LA-6833-MS
Informal Report

UC-32 and UC-34

Issued: June 1977

A Numerical Code for the Three-Dimensional Parabolic Wave Equation

J. C. Goldstein

los alamos
scientific laboratory
of the University of California
LOS ALAMOS, NEW MEXICO 87545

UNITED STATES
ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION
CONTRACT W-7405-ENG. 36

Printed in the United States of America. Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, VA 22161
Price: Printed Copy $3.50 Microfiche $3.00

A NUMERICAL CODE FOR THE THREE-DIMENSIONAL

PARABOLIC WAVE EQUATION

by

J. C. Goldstein

ABSTRACT

This report summarizes various features of a code (originally brought to the Los Alamos Scientific Laboratory (LASL) by F. Tappert of the Courant Institute in New York) designed to solve the three-dimensional parabolic wave equation with an added nonlinear (self-focusing) term. Some exact conservation laws of the full nonlinear equation are considered. The precise numerical method used to solve the equation is explicitly displayed. Comparisons of numerically computed results with exact results for a sample pure diffraction problem are made. A discussion of various input data for the code, which now exists in two different versions, is given.

The intent of this report is to summarize various features of the code brought to the Los Alamos Scientific Laboratory (LASL) by F. Tappert several years ago. There are two versions of the code readily available: (a) Tappert's original version with additional contour and three-dimensional plots which were added by S. J. Gitomer, to be referred to as TAP1 below; (b) a version in which the Fourier manipulation is redone, partially coded in COMPASS, with different graphics output; these modifications were done by D. B. Henderson and we shall refer to this version as TAP2 below.

The code was written by F. Tappert originally to study self-focusing in a nonlinear medium. Since the small-scale instability theory of self-focusing (as given by Suydam in Ref. 1, for example) predicts that an initially axisymmetric light beam will break up into a nonaxisymmetric pattern of filaments as the beam propagates through a nonlinear medium, the code is capable of treating the propagation of a general two-dimensional wave front. The model of the medium nonlinearity in the code reduces to the usual cubic term at low light intensities but saturates at high intensities. Although the code was not intended to treat propagation through laser media, a constant gain (or loss) may be included in the calculation. Only a single wave front is propagated; hence, the nonlinear medium is assumed to respond instantaneously. Only a single polarization component of the electric field is treated. Although general two (transverse)-dimensional wave fronts can be considered, one must recall that the code does solve the paraxial or quasioptical equation rather than the full second-order wave equation so that the general limits of applicability of the paraxial approximation (e.g., limited range of Fresnel numbers in pure diffraction problems) apply.

We proceed to present the quasioptical equation, various general properties, the numerical method of solution, and some examples from diffraction theory alone (no nonlinear medium). Most of these topics are expanded versions of statements made in various notes left here by F. Tappert.

We use the slowly varying envelope representation of the full electric field E.

$$E(x,y,z;\tau) = \frac{1}{2} \mathcal{E}(x,y,z)e^{-i\omega\tau} + C.C. \qquad (1a)$$

$$\tau = t - z/v \quad (1b)$$
$$v = c/n \quad (1c)$$

where n is the linear index of refraction of the medium (only a single medium is treated by the code). The usual treatment (using Eq. (1) in the wave equation, Ref. 1; a somewhat different derivation is given in Ref. 2) then gives the following quasioptical equation for the envelope $E(x,y,z)$.

$$-2ik\frac{\partial E}{\partial z} = \nabla_\perp^2 E + k^2\delta|E|^2 E \quad (2a)$$

$$k = \frac{\omega}{v} = \frac{\omega n}{c} \quad (2b)$$

$$\delta = \frac{n_2}{n} \quad (2c)$$

$$\nabla_\perp^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \quad . \quad (2d)$$

Here n_2 is the nonlinear index of refraction of the medium [using the relation $\epsilon_2 = \frac{4}{3} nn_2$ in Eq. (2) recovers the form of this equation derived in Ref. 1, aside from a definition which interchanges E and E^* in Eq. (1)].

We consider Eq. (2) on a square region of the transverse plane:

$$0 \le x \le \ell \quad (3a)$$

$$0 \le y \le \ell \quad . \quad (3b)$$

Changing to dimensionless variables x', y',

$$\left. \begin{aligned} x' &= \frac{x}{\ell} \\ y' &= \frac{y}{\ell} \end{aligned} \right\} \leftrightarrow \left\{ \begin{aligned} x &= \ell x' \quad (4a) \\ y &= \ell y' \quad (4b) \end{aligned} \right.$$

$$\frac{\partial}{\partial x} = \frac{1}{\ell}\frac{\partial}{\partial x'}$$

$$\frac{\partial^2}{\partial x^2} = \frac{1}{\ell^2}\frac{\partial^2}{\partial x'^2} \quad ,$$

Eq. (2a) becomes

$$-2ik\frac{\partial E}{\partial z} = \frac{1}{\ell^2}\nabla_\perp'^2 E + k^2\delta|E|^2 E \quad . \quad (5)$$

We next rescale z to

$$z' = \frac{z}{k\ell^2} \quad (6)$$

so that Eq. (5) becomes

$$-i\frac{\partial E}{\partial z'} = \frac{1}{2}\nabla_\perp'^2 E + \left[\frac{k^2\ell^2}{2}\delta\right]|E|^2 E \quad . \quad (7)$$

We now define a scaled electric field envelope E' and a new constant β by

$$\beta|E'|^2 = \left[\frac{k^2\ell^2}{2}\delta\right]|E|^2 \quad (8)$$

so that finally the scaled quasioptical equation becomes

$$-i\frac{\partial E'}{\partial z'} = \frac{1}{2}\nabla_\perp'^2 E' + \beta|E'|^2 E' \quad (9a)$$

$$= \frac{1}{2}\nabla_\perp'^2 E' + \frac{\beta|E'|^2}{1+\gamma|E'|^2} E' \quad (9b)$$

$$= \frac{1}{2}\nabla_\perp'^2 E' + \left[\frac{\beta|E'|^2}{1+\gamma|E'|^2} + i\alpha\right] E' \quad . \quad (9c)$$

Here a saturable form of the nonlinearity, parameterized by γ, has been added in Eq. (9b) and a constant gain (or loss), specified by α, has been included in Eq. (9c). Notice that according to the relative signs of Eq. (9c), $\alpha>0$ corresponds to a loss while $\alpha<0$ corresponds to a gain - in contrast to the conventional usage. The three parameters α, β, and γ are referred to by their Greek names in the code.

