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On the Reference Wave Vector of Paraxial Helmholtz Equations

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ON THE REFERENCE WAVE VECTOR OF PARAXIAL HELMHOLTZ EQUATIONS

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Abstract

The reference wave vector of the paraxial Helmholtz equation is determined using various strategies which result all in similar expressions. The effort for its evaluation is so small that the reference wave vector can be adapted for each propagation step of an arbitrary BPM-algorithm.

1 Introduction

The propagation of beams in an inhomogeneous half-space forms one of the canonical problems of integrated optics. The corresponding computer simulation is called beam propagation method (BPM) irrespective of the underlying mathematical procedure [1]. During the last years a couple of new algorithms were developed to extend the range of application to high-contrast step-index waveguide structures [2]. This includes extensions of the split operator technique [3], various algorithms based on explicit and implicit finite differences [4], static and adaptive z-transient variational principles [5], [6] and various algorithms based on the eigenmode analysis such as the method of lines [7]. A BPM benchmark test [9] carried out by many groups has clearly shown that not only the underlying algorithm but also the choice of the reference wave vector substantially affects the accuracy of the simulation results. This influence is well known and has been discussed in previous publications. It was proposed to choose the wave vector of the fundamental mode [8] or an average of the wave vectors of the contributing modes with respect to the underlying waveguide [4]. In the latter paper it was also remarked that the reference wave vector should be chosen such that the variation of the amplitudes becomes minimal in the direction of the wave propagation. It will turn out that exactly this is obtained by one of the strategies proposed in this paper. But in contrast to both of the papers mentioned, no direct spectral analysis of the propagation field is needed.

Within this paper various strategies to choose the reference wave vector are derived on the basis of Maxwell's equations. Although these strategies aim at different properties of the approximated solutions, they all result in similar expressions for the reference wave vector.

2 Vector Helmholtz Equations

The following discussion will be focussed to nonmagnetic and isotropic materials. All charges and currents inside the material are assumed to be described by the dielectric profile ϵ. Furthermore, the discussion is restricted to the time-harmonic behavior which is obtained as a quasi-stationary solution after all relaxation oscillations are completed. Using Gaussian units, the time-harmonic Maxwell's equations governing the electric field $\mathbf{E}$ and the magnetic field $\mathbf{H}$ are given by

$$\text{curl}\,\mathbf{E} = -ik_0\mathbf{H} \tag{1}$$

$$\text{curl}\,\mathbf{H} = ik_0\epsilon\mathbf{E} \tag{2}$$

$$\text{div}\,\epsilon\mathbf{E} = 0 \tag{3}$$

$$\text{div}\,\mathbf{H} = 0 \tag{4}$$

where k_0 designates the free space propagation constant.

The elimination of either the electric or magnetic field from Maxwell's equations leads to the vector Helmholtz equations:

$$\text{curl}\,(\text{curl}\,\mathbf{E}) = k_0^2\epsilon\mathbf{E} \tag{5}$$

$$\text{curl}\left(\frac{1}{\epsilon}(\text{curl}\,\mathbf{H})\right) = k_0^2\mathbf{H}. \tag{6}$$

Utilizing the vector identity $\text{curl}\,(\text{curl}\,\mathbf{A}) = \text{grad}\,(\text{div}\,\mathbf{A}) - \triangle\mathbf{A}$ and the reformulated Maxwell equation $\text{div}\,\mathbf{E} = -\text{grad}\,(\ln\epsilon)\cdot\mathbf{E}$ we can rewrite the vector Helmholtz equations in the alternative form:

$$\triangle\mathbf{E} = -\text{grad}\,\left(\text{grad}\,(\ln\epsilon)\cdot\mathbf{E}\right) - k_0^2\epsilon\mathbf{E} = \mathcal{L}_E\mathbf{E} \tag{7}$$

$$\triangle\mathbf{H} = -\text{grad}\,(\ln\epsilon)\times\text{curl}\,\mathbf{H} - k_0^2\epsilon\mathbf{H} = \mathcal{L}_H\mathbf{H}. \tag{8}$$

In addition to the physical solutions of interest for us the vector Helmholtz equation supports nonphysical, spurious solutions such as magnetic monopoles ($\text{div}\,\mathbf{H} \neq 0$).

