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Free-space wave propagation beyond the paraxial approximation

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Wave propagation in free space is considered without invoking the paraxial approximation. An explanation is provided for the discrepancy which arises when the general formalism is applied to the case of a Gaussian beam.

In optical propagation problems the paraxial approximation is almost invariably made in order to simplify Maxwell's equations. It is known that the paraxial solution is reasonably accurate if the beam half-width w_0 remains larger than the radiation wavelength λ throughout propagation. In some experimental situations it may be necessary to go beyond the paraxial approximation. Starting from Maxwell's equations, Lax *et al.*[1] have developed a general method to obtain corrections to the paraxial solution by expanding the electric field as a power series in terms of a small dimensionless parameter $f=(kw_0)^{-1}$ where $k=2\pi/\lambda$ is the wave number. They treat the vector problem in its full generality and their solution is applicable even to the case of a nonlinear medium. More recently, Davis[2] presented a vector theory of free-space wave propagation after assuming that the electromagnetic vector potential is linearly polarized. When expanded in powers of f, his result agrees with that of Lax *et al.*[1] when the latter is specialized to the vacuum case.

Several authors[3,4] have considered free-space Gaussian-beam propagation within the framework of a scalar theory but without invoking the paraxial approximation. For this case, the solution of the scalar Helmholtz equation subject to the appropriate boundary conditions is required. Agrawal and Pattanayak[3] solved this equation in the positive half-space $z>0$ together with the boundary condition that the scalar field $E(x,y,0)$ is a known function which they took to be a Gaussian. An angular-spectrum method was used to obtain $E(\vec{r})$ which was then expanded as a power series in the expansion parameter f to obtain corrections to the paraxial solution. Couture and Belanger,[4] on the other hand, obtained corrections to the paraxial solution using the perturbation-expansion procedure adopted in Refs. 1 and 2.

Couture and Belanger[4] recently pointed out that the first-order corrections to the paraxial solution obtained in Refs. 2–4 are not identical. They suggested that an additional condition should be imposed to obtain a unique and self-consistent correction by the method of Lax *et al.*[1] The condition imposed by them is an *ad hoc* assumption that the paraxial solution is an exact solution to Maxwell's equations along the axis of propagation. Although they were able to reconcile differences between their and Davis's results,[2] the discrepancy remained with respect to the results obtained by Agrawal and Pattanayak.[3] The purpose of this note is to clarify the situation by providing an alternative explanation for this discrepancy.

For the sake of generality, let us consider the vector theory of electromagnetic wave propagation in free space. It requires the solution of the vector Helmholtz equation

$$(\nabla^2+k^2)\vec{E}(\vec{r})=0\ , \tag{1}$$

subject to the appropriate boundary conditions. Here k is the wave number. The electric vector $\vec{E}$ can be separated in its transverse and longitudinal components

$$\vec{E}=\hat{n}E_t+\hat{z}E_z\ , \tag{2}$$

where the transverse unit vector $\hat{n}$ can, in general, be complex. It is assumed that the optical beam has a uniform polarization so that $\hat{n}$ is independent of the coordinates x and y. For simplicity we restrict our discussion to the case of linear polarization and choose $\hat{n}=\hat{x}$.

Following the formulation of Lax *et al.*,[1] we introduce the dimensionless coordinates

$$\xi=x/w_0,\quad \eta=y/w_0,\quad \zeta=z/l\ , \tag{3}$$

where $l=kw_0^2$ is the diffraction length and w_0 is the beam half-width at some plane $z\geqslant 0$. A consistent solution of Eq. (1) is obtained by expanding E_t and E_z as a power series in small dimensionless perturbation parameter

$$f=w_0/l=(kw_0)^{-1}\ . \tag{4}$$

Only alternate powers of f are found necessary :

$$E_t=\psi e^{ikz}=\left[\sum_{n=0}^{\infty} f^{2n}\psi^{(2n)}\right]e^{ikz}\ , \tag{5}$$

$$E_z=\phi e^{ikz}=\left[\sum_{n=0}^{\infty} f^{2n+1}\phi^{(2n+1)}\right]e^{ikz}\ . \tag{6}$$