Henceforth we shall drop the primes and assume that all quantities are scaled. Equation (9) has the form of a Schrödinger equation: in discussing some of the general properties of this equation, we will symbolize the nonlinear term by $f(|E|^2)$ and consider the equations

$$-i\frac{\partial E}{\partial z} = \frac{1}{2}\nabla_\perp^2 E + f(|E|^2)E \quad (10a)$$

$$i\frac{\partial E^*}{\partial z} = \frac{1}{2}\nabla_\perp^2 E^* + f(|E|^2)E^* \quad . \quad (10b)$$

Here we have obviously set $\alpha\equiv 0$ and thus do not consider the case of constant gain or loss. By analogy with quantum mechanics, we expect that probability or wave function normalization will be a conserved quantity. From Eq. (10) we see that

$$i\left(E^*\frac{\partial E}{\partial z} + E\frac{\partial E^*}{\partial z}\right) = i\frac{\partial}{\partial z}(E^*E) = -\frac{1}{2}E^*\nabla_\perp^2 E + \frac{1}{2}E\nabla_\perp^2 E^*$$
$$= \frac{1}{2}\vec{\nabla}_\perp \cdot \left(E\vec{\nabla}_\perp E^* - E^*\vec{\nabla}_\perp E\right)$$

$$\int dxdy\; i\,\frac{\partial}{\partial z}(E^*E) = i\,\frac{\partial}{\partial z}\int dxdy\; E^*E$$
$$= \frac{1}{2}\int dxdy\; \vec{\nabla}_\perp \cdot \left(E\vec{\nabla}_\perp E^* - E^*\vec{\nabla}_\perp E\right)$$
$$= \frac{1}{2}\int_{\text{bdry}} d\ell\; \hat{n} \cdot \left(E\vec{\nabla}_\perp E^* - E^*\vec{\nabla}_\perp E\right) \quad .$$

Assuming that $E(\vec{r}_\perp, z) \to 0$ as $\vec{r}_\perp \to \infty$ rapidly enough makes the last integral negligibly small in the limit, so that the total power in the beam is conserved.

$$i\,\frac{\partial}{\partial z}\int dxdy|E|^2 = 0 \;\Rightarrow \int dxdy|E|^2 = \text{const.} \quad (11)$$

Notice that this holds even in the presence of the nonlinear term although it has been assumed that f is a real function, that is,

$$f^*\left(|E|^2\right) = f\left(|E|^2\right) \quad . \qquad (12)$$

That is, β and γ of Eq. (9b) are real constants if that explicit form of f is used.

Again by analogy with quantum mechanics, one expects that, in the absence of constant gain or loss, total energy is conserved. We use the analogy to define a total energy <E>, but in view of the "nonlinear potential" term f we allow for a more general energy functional.

$$<E> = \int dxdy\; E^*\left[\frac{1}{2}\nabla_\perp^2 + G(|E|^2)\right]E \quad . \qquad (13)$$

Therefore,

$$i\,\frac{d}{dz}<E> = \int dxdy\Bigg\{\left(i\,\frac{dE^*}{dz}\right)\left[\frac{1}{2}\nabla_\perp^2 + G(u)\right]E$$
$$+ E^*\left[\frac{1}{2}\nabla_\perp^2 + G(u)\right]\left(i\,\frac{dE}{dz}\right)$$
$$+ E^*\left[\frac{dG}{du}\, i\,\frac{du}{dz}\right]E\Bigg\} \quad , \qquad (14)$$

where

$$u = E^*E \qquad (15)$$

$$i\,\frac{du}{dz} = i\left(\frac{dE^*}{dz}E + E^*\,\frac{dE}{dz}\right) \quad . \qquad (16)$$

Using Eq. (10) to compute the field derivatives, we obtain

$$i\,\frac{d}{dz}<E> = \int dxdy\Bigg\{\left(\frac{1}{2}\nabla_\perp^2E^* + fE^*\right)\left(\frac{1}{2}\nabla_\perp^2E + GE\right)$$
$$+\left(\underline{\frac{1}{2}\nabla_\perp^2E^*} + GE^*\right)\left(-\frac{1}{2}\nabla_\perp^2E - fE\right)$$
$$+ E^*\,\frac{dG}{du}\left[\left(\frac{1}{2}\nabla_\perp^2E^* + fE^*\right)E + E^*\left(-\frac{1}{2}\nabla_\perp^2E - fE\right)\right]E\Bigg\} \,,$$

where $\int dxdy\; E^*(\nabla_\perp^2E) = \int dxdy\; (\nabla_\perp^2E^*)E$ has been used in the underlined term. Assembling the terms we find

$$i\,\frac{d}{dz}<E> = \int dxdy\Bigg\{\left(\frac{1}{2}\nabla_\perp^2E^*\right)\left(GE - fE + u\,\frac{dG}{du}\,E\right)$$
$$-\left(\frac{1}{2}\nabla_\perp^2E\right)\left(GE^* - fE^* + u\,\frac{dG}{du}\,E^*\right)\Bigg\} \quad . \qquad (17)$$

Assuming further that

$$G^*(|E|^2 = G(|E|^2) \quad , \qquad (18)$$

we see that in order to have conservation of energy we need to choose G such that it satisfies the following equation.

$$u\,\frac{dG}{du} + G - f = 0 \quad . \qquad (19)$$

Suppose that f may be represented by

$$f(u) = \sum_{n=0}^{\infty} f_n u^n \quad , \qquad (20)$$

where the f_n are real constants. Although this is not the most general form imaginable for the nonlinear term, it does include the explicit form used in the code as in Eq. (9b). Then we may try the following representation of G.

$$G(u) = \sum_{n=0}^{\infty} g_n u^n \quad , \qquad (21)$$

where g_n are real constants. Equation (19) then gives

$$u\sum_{n=0}^{\infty} n g_n u^{n-1} + \sum_{n=0}^{\infty} g_n u^n = \sum_{n=0}^{\infty} f_n u^n \quad .$$

This is satisfied if

$$(n+1)g_n = f_n ; g_n = \frac{1}{n+1} f_n \quad .$$

Obviously this is true if

$$G(u) = \frac{1}{u}\int du f(u) \quad . \tag{22}$$

Explicitly, for the nonlinear terms of Eq. (9a) and (9b), we find the following "potential energy" functionals.

$$G_a(|E|^2) = \frac{\beta}{2}|E|^2 \tag{23a}$$

$$G_b(u) = \frac{1}{u}\int \frac{\beta u du}{1+\gamma u} = \frac{\beta}{\gamma u}\int du\left(1 - \frac{1}{1+\gamma u}\right)$$

$$G_b(u) = \frac{\beta}{\gamma u}\left[u - \frac{1}{\gamma}\ln(1+\gamma u)\right] \quad . \tag{23b}$$

By analogy with quantum mechanics, Eqs. (23a) and (23b) in Eq. (13) give the following explicit forms for the "kinetic energy" TE and the "potential energy" PE.