3 Paraxial Helmholtz Equations

Paraxial approximation apply to fields which can be regarded as weakly disturbed plane waves, i. e. , the electric and magnetic fields can be written as

$$\mathbf{E} = \mathbf{E}_p e^{-i\mathbf{kr}} \tag{9}$$

$$\mathbf{H} = \mathbf{H}_p e^{-i\mathbf{kr}}, \tag{10}$$

where $\mathbf{k}$ represents the wave vector of the reference plane wave and $\mathbf{E}_p$ and $\mathbf{H}_p$ the (slowly varying) amplitudes. Obviously, the choice of the reference plane wave significantly affects the oscillatory behavior of the amplitudes.

The spread of the optical field in an inhomogeneous half-space, i. e. , the propagation of beams, represents the most important area of application of the paraxial Helmholtz equations. The numerical algorithms used for this task are designated as beam propagation methods (BPM). Most of them run stepwise, i. e. , they transport within one propagation step the optical field along the optical axis $\mathbf{e}_z$ from a transverse plane at the longitudinal coordinate z to a transverse plane at $z + \Delta z$. In order to further simplify the following discussion, the dielectric profile is assumed to be only a function of the transverse coordinates which are designated by the position vector $\mathbf{r}_t$ for one propagation step. The equations governing the evolution of the transversal and the longitudinal field components can be then separated.

In the following, the paraxial Helmholtz equations are derived in two different ways. Both approaches result in different strategies in order to find the best reference plane wave.

3.1 Slowly Varying Amplitude Approximation

By using these representations the vector Helmholtz equations can be reformulated in terms of the amplitudes

$$\begin{aligned}\triangle\mathbf{H}_p - 2i\mathbf{k}\cdot\nabla\mathbf{H}_p - k^2\mathbf{H}_p &= \mathcal{L}_H\mathbf{H}_p + i\,\text{grad}\,(\ln\epsilon)\times\mathbf{k}\times\mathbf{H}_p\\ \triangle\mathbf{E}_p - 2i\mathbf{k}\cdot\nabla\mathbf{E}_p - k^2\mathbf{E}_p &= \mathcal{L}_E\mathbf{E}_p + i\,\mathbf{k}\,\text{grad}\,(\ln\epsilon)\cdot\mathbf{E}_p,\end{aligned}$$

which yield after an rearrangement

$$
\begin{aligned}
-2i\mathbf{k}\cdot\nabla\mathbf{H}_p &= \mathcal{L}_H\mathbf{H}_p + (k^2-\triangle_t)\mathbf{H}_p + i\,\mathrm{grad}\,(\ln\epsilon)\times\mathbf{k}\times\mathbf{H}_p - \frac{\partial^2}{\partial z^2}\mathbf{H}_p \\
-2i\mathbf{k}\cdot\nabla\mathbf{E}_p &= \mathcal{L}_E\mathbf{E}_p + (k^2-\triangle_t)\mathbf{E}_p + i\,\mathbf{k}\,\mathrm{grad}\,(\ln\epsilon)\cdot\mathbf{E}_p - \frac{\partial^2}{\partial z^2}\mathbf{E}_p.
\end{aligned}
$$

A unified notation for the two vectorial Helmholtz equations, for the transverse electric and transverse magnetic field, as well as for the scalar Helmholtz equation yields

$$
-2i(\mathbf{k}\cdot\nabla)\mathbf{u}_p = \mathcal{H}\mathbf{u}_p + k^2\mathbf{u}_p - \frac{\partial^2\mathbf{u}_p}{\partial z^2}. \tag{11}
$$

For the further discussion, it will be assumed that the optical field $\mathbf{u}$ is normalized, i. e. ,

$$
\langle\mathbf{u}\mid\mathbf{u}\rangle = \langle\mathbf{u}_p\mid\mathbf{u}_p\rangle = 1. \tag{12}
$$