The paraxial solution $\psi^{(0)}$ and the successive correction terms are obtained by solving the following set of partial differential equations:

$$\left[2i\frac{\partial}{\partial\zeta}+\frac{\partial^2}{\partial\xi^2}+\frac{\partial^2}{\partial\eta^2}\right]\psi^{(0)}=0 \ , \quad (7)$$

$$\left[2i\frac{\partial}{\partial\zeta}+\frac{\partial^2}{\partial\xi^2}+\frac{\partial^2}{\partial\eta^2}\right]\psi^{(2n)}=-\frac{\partial^2\psi^{(2n-2)}}{\partial\zeta^2} \ , \quad n\geq 1 \ . \quad (8)$$

The longitudinal components $\phi^{(2n+1)}$ are obtained in terms of the transverse components using[1]

$$\phi^{(1)}=i\frac{\partial\psi^{(0)}}{\partial\xi} \ , \quad (9)$$

$$\phi^{(2n+1)}=i\frac{\partial\psi^{(2n)}}{\partial\xi}+i\frac{\partial\phi^{(2n-1)}}{\partial\zeta} \ , \quad n>1 \ . \quad (10)$$

It should be noted that the evaluation of the longitudinal components does not require any additional boundary conditions once the transverse components have been obtained after solving Eqs. (7) and (8). The vector field $\vec{E}$ is thus completely known if E_t is specified on some surface which for a plane boundary may be taken to be the plane $z=0$. Since the transverse components evolve along z independently of the longitudinal components, further consideration can be restricted to the transverse part of the electric field only. In other words, the free-space vector problem can be reduced to a scalar problem if the boundary field has uniform polarization in the plane $z=0$.

Let us consider the solution of Eqs. (7) and (8) when $E_t(x,y,0)$ is specified. The knowledge of the boundary field $E_t(x,y,0)=E_b(x,y)$ should provide a unique $E_t(x,y,z)$ for all $z>0$. The boundary field itself may arise due to sources present in the region $z<0$, but its origin is of no concern since Eq. (1) is solved only in the positive half-space.

It is clear that $E_b(x,y)$ should determine the boundary values $\psi^{(2n)}(x,y,0)$ for all n in a unique manner. A basic requirement is that the total field $E_t(x,y,z)$ should reduce to its boundary value $E_b(x,y)$ as $z\rightarrow 0$. This requirement holds for arbitrary values of f. Since E_b is, in general, independent of f, the paraxial solution $\psi(0)$ itself should reduce to E_b as $z\rightarrow 0$. Using Eq. (5) with $z=0$, the boundary conditions are

$$\psi^{(2n)}(x,y,0)=\begin{cases}E_b(x,y), & \text{if } n=0\\ 0, & \text{if } n\geq 1 \ .\end{cases} \quad (11)$$

This is the viewpoint adopted by Agrawal and Pattanayak.[3] One may readily verify from their general solution [Eq. (20) of Ref. 3] that all corrections to the paraxial field vanish at $z=0$. Note that they used an angular-spectrum-representation method. Their method is, however, equivalent to solving the infinite set of partial differential equations (7) and (8) with the boundary condition given by Eq. (11).

We now discuss the solution obtained by Couture and Belanger.[4] They do not solve Eq. (1) from the boundary-value viewpoint as discussed above. A solution of the scalar Helmholtz equation is sought in the entire space. The boundary conditions are used at infinity by requiring that the field $E_t(x,y,z)$ behaves as an outgoing spherical wave for large z. Equation (7) is known[5,6] to have Hermite-Gauss functions as its solutions. This countably infinite set of paraxial solutions (often called the "free-space eigenmodes") is complete and has proven to be a useful basis in optical-resonator problems.[7,8] The question addressed in Ref. 4 is how this set of eigenmodes is modified when the corrections arising from Eq. (8) are incorporated. In order to be able to solve Eq. (8) an additional condition on $\psi^{(2n)}$ is needed. Couture and Belanger introduce an *ad hoc* assumption that along the z axis