$$TE = \int dxdy\, E^* \frac{1}{2}\nabla_\perp^2 E = -\frac{1}{2}\int dxdy\, (\vec{\nabla}_\perp E^*)\cdot(\vec{\nabla}_\perp E)$$

$$TE = -\frac{1}{2}\int dxdy|\vec{\nabla}_\perp E|^2 \tag{24}$$

$$PE = \int dxdy\, E^* G\left(|E|^2\right)E = \frac{\beta}{2}\int dxdy\left(|E|^2\right)^2 \tag{25a}$$

$$= \frac{\beta}{\gamma}\int dxdy\left[|E|^2 - \frac{1}{\gamma}\ln\left(1+\gamma|E|^2\right)\right] \quad . \tag{25b}$$

From Eqs. (17) and (19) we have that

$$\langle E\rangle = TE + PE = \text{constant} \quad . \tag{26}$$

This affords another check, in addition to Eq. (11), on the numerical accuracy of the code. Again, Eq. (26) is a general result which does not depend on the exact form of the nonlinearity f, provided f satisfies the reality condition of Eq. (12). Recall that we are taking $\alpha \equiv 0$ in these considerations, so that there is no constant gain or loss. Apparently, in the code the algebraic sign of the quantities TE and PE are opposite to that indicated in Eq. (24) and Eq. (25). <E> is called EN in the code.

Both properties of Eq. (11) and Eq. (26) were stated in Tappert's notes but not explicitly proved. Another relation stated but not proved in those notes is the following: let us define

$$r_0^2 = \frac{\int dxdy\left(x^2+y^2\right)|E(x,y;z)|^2}{\int dxdy|E(x,y;z)|^2} \quad . \tag{27}$$

The claim is then stated that

$$\frac{d^2}{dz^2}\left(r_0^2\right) = 4\ \langle E\rangle \quad . \tag{28}$$

From Eq. (26), the right-hand side of Eq. (28) is implied to be constant in z.

To investigate the validity of Eq. (28), it is convenient to return to the formalism of quantum mechanics. To this end we define a Hamiltonian H

$$H = \frac{p^2}{2m} + V \tag{29}$$

and a momentum operator

$$\vec{p} = \frac{\hbar}{i}\vec{\nabla} \quad . \tag{30}$$

The Schrödinger equation for the wave function ψ is thus

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi$$

$$= \left(\frac{\vec{p}\cdot\vec{p}}{2m} + V\right)\psi \tag{31a}$$

$$-i\hbar\frac{\partial\psi^*}{\partial t} = H\psi^* = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi^* = \left(\frac{\vec{p}\cdot\vec{p}}{2m} + V\right)\psi^* \tag{31b}$$

assuming

$$V^* = V \quad . \tag{32}$$

Since the denominator of Eq. (27) is z independent by Eq. (11), it is sufficient to consider the numerator only. Since Eq. (31) is identical to Eq. (10) with the replacements $t = z$, $\psi = E$, $\hbar = m = 1$, we will continue to use the quantum mechanics notation and make these replacements at the end of the calculation. Thus, we define

$$\bar{r}_0^2 = \int d\tau\psi^* r^2\psi \tag{33}$$

and consider its t dependence.

$$\frac{\partial}{\partial t}\,\bar{r}_0^{\,2} = \int d\tau \left[\left(\frac{\partial\psi^*}{\partial t}\right) r^2\psi + \psi^* r^2\left(\frac{\partial\psi}{\partial t}\right)\right] \quad .$$

In what follows we use the notation A_i for the components of a vector $\vec{A}$ and assume summations over all repeated indices. Thus

$$\frac{\partial}{\partial t}\,\bar{r}_0^{\,2} = \int d\tau \left\{\left(-\frac{1}{i\hbar}\right)\left[\left(\frac{p_k p_k}{2m} + V\right)\psi^*\right] r^2\psi + \psi^* r^2\left(\frac{1}{i\hbar}\right)\left[\left(\frac{p_k p_k}{2m} + V\right)\psi\right]\right\}$$

$$= \frac{1}{2mi\hbar}\int d\tau \left\{\left(-p_k p_k \psi^*\right) r^2\psi + \psi^* r^2\left(p_k p_k \psi\right)\right\}$$

$$= \frac{1}{2mi\hbar}\int d\tau \left\{-\left(p_k p_k \psi\right)^* r^2\psi + \psi^* r^2\left(p_k p_k \psi\right)\right\} \quad .$$

Now, since

$$\int d\tau \left(p_k\psi\right)^*\psi = \int d\tau\, \psi^*\left(p_k\psi\right) \quad , \tag{34}$$

we get

$$\frac{\partial}{\partial t}\,\bar{r}_0^{\,2} = \frac{1}{2mi\hbar}\int d\tau \left\{-\left(p_k\psi\right)^* p_k r^2\psi + \psi^* r^2 p_k p_k \psi\right\} \quad . \tag{35}$$

Recalling the commutation relations

$$\left[r_i, p_j\right] = i\hbar\,\delta_{ij} = -\left[p_j, r_i\right] \quad , \tag{36}$$

we calculate

$$\left[p_k, r_i r_i\right] = \left[p_k, r_i\right] r_i + r_i\left[p_k, r_i\right] = -2i\hbar\, r_k$$

so that Eq. (35) is rewritten as

$$\frac{\partial}{\partial t}\,\bar{r}_0^{\,2} = \frac{1}{2mi\hbar}\int d\tau \Big\{-\left(p_k\psi\right)^*\left(r^2 p_k - 2i\hbar\, r_k\right)\psi$$

$$+ \psi^*\left(p_k r^2 + 2i\hbar\, r_k\right) p_k\psi\Big\}$$

$$= \frac{1}{2mi\hbar}\, 2i\hbar \int d\tau \left\{\left(p_k\psi\right)^* r_k\psi + \psi^* r_k\left(p_k\psi\right)\right\}$$

$$\frac{\partial}{\partial t}\,\bar{r}_0^{\,2} = \frac{1}{m}\int d\tau\, r_k \left\{\left(p_k\psi\right)^*\psi + \psi^*\left(p_k\psi\right)\right\} \tag{37a}$$

$$\frac{\partial}{\partial t}\,\bar{r}_0^{\,2} = 2\int d\tau\, \vec{r}\cdot\vec{J} \quad , \tag{37b}$$

where $\vec{J}$ is the current density

$$\vec{J} = \mathrm{Re}\,\psi^*\,\frac{\vec{p}}{m}\,\psi = \frac{1}{2m}\left(\psi^*\vec{p}\psi - \psi\vec{p}\psi^*\right) \quad . \tag{38}$$