For the vector $\mathbf{H}$-field and vector $\mathbf{E}$-field formulations of the vector Helmholtz equation the amplitude vector $\mathbf{u}_p$ stands for the transverse components of the magnetic and electric fields. The corresponding operators $\mathcal{H}_H$ and $\mathcal{H}_E$ are:

$$
\mathcal{H}_H = \mathcal{L}_H - \triangle_t + i\,\mathrm{grad}\,(\ln\epsilon)\times\mathbf{k}_t\times \tag{13}
$$

$$
\mathcal{H}_E = \mathcal{L}_E - \triangle_t + i\,\mathbf{k}_t\mathrm{grad}\,(\ln\epsilon)\cdot \tag{14}
$$

For the scalar Helmholtz equation we obtain

$$
\mathcal{H}_s = -\triangle_t - k_0^2\epsilon. \tag{15}
$$

Within the framework of the paraxial approximation the amplitudes are assumed to be slowly varying. In consequence, the second derivative of the amplitude $\partial^2\mathbf{u}_p/\partial z^2$ is neglected. By using the unified formulation (11), the paraxial Helmholtz equation for the amplitudes can be formulated as

$$
-2i(\mathbf{k}\cdot\nabla)\mathbf{u_p} = \mathcal{H}\mathbf{u_p} + k^2\mathbf{u}_p. \tag{16}
$$

It should be noted, that the left hand side of this equation contains all first order derivatives of the amplitudes and that the operator $\mathcal{H}$ acts only on the transverse coordinates.

3.2 Expansion of Operators

Now the paraxial Helmholtz equation will be derived by expanding the square root operator into a Taylor series. The vector Helmholtz equation for the transverse field components can be written as

$$
\begin{aligned}
\frac{\partial^2\mathbf{u}}{\partial z^2} &= \mathcal{H}\mathbf{u} \\
&= -k^2(1+\mathcal{P})\mathbf{u},
\end{aligned} \tag{17}
$$

where the operator $\mathcal{P}$ is given by

$$\mathcal{P} = -\frac{k^2 + \mathcal{H}}{k^2}. \tag{18}$$

Equation (17) implies that the reference wave is running in z-direction. The formal square root of Equation (17) yields a first order partial differential equation with respect to the longitudinal coordinate z. The (nonlocal) square root operator can then be approximated by a formal Taylor series of the local differential operator $\mathcal{P}$

$$\frac{\partial \mathbf{u}}{\partial z} = \pm ik\sqrt{1+\mathcal{P}}\mathbf{u} \tag{19}$$

$$= \pm ik(1 + \frac{1}{2}\mathcal{P} - \frac{1}{8}\mathcal{P}^2 + \ldots)\mathbf{u}. \tag{20}$$

Since the operator $\mathcal{P}$ describes a small perturbation only the leading terms of the Taylor expansion must be taken into account. The restriction to forward propagating waves leads to the paraxial Helmholtz equation

$$\frac{\partial \mathbf{u}}{\partial z} = -ik(1 + \frac{1}{2}\mathcal{P})\mathbf{u}. \tag{21}$$

By replacing the rapidly varying field $\mathbf{u}$ by its slowly varying amplitudes $\mathbf{u}_p$ we obtain the paraxial Helmholtz equation for the amplitude derived in the previous section.

4 Adaption of Gradients

The full propagator for the Helmholtz equation is based on both the optical field $\mathbf{u}$ and its derivative $\partial \mathbf{u}/\partial z$. The paraxial Helmholtz equation, however, represents a first order differential equation with respect to the coordinate z, i. e. , the solution depends only on the initial field $\mathbf{u}$. Thus, the paraxial approximation can be optimized by adapting the gradient $\partial \mathbf{u}/\partial z$ obtained from the paraxial Helmholtz equation to its true value as close as possible.