$$\psi^{(2n)}(0,0,z)=0, \quad n\geq 1 \quad (12)$$

holds for all values of z. [This replaces Eq. (11).] They then show that when all corrections are incorporated the lowest-order free-space eigenmode corresponds to the field[4]

$$E_t(x,y,z)\sim \exp(ikR_c)/R_c \ , \quad (13)$$

where

$$R_c=[x^2+y^2+(z+il)^2]^{1/2} = l[(\zeta+i)^2+f^2(\xi^2+\eta^2)]^{1/2} \quad (14)$$

is the complex source point. When Eq. (13) is expanded in powers of f the zeroth-order term corresponds to the lowest-order Hermite-Gauss eigenmode.

It is clear from the above discussion that Refs. 3 and 4 solve different problems. Nonetheless, it is of some interest to investigate what boundary condition at the plane $z=0$ is required to obtain the solution given by Eq. (13). We note that Eq. (13) can be separated into a paraxial part and a nonparaxial part for all z. In particular, it is possible to expand the derived boundary field $E_t(x,y,0)$ in powers of the dimensionless parameter $f=(kw_0)^{-1}$. We obtain [cf. Eq. (18) of Ref. 4]

$$E_t(x,y,0)=\sum_{n=0}^{\infty}f^{2n}E_b^{(2n)}(x,y) \equiv Ce^{-\rho^2}\sum_{n=0}^{\infty}(f\rho)^{2n}L_n^n(\rho^2) \ , \quad (15)$$

where $L_n^n(\rho^2)$ is the associated Laguerre polynomial, C is a constant, and this expansion converges for $\rho^2=\xi^2+\eta^2<f^{-2}$. When we put $z=0$ in Eq. (5) and use Eq. (15), a term-by-term comparison yields the

prescription

$$\psi^{(2n)}(x,y,0)=E_b^{(2n)}(x,y)=Ce^{-\rho^2}\rho^{2n}L_n^n(\rho^2) \qquad (16)$$

for all n. It is not difficult to verify that, when Eq. (8) is solved using the boundary condition (16), the various corrections $\psi^{(2n)}$ do indeed turn out to be those given in Ref. 4, which simply shows the self-consistency of the scheme. It should be noted from Eq. (16) that $E_b^{(2n)}(0,0)=0$ for $n\geq 1$. This is, however, a consequence of the ansatz, Eq. (12), under which Eq. (13) was derived. The fact that the expression [Eq. (13)] for E_t is singular when $\zeta=0$ and $\rho=1/f$ indicates a nonphysical character to the boundary condition used by Couture and Belanger.[4]

We can now summarize the situation as follows. References 3 and 4 both solve the problem of free-space propagation of a Gaussian beam beyond the paraxial approximation. The different results obtained correspond to solving Eqs. (7) and (8) with the differnt boundary conditions given by Eqs. (11) and (16), respectively. Note that, in contrast to the remarks made in Ref. 4, Agrawal and Pattanayak's result is different not because of different approximations or because of mixing of different-order Hermite-Gauss modes but because they solve a different boundary-value problem, namely, one in which the field is specified on an input plane. Another important point to note is that the solution obtained in Ref. 3 is a unique solution of the Helmholtz equation (1) once the boundary field has been specified. On the other hand, the complex-source-point spherical-wave solution, Eq. (13), is obtained under the ansatz (12). This ansatz does not appear to be unique. A different ansatz will give rise to a different solution of the Helmholtz equation. In any case, the claim made by Couture and Belanger[4] that the condition (12) *must* be added in order to obtain a unique answer by the method of Lax *et al.*[1] is not generally true because a unique answer is always obtained by using the boundary condition given by Eqs. (6) without requiring their ansatz.

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