Continuing, we have from Eq. (37) and Eq. (31):

$$\frac{\partial^2}{\partial t^2}\,\bar{r}_0^{\,2} = \frac{1}{m}\int d\tau\, r_k \Bigg\{\left(p_k\frac{\partial\psi}{\partial t}\right)^*\psi + \left(p_k\psi\right)^*\frac{\partial\psi}{\partial t}$$

$$+ \frac{\partial\psi^*}{\partial t}\left(p_k\psi\right) + \psi^*\left(p_k\frac{\partial\psi}{\partial t}\right)\Bigg\}$$

$$\frac{\partial^2}{\partial t^2}\,\bar{r}_0^{\,2} = \frac{1}{m}\int d\tau\, r_k \Bigg\{\left[p_k\frac{1}{i\hbar}\left(\frac{p_j p_j}{2m} + V\right)\psi\right]^*$$

$$+ \left(p_k\psi\right)^*\frac{1}{i\hbar}\left(\frac{p_j p_j}{2m} + V\right)\psi$$

$$- \frac{1}{i\hbar}\left[\left(\frac{p_j p_j}{2m} + V\right)\psi^*\right]\left(p_k\psi\right)$$

$$+ \psi^*\left[p_k\frac{1}{i\hbar}\left(\frac{p_j p_j}{2m} + V\right)\psi\right]\Bigg\}$$

$$\frac{\partial^2}{\partial t^2}\,\bar{r}_0^{\,2} = \frac{1}{2m^2 i\hbar}\int d\tau\, r_k \Big\{-\left(p_k p_j p_j\psi\right)^*$$

$$+ \left(p_k\psi\right)^*\left(p_j p_j\psi\right) - \left(p_j p_j\psi^*\right)\left(p_k\psi\right) + \psi^*\left(p_k p_j p_j\psi\right)\Big\}$$

$$+ \frac{1}{i\hbar m}\int d\tau\, r_k \Big\{\left(-p_k V\psi\right)^*\psi + \left(p_k\psi\right)^* V\psi - V\psi^*\left(p_k\psi\right)$$

$$+ \psi^*\left(p_k V\psi\right)\Big\} \quad . \tag{39a}$$

We define these two parts to be T_1 and T_2, respectively:

$$\frac{\partial^2}{\partial t^2}\bar{r}_0^{\,2} = T_1 + T_2 \quad . \tag{39b}$$

First consider T_1, being careful of the order of the terms we get.

$$T_1 = \frac{1}{2m^2 i\hbar}\int d\tau\Big\{-\left(p_k p_j p_j \psi\right)^* r_k \psi + \left(p_k\psi\right)^* r_k\left(p_j p_j \psi\right) - \left(p_j p_j\psi\right)^* r_k\left(p_k\psi\right) + \psi^* r_k\left(p_k p_j p_j \psi\right)\Big\} \quad .$$

By reordering the terms, keeping Eq. (34) in mind, we get

$$T_1 = \frac{1}{2m^2 i\hbar}\int d\tau\Big\{\psi^* p_k r_k p_j p_j \psi - \psi^* p_j p_j p_k r_k \psi + \psi^* r_k p_k p_j p_j \psi - \psi^* p_j p_j r_k p_k \psi\Big\}$$

$$= \frac{1}{2m^2 i\hbar}\int d\tau\Big\{\psi^*\left[p_k r_k, p_j p_j\right]\psi + \psi^*\left[r_k p_k, p_j p_j\right]\psi\Big\} \quad .$$

Now $r_k p_k = p_k r_k + \left[r_k, p_k\right]$; since the commutator $\left[p_k, p_k\right]$ is a c-number via Eq. (36), it commutes with $p_j p_j$ in the second term. Thus we may write

$$T_1 = \frac{1}{m^2 i\hbar}\left\langle\left[p_k r_k, p_j p_j\right]\right\rangle \quad . \tag{40}$$

Now

$$\left[p_k r_k, p_j p_j\right] = \left[p_k r_k, p_j\right]p_j + p_j\left[p_k r_k, p_j\right]$$

$$= -\left[p_j, p_k r_k\right]p_j - p_j\left[p_j, p_k r_k\right]$$

$$= -\Big\{\Big(\left[p_j, p_k\right]r_k + p_k\left[p_j, r_k\right]\Big)p_j + p_j\Big(\left[p_j, p_k\right]r_k + p_k\left[p_j, p_k\right]\Big)\Big\}$$

$$= -p_k\left(-i\hbar\delta_{jk}\right)p_j - p_j p_k\left(-i\hbar\delta_{jk}\right) \quad .$$

Therefore we get

$$\left[p_k r_k, p_j p_j\right] = 2i\hbar p_k p_k$$

and T_1 becomes, using Eq. (40),

$$T_1 = \frac{2}{m^2}\left\langle p_k p_k\right\rangle \quad . \tag{41}$$

We next consider the term T_2: again taking care to preserve the correct ordering of terms from Eq. (39a) we have

$$T_2 = \frac{1}{i\hbar m}\int d\tau\Big\{-\left(p_k V\psi\right)^* r_k\psi + \left(p_k\psi\right)^* r_k V\psi - r_k V\psi^*\left(p_k\psi\right) + r_k\psi^*\left(p_k V\psi\right)\Big\}$$

$$= \frac{1}{i\hbar m}\int d\tau\Big\{-\psi^* V p_k r_k\psi + \psi^* p_k r_k V\psi - \psi^* V r_k p_k\psi + \psi^* r_k p_k V\psi\Big\}$$

$$= \frac{1}{i\hbar m}\int d\tau\Big\{\psi^*\left(r_k p_k V - V r_k p_k\right)\psi + \psi^*\left(p_k r_k V - V p_k r_k\right)\psi\Big\}$$

$$= \frac{1}{i\hbar m}\Big\{\left\langle\left[r_k p_k, V\right]\right\rangle + \int d\tau\Big[\left(V r_k p_k\psi\right)^* - \left(r_k p_k V\psi\right)^*\psi\Big]\Big\}$$

$$= \frac{1}{i\hbar m}\Big\{\left\langle\left[r_k p_k, V\right]\right\rangle + \int d\tau\Big[\left(V r_k p_k\psi\right)\psi^* - \left(r_k p_k V\psi\right)\psi^*\Big]^*\Big\}$$

$$= \frac{1}{i\hbar m}\Big\{\left\langle\left[r_k p_k, V\right]\right\rangle - \left\langle\left[r_k p_k, V\right]\right\rangle^*\Big\}$$

$$T_2 = \frac{2}{m\hbar}\,\mathrm{Im}\left\langle\left[r_k p_k, V\right]\right\rangle \quad . \tag{42}$$