4.1 Adaption of the Gradient $\partial u/\partial z$

For the derivation started now, it is assumed that the scalar optical field u and its paraxial approximation coincide at the initial plane $z = z_0$. It is furthermore assumed that the partial derivative $\partial u/\partial z$ is also known at the initial plane. The transformation between the optical field and its amplitude is given by

$$u = u_p e^{-i\mathbf{kr}}.$$

The gradient can then be formulated as

$$\frac{\partial u}{\partial z} = \frac{\partial u_p}{\partial z} e^{-i\mathbf{kr}} - ik_z u.$$

Thus, the condition

$$\left\| \frac{\partial u}{\partial z} - \left(\frac{\partial u_p}{\partial z} e^{-i\mathbf{kr}} - ik_z u \right) \right\| \to \min$$

represents a well suited analytical formulations of this optimization problem. By using another formulation of the varying amplitude approximation

$$\left\| \frac{\partial u_p}{\partial z} \right\| \ll \| k_z u_p \|$$

this criterion can be essentially simplified to

$$\left\| \frac{\partial u}{\partial z} + ik_z u \right\| \to \min . \tag{22}$$

4.2 Adaption of the Reference Plane Wave

Consider a transverse vector $\mathbf{r_0}$ describing an arbitrary position in the plane $z = z_0$ and a transverse vector $\mathbf{r}_0 + \mathbf{s}$ describing a position in the plane $z = z_0 + \Delta z$. The scalar field $u(\mathbf{r}_0) + \mathbf{s}$ can be approximated in the region close to $\mathbf{r_0}$ by

$$u(\mathbf{r}_0 + \mathbf{s}) \approx u(\mathbf{r}_0) + \mathbf{s} \cdot \operatorname{grad} u(\mathbf{r}_0) \tag{23}$$

The corresponding approximation for the reference plane wave yields

$$\begin{aligned} \tilde{u}(\mathbf{r}_0 + \mathbf{s}) &\approx u(\mathbf{r}_0) \exp(-i\mathbf{ks}) \\ &\approx u(\mathbf{r}_0) + \mathbf{s} \cdot (-i\mathbf{k}) u(\mathbf{r}_0). \end{aligned}$$

In order to find the best overall approximation the reference wave vector is be chosen such that

$$\operatorname{grad} u + i\mathbf{k}u \to \text{small for all } \mathbf{r_0}.$$

A natural mathematical implementation of this condition results in

$$\| \operatorname{grad} u + i\mathbf{k}u \| \to \min . \tag{24}$$

If the coordinate system is oriented such that the reference wave vector is parallel to the z-axis ($\mathbf{k} = k_z \mathbf{e}_z$) we recover the condition derived in the previous section (see Equation (22)).

The calculated minimum can be also be used to estimate the error for the field evolution along the z-axis. The corresponding error indicator e is given by

$$e = \left\| \frac{\partial u_p}{\partial z} \right\| .$$

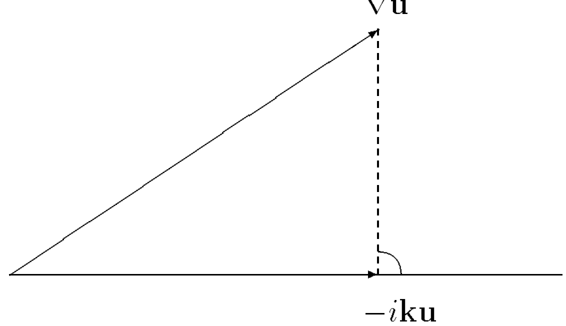

FIG. 1. *Orthogonal projection from* $\nabla\mathbf{u}$ *to* $\mathbf{ku}$

Usually, the paraxial approximation results mainly in deviations of the phase fronts. The corresponding phase error can then be written as

$$\Delta\phi = \sum_l e_l \Delta z_l.$$

In contrast to the minimization of the z-component of the group velocity presented in the previous section this approach aims at the reduction of the vectorial group velocity of the amplitudes. Although both strategies are equivalent with respect to their approximation quality, the numerical effort for the second strategy may be much smaller, especially in the context of adaptive algorithms. For a given discretization error, namely, small overall group velocities, i. e. , small variations of the amplitudes, result in a small number of transverse discretization points and in larger possible step sizes at the same time.

