 4 for a detailed discussion). In Fig. 2.6a only guided modes were taken into account, whereas in Fig. 2.6b also radiation modes were considered. In both cases we did not use
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Figure 2.4 Mode profiles $\phi_m(x)$ calculated for a waveguide with a stepped refractive-index profile, with $n_1 = 1$, $n_2 = 1 - 2.57 \times 10^{-6}$, $W = 400$ nm and $\lambda = 0.0931$ nm. The dependence of the mode profiles on the step size $\Delta x$ is shown for the modes (a) $m = 0$, (b) $m = 4$ and (c) $m = 6$. The vertical lines indicate the boundaries between the guiding layer and the cladding. (d) The propagation constant $\beta_m$ as a function of mode number for $\Delta x = 6$ nm. The size of the computational window was $6W$. 

- For $\Delta x = 6$ nm:
  - (a) $m = 0$
  - (b) $m = 4$
  - (c) $m = 6$

- Vertical lines indicate boundaries.

- The propagation constant $\beta_m$ is shown as a function of mode number $m$.
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Figure 2.5 (a) $\beta_m$ calculated as a function of the step size $\Delta x$ for $m = 0, 1, 2, \ldots, 15$ ($m_{\text{max}} = 19$), using the same parameters as in Fig. 2.4. (b) Relative error of the propagation constant, $|\beta_m - \beta_m^c|/\beta_m^c$, as a function of $\Delta x$ for $m = 0$ and $m = 13$. For $\beta_m^c$ we took the $\beta_m$ value found for $\Delta x = 1.5$ nm.

the second term on the right-hand-side of Eq. (2.15) but only the first term with $m_{\text{max}} = 19$ and $m_{\text{max}} = 40$, respectively. As expected, the intensity in Fig. 2.6a is confined within the guiding layer. In Fig. 2.6b, also intensity outside the guiding layer is observed. This is due to the excitation of radiation modes by the incident field profile. In the absence of absorption, the radiation modes exit the waveguide without attenuation.

Comparing Figs. 2.6a and 2.6b, we only observe small differences between the intensity distributions within the waveguide. This indicates that the field within the guiding layer is accurately described by an expansion of the wave field in terms of guided modes only.

2.5.2 Solving coupled mode equations

We describe waveguiding in terms of coupled modes in order to understand the coupling mechanism due to variations in the refractive-index profile. In the following we solve the set of coupled differential equations Eq. (2.23). Let us consider a refractive-index profile $n = n(x)$. In this case the coupling coefficients $\Gamma_{mk}$ in Eq. (2.24) are constants.
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Calculated intensity distribution $|\Psi(x,z)|^2$ within a waveguide having a stepped refractive index profile ($n_1 = 1$ and $n_2 = 1 - 2.57 \times 10^{-6}$) and a guiding layer of width $W = 400$ nm. The incident field, with $\lambda = 0.0931$ nm, was chosen so as to excite both $TE_3$ and $TE_4$. In (a) only guided modes were taken into account and in (b) also radiation modes were considered. The step sizes are $\Delta x = 6$ nm and $\Delta z = 0.01$ mm and the computational window ranged from $-1000$ nm to 1200 nm.

Figure 2.6
In order to solve the set of equations Eq. (2.23),

$$\frac{dc_k}{dz} = \sum_{m=0}^{\infty} \Gamma_{mk} c_m \exp(i(\beta_k - \beta_m)z),$$  \hspace{1cm} (2.35)

we substitute

$$c_m(z) = a_m(z)e^{i\beta_m z}.$$  \hspace{1cm} (2.36)

This results in

$$\frac{da_k(z)}{dz} = \sum_{m=0}^{\infty} (\Gamma_{mk} - i\beta_m \delta_{mk}) a_m(z).$$  \hspace{1cm} (2.37)