Now, since

$$\left[r_k p_k, V\right] = -\left[V, r_k\right]p_k - r_k\left[V, p_k\right]$$

and since $\left[V, r_k\right] = 0$ and $\left[p_k, F\right] = \left(p_k F\right)$ where F is any c-number function of coordinates, we have that

$$\left[r_k p_k, V\right] = r_k\left(p_k V\right) \quad . \tag{43}$$

Returning to explicit differential operator representation of $\vec{p}$, we get from Eqs. (43) and (42):

$$T_2 = \frac{2}{m\hbar}\,\mathrm{Im}\int d\tau\psi^* r_k\left(p_k V\right)\psi = \frac{2}{m\hbar}\,\mathrm{Im}\int d\tau u r_k\left(p_k V\right)$$

$$= \frac{2}{m\hbar}\,\mathrm{Im}\,\frac{\hbar}{i}\int d\tau u r_k\left(\partial_k V\right) = -\frac{2}{m}\int d\tau u r_k\left(\partial_k V\right) \quad , \tag{44}$$

where

$$\partial_k = \frac{\partial}{\partial r_k}$$

and, as in Eq. (15),

$$u = \psi^*\psi \quad .$$

Suppose we find a function h which satisfies

$$ur_k\left(\partial_k V\right) = r_k\left(\partial_k h\right) \quad . \tag{45}$$

We assume that the potential V can be expanded into a series in powers of u, as done above in Eq. (20) for the "potential" $f\left(|E|^2\right)$.

$$V = \sum_{n=0}^{\infty} V_n u^n \tag{46}$$

$$\partial_k V = \sum_{n=0}^{\infty} V_n n u^{n-1}\left(\partial_k u\right)$$

$$u\partial_k V = \sum_{n=0}^{\infty} V_n n u^n\left(\partial_k u\right) \quad .$$

It is obvious then that if h also can be expanded into a power series in u, Eq. (45) is satisfied provided that expansion is

$$h = \sum_{n=0}^{\infty} V_n \frac{n}{n+1} u^{n+1} \quad . \tag{47}$$

Therefore, assuming representations of Eqs. (46) and (47), we can write

$$T_2 = -\frac{2}{m}\int d\tau u r_k\left(\partial_k V\right) = -\frac{2}{m}\int d\tau r_k\left(\partial_k h\right). \tag{48}$$

Now, since $\partial_k\left(r_k h\right) = \left(\partial_k r_k\right)h + r_k\left(\partial_k h\right)$, and for the case of two transverse dimensions only (k=1,2), we get

$$T_2 = -\frac{2}{m}\int d\tau\left[\partial_k\left(r_k h\right) - 2h\right] \quad .$$

Assuming that $\psi \to 0$ as $\vec{r} \to \infty$ in a strong enough way, the first term will vanish in the limit and we are left with

$$T_2 = \frac{4}{m}\int d\tau h \quad . \tag{49}$$

Again, for the "potential" V represented in Eq. (46), this becomes

$$T_2 = \frac{4}{m}\int d\tau \sum_{n=0}^{\infty} V_n \frac{n}{n+1} u^{n+1} \quad . \tag{50}$$

From Eqs. (39b), (41), and (50), using the transcriptions t = z, ħ = m = 1, we recover $\left(Pr_0{}^2\right)$ from $\bar{r}_0{}^2\left(\psi{=}E\right)$ and we have derived the result

$$\frac{\partial^2}{\partial z^2}\left(Pr_0{}^2\right) = T_1 + T_2$$

$$= 4TE + 4\int d\tau \sum_{n=0}^{\infty} f_n \frac{n}{n+1} u^{n+1} \quad , \tag{51}$$

where P is defined below in Eq. (56) and is a constant by Eq. (11) (and is the total power in the beam divided by cn/8π), and where TE is given in Eq. (24) and we have returned to the notation and expansion of Eqs. (10) and (20). Recall that, from Eqs. (22) and (25), the "potential energy" term is given by

$$PE = \int d\tau E^* G(u) E = \int d\tau u \sum_{n+1}^{\infty} f_n \frac{1}{n+1} u^n \quad . \tag{52}$$

It is apparent on comparing Eq. (51) and Eq. (52) that the second term of Eq. (51) is not equal in general to PE. However, in the special circumstance that the expansion of Eq. (20) has only one term, corresponding to n=1, as is the case in Eq. (9a) which is the most frequently studied form of the quasioptical equation with a self-focusing nonlinearity, we have

$$f_1 = \beta \tag{53}$$

$$\frac{\partial^2}{\partial z^2}\left(Pr_0{}^2\right) = 4TE + 4\int d\tau \frac{\beta}{2} u^2 \tag{54}$$

$$PE = \int d\tau u \frac{\beta}{2} u = \frac{\beta}{2}\int d\tau u^2$$

so that in fact, using the definition in Eq. (26), we obtain

$$\frac{\partial^2}{\partial z^2}\left(Pr_0{}^2\right) = 4\langle E\rangle = \text{constant} \quad , \tag{55}$$

which is essentially the expression in Eq. (28) that we set out to investigate.

Therefore, it appears that Eq. (55) is not in general true. That is, in contrast to the properties of Eqs. (11) and (26) [for circumstances in which the nonlinear term f satisfies Eq. (12) and can be represented by Eq. (20)] which are true in the presence of a general class of nonlinearities, the property of Eq. (55) appears to be valid only in the circumstance that Eq. (53) is the only nonvanishing term of the expansion of Eq. (20).

Equation (55), together with Eq. (37) as written in terms of the variables of the electromagnetic wave problem rather than the quantum mechanical analogs, apparently form the "moment theory" of self-focusing. This is utilized by Suydam in Ref. 1 where the origin of this theory is cited as an untranslated Russion article by Vlasov, Petrishchev, and Talanov.[3] The present author does not read Russian and therefore thought it useful to present his own derivation of these (possibly well-known) results.

Two other quantities are kept track of in the code. Defining

$$P = \int dxdy \ |E|^2 \ , \tag{56}$$

they are

$$\frac{1}{r_1^{\ 2}} = \frac{TE}{P} \tag{57}$$

$$r_2^{\ 2} = \frac{P}{|E(0,0,z)|^2}$$

where again the code uses the negative of Eq. (24) as the definition of TE.