4.3 Vectorial Approach

The vectorial approach represents a straightforward generalization of the scalar approach. As in the previous section expansions of the optical field and the reference plane wave around $\mathbf{r}_0$ are compared.

$$\mathbf{u}(\mathbf{r}+\mathbf{s}) \approx \mathbf{u}(\mathbf{r}_0) + \mathbf{s}\cdot(\nabla\mathbf{u}(\mathbf{r}_0)) \tag{25}$$

The Taylor expansion for the reference plane wave is given by

$$\begin{aligned}\tilde{\mathbf{u}}(\mathbf{r}_0+\mathbf{s}) &\approx \mathbf{u}(\mathbf{r}_0)\exp(-i\mathbf{k}\mathbf{s})\\ &\approx \mathbf{u}(\mathbf{r}_0) + \mathbf{s}\cdot(-i\mathbf{k}\mathbf{u}(\mathbf{r}_0)).\end{aligned}$$

Obviously, the matching condition for the vector fields

$$\|\nabla\mathbf{u} + i\mathbf{k}\mathbf{u}\| \to \min \tag{26}$$

represents a natural generalization of the scalar case.

4.4 Optimization

Equation (26) covers all the optimization strategies derived before. The calculation of the minimum by deriving Equation (26) with respect to the real and imaginary parts of reference wave vector is straightforward but somewhat lengthy.

The same result may be derived by applying the projection theorem (see [10]), i. e. , we consider the orthogonal projection of a vector of a given space into a subspace. Here, the larger space is the Hilbert space defined by all tensors $\nabla \mathbf{u}$ of functions $\mathbf{u}(\mathbf{r})$ which coincide at $z = z_0$. This space is approximated by the tensors $-i\mathbf{k}\mathbf{u}$ (with arbitrary wave vectors). The wave vector $\mathbf{k}$ has to be chosen such to make the distance between $\nabla \mathbf{u}$ and $-i\mathbf{k}\mathbf{u}$ a minimum in the Hilbert space (see Fig. 1). The projection theorem states that the expression (26) has a minimum if the orthogonality condition

$$\langle \mathbf{k}\mathbf{u} \mid \nabla \mathbf{u} + i\mathbf{k}\mathbf{u} \rangle = 0 \tag{27}$$

is satisfied. The evaluation of the tensor components

$$\langle k_j u_l \mid \nabla_j u_l + i k_j u_l \rangle = k_j^* \left(\langle u_l \mid \nabla_j u_l \rangle + i k_j \right)$$

leads to the final expression

$$\mathbf{k} = \langle \mathbf{u} \mid i\nabla \mathbf{u} \rangle \, . \tag{28}$$

In physical terms: the reference wave vector should be adapted to the mean value of the momentum operator.

It should be noted that Equation (28) can also be applied to lossy media. The optimization will then result in complex reference wave vectors. The condition can also be reformulated in terms of the amplitudes by using

$$\begin{aligned}
\nabla \mathbf{u}\big|_{z=z_0} &= \left(\nabla \mathbf{u}_p - i\mathbf{k}\mathbf{u}_p\right)_{z=z_0} \exp(-i\mathbf{k}_t \cdot \mathbf{s}_t) \\
\langle \mathbf{u} \mid \nabla \mathbf{u} \rangle_{z=z_0} &= \Big\langle \mathbf{u}_p \exp(-i\mathbf{k}_t \cdot \mathbf{s}_t) \,\Big|\, \left(\nabla \mathbf{u}_p - i\mathbf{k}\mathbf{u}_p\right)_{z=z_0} \exp(-i\mathbf{k}_t \cdot \mathbf{s}_t) \Big\rangle \\
&= \langle \mathbf{u}_p \mid \nabla \mathbf{u}_p \rangle - i\mathbf{k}.
\end{aligned}$$

The final form of the condition is given by

$$\mathbf{0} = \langle \mathbf{u}_p \mid i\nabla \mathbf{u}_p \rangle \, . \tag{29}$$

In physical terms: the mean value of the momentum operator formed with amplitudes should vanish.

By using Equation (16), the best reference wave vector obtained by the adaption of gradients can also be expressed in terms of the Hamiltonian of the underlying Helmholtz equation. The resulting expression is

$$k^2 = -\langle \mathbf{u}_p \mid \mathcal{H}\mathbf{u}_p \rangle \, , \tag{30}$$

i. e. , the square of the reference wave vector should be given by the mean value of the Hamiltonian.

For a waveguide, which is excited with an eigenmode with an effective index n_l, Equation (30) leads to $k = n_l k_0$.