This is a matrix equation,

$$\frac{d\mathbf{a}(z)}{dz} = -i\mathbf{Q} \cdot \mathbf{a}(z),$$  \hspace{1cm} (2.38)

with the $z$-independent matrix elements defined as

$$Q_{mk} = i\Gamma_{mk} + \beta_m \delta_{mk}$$  \hspace{1cm} (2.39)

and the column vector $\mathbf{a}$ given by $\mathbf{a}(z) = (a_0(z), a_1(z), \ldots)$. The solution to Eq. (2.38) is given by

$$\mathbf{a}(z) = \exp(-i\mathbf{Q}z) \cdot \mathbf{a}(0) = \sum_{p=0}^{\infty} e^{-i\lambda_p z} \left[ \mathbf{v}_p^T \cdot \mathbf{a}(0) \right] \mathbf{v}_p,$$  \hspace{1cm} (2.40)

where $\{\lambda_p\}$ and $\{v_p\}$ are the eigenvalues and eigenvectors of the matrix $\mathbf{Q}$, respectively. Numerically, these are obtained as discussed in section 2.5.1. The electric field amplitude follows from

$$\Psi(x, z) = \sum_{m=0}^{\infty} a_m(z) \phi_m(x),$$  \hspace{1cm} (2.41)

where $\{a_m(z)\}$ are the components of $\mathbf{a}(z)$ as calculated from Eq. (2.40), and $\{\phi_m\}$ the modes for a waveguide with a refractive-index profile $n = n_0(x)$.

### 2.5.3 Finite difference beam propagation method (FD-BPM)

In order to evaluate the field profile within a waveguide having a refractive-index profile $n = n(x, z)$, we have to solve the differential equation (2.29) numerically. This is accomplished by approximating the derivatives with finite-difference expressions. Therefore, we discretize the field amplitude, $\psi(x, z) =$
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\[ \psi(x_0 + i \Delta x, z_0 + j \Delta z) \equiv \psi_1^i, \] with \( x_0 \) and \( z_0 \) the lower limits of \( x \) and \( z \), respectively, and \( i = 0, 1, ..., N - 1 \) and \( j = 0, 1, ..., N_z - 1 \). Applying the discretisation, as given in Eq. (2.31), to Eq. (2.29), we obtain the following matrix equation

\[ \frac{\partial \psi^j}{\partial z} = \frac{i}{2k_0} M' \psi^j, \] (2.42)

where \( \psi^j = (\psi_0^j, ..., \psi_{N-1}^j) \). The \( N \times N \) matrix \( M' \) is tri-diagonal with the following non-zero matrix elements:

\[ M'_{i,i} = \frac{2}{(\Delta x)^2} - k_0^2 \left[ n(x_i)^2 - 1 \right], \] (2.43a)

\[ M'_{i,i-1} = M'_{i,i+1} = -\frac{1}{(\Delta x)^2}. \] (2.43b)

If we would assume the fields to be zero for \( x_{-1} \) and \( x_N \), unwanted reflections of waves propagating towards the boundaries of the computational window would occur. In order to avoid this, we employed so-called transparent boundary conditions [23]. These are valid under the assumption that close to the boundary the field is a plane wave, i.e.

\[ \frac{\psi_{i+1}^j}{\psi_i^j} = \frac{\psi_{i+1}^j}{\psi_i^j} = \exp(ik_x \Delta x) \equiv q_0 \] (2.44)

and similarly for the boundary values for \( i = N - 1 \). The boundary conditions are implemented by replacing \( M'_{0,0} \) and \( M'_{N-1,N-1} \) with the following expressions:

\[ M'_{0,0} = \frac{2}{(\Delta x)^2} - k_0^2 \left[ n(x_0)^2 - 1 \right] + q_0 \] (2.45a)

\[ M'_{N-1,N-1} = \frac{2}{(\Delta x)^2} - k_0^2 \left[ n(x_{N-1})^2 - 1 \right] + q_{N-1} \] (2.45b)