We next turn to the method of solution of Eq. (10): we rewrite that equation as

$$\frac{\partial E}{\partial z} = i\Big(A + B(z)\Big)E \tag{58a}$$

$$A = \frac{1}{2}\nabla_\perp^{\ 2} \tag{58b}$$

$$B(z) = f\left(|E(\vec{r},z)|^2\right) \ . \tag{58c}$$

The approximate solution of Eq. (58) is

$$E\left(\vec{r},z_0 + \Delta z\right) \approx e^{i\Delta z\left(A + B\left(z_0\right)\right)} E\left(\vec{r},z_0\right) \tag{59}$$

since as

$$\Delta z \to 0$$

$$\lim_{\Delta z \to 0} \frac{E\left(\vec{r},z_0 + \Delta z\right) - E\left(\vec{r},z_0\right)}{\Delta z}$$

$$= i\left(A + B\left(z_0\right)\right)E\left(\vec{r},z_0\right) + O(\Delta z)\left[A,B\left(z_0\right)\right]E\left(\vec{r},z_0\right) \ . \tag{60}$$

Notice that since $[A,B] \neq 0$, the full Baker-Hausdorff expansion must be used. As in Eq. (60), the commutator terms are higher order in Δz in that expansion so that as $\Delta z \to 0$ we drop them and approximate Eq. (59) by

$$E\left(\vec{r},z_0 + \Delta z\right) \simeq e^{i\Delta zB} e^{i\Delta zA} E\left(\vec{r},z_0\right) \ . \tag{61}$$

In order to evaluate the action of the first exponential, in view of Eq. (58b), we make use of a Fourier transform in the transverse coordinate $\vec{r}$: we define the transform $\tilde{E}\left(\vec{k}_\perp,z_0\right)$ of $E\left(\vec{r},z_0\right)$ by

$$\tilde{E}\left(\vec{k}_\perp,z_0\right) = \int d^2r \ e^{-i\vec{k}_\perp\cdot\vec{r}} E\left(\vec{r},z_0\right) \tag{62a}$$

$$E\left(\vec{r},z_0\right) = \int \frac{d^2k_\perp}{(2\pi)^2} e^{i\vec{k}_\perp\cdot\vec{r}} \tilde{E}\left(\vec{k}_\perp,z_0\right) \ . \tag{62b}$$

Thus

$$\nabla_\perp^{\ 2}E\left(\vec{r},z_0\right) = \int \frac{d^2k_\perp}{(2\pi)^2}\left(-k_\perp^{\ 2}\right)e^{i\vec{k}_\perp\cdot\vec{r}} \tilde{E}\left(\vec{k}_\perp,z_0\right)$$

so that expanding the exponential operator in Eq. (61) gives

$$e^{i\frac{\Delta z}{2}\nabla_\perp^{\ 2}} E\left(\vec{r},z_0\right)$$

$$= \int \frac{d^2k_\perp}{(2\pi)^2} e^{-i\frac{\Delta z}{2}k_\perp^{\ 2}} e^{i\vec{k}_\perp\cdot\vec{r}} \tilde{E}\left(\vec{k}_\perp,z_0\right) \ .$$

Therefore, from Eq. (61), we find that

$$E\left(\vec{r},z_0 + \Delta z\right) = e^{i\Delta zf\left(\left|E\left(\vec{r},z_0\right)\right|^2\right)}$$

$$\cdot \int \frac{d^2k_\perp}{(2\pi)^2} e^{-\frac{i}{2}\Delta zk_\perp^{\ 2}} e^{i\vec{k}_\perp\cdot\vec{r}} \tilde{E}\left(\vec{k}_\perp,z_0\right) \ . \tag{63}$$

If we define $Q(\vec{r})$ by

$$Q\left(\vec{r}\right) = \int \frac{d^2k_\perp}{(2\pi)^2} e^{-i\frac{\Delta z}{2}k_\perp^{\ 2}} e^{i\vec{k}_\perp\cdot\vec{r}} \tilde{E}\left(\vec{k}_\perp,z_0\right) \tag{64}$$

and then recognize that, from Eq. (63),

$$\left|E\left(\vec{r},z + \Delta z\right)\right|^2 = \left|Q\left(\vec{r}\right)\right|^2 \tag{65}$$

for nonlinear potentials f satisfying the reality condition in Eq. (12), we therefore can write that, using the representation of Eq. (20),

$$f\left(\left|E\left(\vec{r},z_0\right)\right|^2\right) = \sum_{n=0}^{\infty} f_n\left(\left|Q\left(\vec{r}\right)\right|^2\right)^n \quad . \qquad (66)$$

In particular, for the particular f used in Eq. (9b), we have

$$f\left(\left|E\left(\vec{r},z_0\right)\right|^2\right) \equiv F\left(\vec{r},z_0\right) = \frac{\beta\left|Q\left(\vec{r}\right)\right|^2}{1 + \gamma\left|Q\left(\vec{r}\right)\right|^2} \qquad (67)$$

so that the solution of Eq. (63) may be written in this case as

$$E\left(\vec{r},z_0 + \Delta z\right) = e^{i\Delta z F\left(\vec{r},z_0\right)} Q\left(\vec{r}\right) \qquad (68a)$$

$$E\left(\vec{r},z_0 + \Delta z\right) = e^{-\alpha\Delta z} e^{i\Delta z F\left(\vec{r},z_0\right)} Q\left(\vec{r}\right) \quad . \qquad (68b)$$

Equation (68b) includes the constant gain or loss term of Eq. (9c).

The Fourier integrals of Eq. (62) of course cannot be evaluated exactly. To do them numerically requires use of the finite Fourier transform. This expansion is on a finite mesh: for a function H(x) of one variable x which is periodic with period p_x, the transform pair may be defined by $\left(H\left(x + p_x\right) = H(x)\right)$

$$\Delta x = \frac{p_x}{N_x}\,; N_x = \text{positive integer} \qquad (69a)$$

$$H(n\Delta x) = \sum_{m=1}^{N_x} e^{i\left(\frac{2\pi}{p_x} m\right)n\Delta x}\, \tilde{H}\left(\frac{2\pi}{p_x} m\right) \qquad (69b)$$

$$\tilde{H}\left(\frac{2\pi}{p_x} m\right) = \frac{1}{N_x}\sum_{n=1}^{N_x} e^{-i\left(\frac{2\pi}{p_x} m\right)n\Delta x} H(n\Delta x) \quad . \qquad (69c)$$

By using the relation $\sum_{m=1}^{N} s^n = \frac{s}{1-s}\left(1 - s^N\right)$ one can explicitly verify that Eqs. (69b) and (69c) are the correctly normalized transforms by substituting Eq. (69c) into Eq. (69b).