5 Adaption of Mean Values

5.1 Annihilation of the Mean Perturbation

The Taylor expansion of a square root (see Equation (20)) converges increasingly faster for decreasing perturbations $\mathcal{P}$. Therefore, it is natural to choose the reference wave vector k such that the mean perturbation vanishes, i. e. ,

$$\langle \mathbf{u} \mid \mathcal{P}\mathbf{u} \rangle = 0$$

which in turn yields

$$k^2 = -\langle \mathbf{u_p} \mid \mathcal{H}\mathbf{u_p} \rangle .$$

For vanishing transverse components, this condition yields again Equation (30).

5.2 Adaption of the Mean Dielectric Constant

The adaption of the mean dielectric constant obtained from the paraxial approximation to its true value, i. e. , the adaption of the centers of the excited modes to each other, represents another strategy for choosing the reference wave vector. A comparison of the right hand side of the full Helmholtz equation (17) with the square of the paraxial approximation (21) yields the following condition

$$\left| \left\langle \mathbf{u} \,\middle|\, k^2 \mathcal{P}^2 \mathbf{u} \right\rangle \right| \to \min . \tag{31}$$

The mean value of the expression $k^2\mathcal{P}^2$ will not vanish in general as long as the reference wave vector $\mathbf{k}$ is real and the operator $\mathcal{H}$ is self-adjoint. Therefore, the following condition results in the best adaption of the mean dielectric constant

$$\frac{\partial}{\partial k} \left\langle \mathbf{u} \,\middle|\, k^2 \mathcal{P}^2 \mathbf{u} \right\rangle = 0.$$

The evaluation of this expression yields

$$\begin{aligned} 0 &= \frac{\partial}{\partial k} \left\langle \mathbf{u} \,\middle|\, k^2 \mathcal{P}^2 \mathbf{u} \right\rangle \\ &= \frac{\partial}{\partial k} \left\langle \mathbf{u} \,\middle|\, k^2 \left(\frac{\mathcal{H}}{k^2} - 1 \right)^2 \mathbf{u} \right\rangle , \end{aligned}$$

and finally

$$k^4 = \left\langle \mathbf{u} \,\middle|\, \mathcal{H}^2 \mathbf{u} \right\rangle . \tag{32}$$

For a waveguide, which is excited with an eigenmode with an effective index n_l, Equation (32) again leads to a reference wave vector $k = n_l k_0$.

6 Conclusions

Various strategies to choose the reference wave vector have been presented within the framework of this paper. Any of the choices looks heuristic since it is implicitly assumed that the adaption of a single property would result in an overall optimization of the paraxial solution. However, for realistic problems all strategies presented here result in similar criteria as can be seen by applying them to a waveguide structure which is excited by an eigenmode. Therefore, it is allowed to assume that each criterion will result in a good overall optimization of the paraxial solution.

For the application in simulation programs practical criteria such as the numerical effort will determine the final choice.

Although the expressions for the reference wave vector presented here apply to the paraxial Helmholtz equation, they can also be used for more sophisticated approaches such as the wide angle approximations [11].

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Appendix

For the calculation of the approximation error a norm needs to be defined. In Hilbert spaces a norm is induced by a scalar product. For scalar functions $u(r_t)$, $v(r_t)$ it is, as usual, defined by

$$\langle u \mid v \rangle = \int u^*(\mathbf{r}_t) \cdot v(\mathbf{r}_t)\, d^2 r_t .$$

For vector functions $\mathbf{u}(\mathbf{r}_t)$, $\mathbf{v}(\mathbf{r}_t)$ it is defined by

$$\langle \mathbf{u} \mid \mathbf{v} \rangle = \int \mathbf{u}^*(\mathbf{r}_t) \cdot \mathbf{v}(\mathbf{r}_t)\, d^2 r_t = \sum_j \langle u_j \mid v_j \rangle \, .$$

For tensor functions $u(\mathbf{r}_t)$, $v(\mathbf{r}_t)$ it is defined by

$$\langle u \mid v \rangle = \int \sum_{i,j} u_{ij}^*(\mathbf{r}_t) \cdot v_{ij}(\mathbf{r}_t)\, d^2 r_t = \sum_{i,j} \langle u_{ij} \mid v_{ij} \rangle \, .$$

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