By integrating Eq. (2.42) with the use of the implicit Crank-Nicholson scheme [19, 22] we obtain a stable algorithm [22]. It consists of solving

\[ \psi^{i+1} - \psi^i = \frac{i \Delta z}{2k_0} M' \left( \frac{\psi^i + \psi^{i+1}}{2} \right), \] (2.46)

for \( \psi^{i+1} \). In essence, the solution found for \( z = z_j \) is propagated forward to \( z = z_{j+1} \) by means of

\[ \psi^{i+1} = \left( I + \frac{i \Delta z}{4k_0} M' \right)^{-1} \left( I - \frac{i \Delta z}{4k_0} M' \right) \cdot \psi^i, \] (2.47)
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Figure 2.7 Intensity distribution $|\Psi(x,z)|^2$, calculated with the FD-BPM, within a waveguide having a stepped refractive index profile ($n_1 = 1$, $n_2 = 1 - 2.57 \times 10^{-6} + i 1.25 \times 10^{-8}$ and $W = 400$ nm). The step sizes $\Delta x$ and $\Delta z$ were 6 nm and 0.01 mm, respectively. The computational window ranged from -1000 nm to 1200 nm and the incident field, with $\lambda = 0.0931$ nm, was chosen to excite both the modes $TE_3$ and $TE_4$.

where $I$ denotes the identity matrix. With Eq. (2.47), the problem of solving a complex differential equation is reduced to inverting the matrix $I + (i\Delta z/4k_0)M'$. Numerically this is not a difficult task.

As for the FD-MS, we have to check the convergence of the obtained solution. Here, three parameters influence the convergence: $\Delta x$, $\Delta z$ and the size of the computational window. In practice, we repeat the calculations with reduced step sizes until the solution converges. The size of the computational window must be sufficiently large so as to avoid reflections of waves from its boundaries, which may occur in spite of the use of transparent boundary conditions.

For illustration, we consider the same waveguiding conditions as were assumed for the calculations shown in Fig. 2.6. We added a imaginary part to the refractive index of the cladding so as to include absorption. The intensity distribution within the guiding layer is the same as the distribution obtained with FD-MS, compare
Figure 2.8 (a) The spherical waves emitted by a point within the exit plane of the waveguide are also reflected, causing interference between the reflected and non-reflected wave fronts. (b) The far-field angular intensity distributions are calculated from the overlap between the field distribution at the waveguide exit $\Psi(x, L)$ and the 'modes' $\phi_e(x)$ allowed within the half-space behind the waveguide exit.

Fig. 2.7 and Fig. 2.6b. However, because of absorption, waves propagating within the cladding are attenuated and do not reach the waveguide exit.

Extremely small step sizes $\Delta x$ and $\Delta z$ result in unacceptably long computation times. Although this problem did not occur for the refractive index profiles considered in this thesis, there are ways to reduce the computation time to an acceptable level. One of them is to approximate $\partial^2 \psi/\partial z^2$ (see Section 2.4), which allows for greater step sizes. Another option is to use a non-uniform discretisation such that a small step size $\Delta x$ or $\Delta z$ is chosen in regions where the refractive index varies rapidly over small distances in the $x$ or $z$ direction, respectively.

2.6 Propagation of waves emerging from the waveguide

Experimentally, we identify the modes exiting the waveguide by measuring the intensity of the outgoing wave field as a function of the angle $\theta_e$ (see Fig. 2.8a). With the detector placed in the far field, such angular intensity distributions correspond to Fraunhofer diffraction patterns. Comparing the measured patterns with
patterns deduced from calculated field distributions at the exit of the waveguide \( \Psi(x, L) \), in combination with a search for the best fit, we are able to deduce the refractive index profile of the waveguide (see e.g. chapter 6).