Thus, for a two-dimensional function $E\left(\vec{r}\right) = E(x,y)$, we may define the finite Fourier transform pair similarly [we assume that E is periodic in x and y with periods p_x and p_y, $E\left(x + p_x, y + p_y\right) = E(x,y)$]:

$$\Delta x = \frac{p_x}{N_x};\ N_x = \text{positive integer} \qquad (70a)$$

$$\Delta y = \frac{p_y}{N_y};\ N_y = \text{positive integer} \qquad (70b)$$

$$E(n\Delta x,m\Delta y) = \sum_{k=1}^{N_x}\sum_{\ell=1}^{N_y} e^{i\left(\frac{2\pi}{p_x} k\right)n\Delta x} \cdot e^{i\left(\frac{2\pi}{p_y} \ell\right)m\Delta y}\, \tilde{E}\left(\frac{2\pi}{p_x} k, \frac{2\pi}{p_y} \ell\right) \qquad (70c)$$

$$\tilde{E}\left(\frac{2\pi}{p_x} k, \frac{2\pi}{p_y} \ell\right) = \frac{1}{N_x N_y}\sum_{n=1}^{N_x}\sum_{m=1}^{N_y} e^{-i\left(\frac{2\pi}{p_x} k\right)n\Delta x} \cdot e^{-i\left(\frac{2\pi}{p_y} \ell\right)m\Delta y}\, E(n\Delta x,m\Delta y) \quad . \qquad (70d)$$

Since $\vec{k}_\perp = \frac{2\pi}{p_x} k\hat{i} + \frac{2\pi}{p_y} \ell\hat{j}$, $k_\perp^{\,2} = \left(\frac{2\pi}{p_x} k\right)^2 + \left(\frac{2\pi}{p_y} \ell\right)^2$ and analogous to Eq. (64) we get

$$Q(n\Delta x,m\Delta y) = \sum_{k=1}^{N_x}\sum_{\ell=1}^{N_y} e^{i\left(\frac{2\pi}{p_x} k\right)n\Delta x}\, e^{i\left(\frac{2\pi}{p_y} \ell\right)m\Delta y} \cdot e^{-\frac{i\Delta z}{2}\left\{\left(\frac{2\pi}{p_x} k\right)^2 + \left(\frac{2\pi}{p_y} \ell\right)^2\right\}}\, \tilde{E}\left(\frac{2\pi}{p_x} k, \frac{2\pi}{p_y} \ell\right) \qquad (71)$$

and similarly to Eq. (67)

$$F(n\Delta x,m\Delta y;z_0) = \frac{\beta\left|Q(n\Delta x,m\Delta y)\right|^2}{1 + \gamma\left|Q(n\Delta x,m\Delta y)\right|^2} \qquad (72)$$

so that the solutions in Eq. (68) become

$$E(n\Delta x,m\Delta y;z_0 + \Delta z) = e^{i\Delta z F(n\Delta x,m\Delta y;z_0)} Q(n\Delta x,m\Delta y) \qquad (73a)$$

$$E(n\Delta x,m\Delta y;z_0 + \Delta z) = e^{-\alpha\Delta z} e^{i\Delta z F(n\Delta x,m\Delta y;z_0)} Q(n\Delta x,m\Delta y) \quad . \qquad (73b)$$

This is explicitly the solution evaluated by the code. That is, given an initial field $E(x,y;0)$, $\tilde{E}(x,y;0)$ is computed via Eq. (70d). Q is then computed from Eq. (71), F from Eq. (72), and $E(x,y;\Delta z)$ is then evaluated from Eq. (73b). The procedure is then iterated until the number of longitudinal steps specified in the input data (parameter NZ in the code) is reached. Appendix A gives a full list of input parameters and their meaning.

We have made some checks of the numerical accuracy of this code. Since exact analytic solutions to the complete (diffraction plus self-focusing) Eq. (9) are not known, we have limited ourselves to examining diffraction problems only with no nonlinear index effects. Notice that when $f\equiv 0$, Eq. (63) is the exact solution of Eq. (58) (with $B\equiv 0$) for arbitrary Δz..

The Kirchhoff-Fresnel diffraction integral for the field envelope $\mathcal{E}(x,y;z)$ resulting from an initial field $\mathcal{E}(x',y';0)$ present in a plane slit aperture located at z=0 is

$$\mathcal{E}(x,y;z) = \left(-\frac{ia}{\pi}\right) e^{-i\left(x^2+y^2\right)} \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dy'$$

$$\cdot\, \mathcal{E}(x',y';0) e^{-i(a-b)\left(x'^2+y'^2\right)} e^{2ia(xx'+yy')} \tag{74a}$$

$$a = \frac{\pi}{\lambda z} \tag{74b}$$

$$b = \frac{\pi}{\lambda F} \quad . \tag{74c}$$

Here F is the initial focal length of the wave ($F \to \infty$ or $b \to 0$ corresponds to a plane wave at the aperture). Since the code can consider only a finite plane region, we choose the initial field envelope to have a Gaussian profile in $x'\left(\theta(x) = 1 \text{ for } x > 0\right.$ and $\left.\theta(x) = -1 \text{ for } x < 0\right)$ and a width L in y'.

$$\mathcal{E}(x',y';0) = \mathcal{E}_0 e^{-\frac{1}{2}\left(\frac{x'}{w_x}\right)^2} \left[\theta\left(y' + \frac{L}{2}\right) - \theta\left(y' - \frac{L}{2}\right)\right]. \tag{75}$$

In subsequent comparisons with numerical results, w_x will be chosen to be much smaller than the finite width of the region from which the numerical solution is obtained. Next, we scale the coordinates x',y' by half the slit width L/2; notice that this is not quite the scaling defined in Eq. (4) which is used in the code.

$$\bar{x} = \frac{x}{L/2} \; , \; \bar{x}' = \frac{x'}{L/2} \tag{76a}$$

$$\bar{y} = \frac{y}{L/2} \; , \; \bar{y}' = \frac{y'}{L/2} \tag{76b}$$

$$\mathcal{E}(\bar{x}',\bar{y}';0) = \mathcal{E}_0 e^{-\frac{1}{2}\left(\frac{L/2}{w_x}\bar{x}'\right)^2} \left[\theta(\bar{y}'+1) - \theta(\bar{y}'-1)\right] \tag{77}$$

Substituting Eqs. (76) and (77) into Eq. (74), we obtain

$$\mathcal{E}(\bar{x},\bar{y};z) = \left(-\frac{ia}{\pi}\right)\left(\frac{L}{2}\right)^2 \mathcal{E}_0 e^{-ia\left(\frac{L}{2}\right)^2\left(\bar{x}^2+\bar{y}^2\right)} I_x I_y \tag{78a}$$

$$I_x = \int_{-\infty}^{\infty} d\bar{x}' e^{-\frac{1}{2}\left(\frac{L/2}{w_x}\bar{x}'\right)^2} \cdot e^{-i(a-b)\left(\frac{L}{2}\right)^2\bar{x}'^2 + 2ia\left(\frac{L}{2}\right)^2\bar{x}\bar{x}'} \tag{78b}$$

$$I_y = \int_{-1}^{+1} d\bar{y}' \, e^{-i(a-b)\left(\frac{L}{2}\right)^2\bar{y}'^2 + 2ia\left(\frac{L}{2}\right)^2\bar{y}\bar{y}'} \quad . \tag{78c}$$