In order to calculate the Fraunhofer diffraction patterns correctly we have to take into account the reflections of outgoing waves from the lower surface (see Fig. 2.8a). Therefore, let us consider, within the exit plane of the waveguide, a ribbon along the y-direction at a position \( x \) with an infinitesimal width \( dx \). Such a ribbon emits a cylindrical wave. For angles \( \theta_e > 0 \), the far-field amplitude due to the cylindrical waves emitted from positions \( x > 0 \), is given by [6]

\[
A(\theta_e) = \left( \frac{i}{R\lambda} \right)^{1/2} e^{-ik_0R} \int_0^\infty \Psi(x, L) \cdot e^{-ik_0\theta_e x} dx,
\]

(2.48)

with \( R \gg W^2/\lambda \) the distance between the waveguide exit and the detector. The far-field amplitude due to the reflected waves is given by

\[
A_r(\theta_e) = \left( \frac{i}{R\lambda} \right)^{1/2} e^{-ik_0R} \int_0^\infty \Psi(x, L) \cdot r e^{ik_0\theta_e x} dx.
\]

(2.49)

Here, \( r \) is the complex amplitude reflection coefficient of the reflecting surface, which is given by Eqs. (2.10) and (2.11). Due to the evanescent waves, the field amplitude is not exactly zero within the lower plate. Hence, we also have to include the cylindrical waves originating from positions \( x < 0 \). Their far-field amplitude after transmittance through the surface is given by

\[
A_t(\theta_e) = \left( \frac{i}{R\lambda} \right)^{1/2} e^{-ik_0R} \int_{-\infty}^0 \Psi(x, L) \cdot t e^{-ik_0\theta_e x} dx,
\]

(2.50)

where \( t = 1 + r \) is the complex amplitude transmission coefficient [10]. By adding the three contributions, we obtain the following expression for the far-field angular intensity distribution [6]:

\[
I(\theta_e) = \left| \left( \frac{i}{R\lambda} \right)^{1/2} e^{-ik_0R} \left[ \int_0^\infty \Psi(x, L) \cdot (e^{-ik_0\theta_e x} + r e^{ik_0\theta_e x}) dx \right. \\
\left. + \int_{-\infty}^0 \Psi(x, L) \cdot t e^{-ik_0\theta_e x} dx \right] \right|^2.
\]

(2.51)

For illustration, we assume that the penetration depth of the x rays into the lower surface is zero, i.e. \( \phi = \pi \). In this case, \( r = -1 \) and \( t = 0 \), which reduces Eq.
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Figure 2.9 (a) Calculated intensity of the wave field ($\lambda = 0.0931$ nm) in the vicinity of the waveguide exit ($n_1 = 1$, $n_2 = 1 - 2.57 \times 10^{-6}$ and $W = 400$ nm). (b) Fraunhofer diffraction pattern calculated using Eq. (2.53).

Examine this expression, we note that $\sin(k_0 \theta_e x)$ gives the $x$-dependence of the 'modes' allowed within the half-space behind the waveguide exit (see Fig. 2.8b). In general, the intensity distribution is proportional to the overlap of the field amplitude at the exit of the waveguide and the modes $\phi_e(x)$, i.e.

$$I(\theta_e) = 4 \left| \left( \frac{i}{RL} \right)^{1/2} e^{-ik_0 R} \int_{0}^{\infty} \Psi(x, L) \sin(k_0 \theta_e x) dx \right|^2 .$$

(2.52)

The $\phi_e(x)$ may be interpreted as the modes of a waveguide with infinite gap width $W$. The angular spacing between the corresponding mode angles $\Delta \theta_m = \lambda/2W$ (see Eq. (2.13)) is infinitesimally small, so that the modes form a continuum.

To illustrate the above, we calculated the intensity of the field $|\Psi(x, z)|^2$ near the exit of an empty waveguide (Fig. 2.9a). We excited a TE$_2$ mode at the entrance of the waveguide, which reaches the exit undisturbed. The angle $\theta_e$ at which the intensity is seen to exit the waveguide, equals the mode angle $\theta_2$ of the TE$_2$ mode. This is also clear from the diffracted intensity shown in Fig. 2.9b, which exhibits a maximum at $\theta_e = \theta_2$. As expected, there is no intensity at other mode angles.
The subsidiary diffraction maxima are due to the finite extent of the wave field across the exit plane.