We are interested only in the intensity at the center ($\bar{x}$=0,$\bar{y}$=0) of the diffraction pattern. Thus, we need only

$$I_x(\bar{x}=0) = \int_{-\infty}^{\infty} d\bar{x}' \exp\left\{-\left[\frac{1}{2}\left(\frac{L/2}{w_x}\right)^2 + i(a-b)\left(\frac{L}{2}\right)^2\right]\bar{x}'^2\right\}$$

$$= \left[\frac{\pi}{\frac{1}{2}\left(\frac{L/2}{w_x}\right)^2 + i(a-b)\left(\frac{L}{2}\right)^2}\right]^{1/2} .$$

Writing this result in amplitude and phase form gives

$$I_x(\bar{x}=0) = \frac{\sqrt{\pi}}{\left[\frac{1}{4}\left(\frac{L/2}{w_x}\right)^4 + (a-b)^2\left(\frac{L}{2}\right)^4\right]^{1/4}} e^{i\frac{\theta}{2}} \tag{79a}$$

$$\tan\theta = -2w_x^2(a-b) \quad . \tag{79b}$$

Turning next to the $\bar{y}'$ integral, we need only

$$I_y(\bar{y} = 0) = \int_{-1}^{+1} d\bar{y}' \, e^{-i(a - b)\left(\frac{L}{2}\right)^2 \bar{y}'^2}$$

$$= 2\int_0^1 d\bar{y}' \left\{ \cos\left[(a - b)\left(\frac{L}{2}\right)^2 \bar{y}'^2\right] - i \sin\left[(a - b)\left(\frac{L}{2}\right)^2 \bar{y}'^2\right] \right\}.$$

We next define the variable u by

$$\frac{\pi}{2} u^2 = (a - b)\left(\frac{L}{2}\right)^2 \bar{y}'^2 \tag{80}$$

and get

$$I_y(\bar{y} = 0) = 2\left[\frac{\pi/2}{(a - b)\left(\frac{L}{2}\right)^2}\right]^{1/2} \cdot \int_0^\omega du \left\{ \cos\left(\frac{\pi}{2} u^2\right) - i \sin\left(\frac{\pi}{2} u^2\right) \right\}$$

where

$$\omega = \left[\frac{(a - b)\left(\frac{L}{2}\right)^2}{\pi/2}\right]^{1/2} .$$

The Fresnel sine and cosine integrals $S(\omega)$ and $C(\omega)$ are defined by

$$S(\omega) = \int_0^\omega du \, \sin\left(\frac{\pi}{2} u^2\right) \tag{81a}$$

$$C(\omega) = \int_0^\omega du \, \cos\left(\frac{\pi}{2} u^2\right) . \tag{81b}$$

We now define the Fresnel number N_F by

$$N_F = \frac{(L/2)^2}{\lambda}\left(\frac{1}{z} - \frac{1}{F}\right) = N_F{}^o\left(1 - \frac{z}{F}\right) \tag{82a}$$

$$N_F{}^o = \frac{(L/2)^2}{\lambda z} \tag{82b}$$

so that finally

$$I_y(\bar{y} = 0) = \sqrt{\frac{2}{N_F}} \left\{ C(\omega) - iS(\omega) \right\} \tag{82c}$$

$$\omega = \sqrt{2N_F} \quad . \tag{82d}$$

The on-axis intensity will be

$$I(\bar{x} = \bar{y} = 0; z) = \frac{c}{8\pi} \left| E(\bar{x} = \bar{y} = 0; z \right|^2 \quad .$$

Calling $I_0 = \frac{c}{8\pi} |E_0|^2$, we find from Eqs. (78), (79), and (82)

$$\frac{I(\bar{x} = \bar{y} = 0; z)}{I_0} = 2\left(\frac{N_F{}^o}{N_F}\right)^2 \left\{ \frac{\pi N_F \left[\frac{2w_x{}^2}{(L/2)^2}\right]}{\sqrt{1 + \left[\pi N_F \frac{2w_x{}^2}{(L/2)^2}\right]^2}} \right\} \cdot \left\{ C^2\left(\sqrt{2N_F}\right) + S^2\left(\sqrt{2N_F}\right) \right\} \quad . \tag{83}$$

To compare some numerical results with Eq. (83), the following specific calculations were done: as in Eq. (3), a square region of side ℓ in the transverse plane was considered. In particular,

$$\frac{L/2}{\ell} = 0.2 \tag{84}$$

$$\frac{w_x}{\ell} = 0.1473591669 \tag{85}$$

were chosen. Equation (85) means that the electric field amplitude at the edge of the computational region in the x direction is down to 3.162277×10^{-3} of the central amplitude. A plane wave $F \rightarrow \infty$ was chosen ($N_F \rightarrow N_F{}^o$) and the patterns at distances z corresponding to several different Fresnel numbers were computed. As we have already noted above, Eq. (63) is the exact solution of Eq. (58) with no non-linear term present ($B \equiv 0$ in Eq. (58)) for arbitrary Δz, so these calculations were all done in a single step. The patterns were evaluated at the scaled distances z' given by $z' = z/k\ell^2 = n \cdot 9.947183943 \times 10^{-5}$ where n = 1,2,3,4,5,6,7,8. These distances correspond to Fresnel numbers:

TABLE I

COMPARISON OF RATIO OF CENTRAL INTENSITY
TO INITIAL CENTRAL INTENSITY
FOR VARIOUS FRESNEL NUMBERS

N_F	Exact	TAP1	TAP2
∞	1.000000	1.000000	1.000000
64	0.9451652	1.004437	1.004238
32	0.92315958	1.027129	1.026721
21 1/3	0.96998127	0.8243172	0.8238254
16	0.8925561	0.9684277	0.9676574
12.8	0.9590980	1.172372	1.171207
10 2/3	1.1973	1.218176	1.216723
9.1428	1.073	1.013224	1.011814
8	0.84995	0.8971402	0.8957135

$$N_F{}^0 = \frac{(L/2)^2}{\lambda z} = \frac{64}{n}$$

$= 64, 32, 21\ 1/3, 16, 12.8, 10\ 2/3, 9.1428, 8$.

These calculations were done with the maximum resotion available, namely, using a grid of 256 x 256 points in the transverse plane. Both versions of the code were used, Tappert's "original" version (with additional graphics capability added by S. J. Gitomer), which we refer to as TAP1, and D. B. Henderson's considerably recoded and speeded up version, which we refer to as TAP2. The results are shown in Table I in which the numerical results are compared to each other and the exact results using Eq. (83). Values of the Fresnel integrals were taken from Ref. 4. No elaborate interpolations were done in computing the "exact" results, so that they are surely not accurate to six figures. However, it may be seen that six figures of accuracy are not needed to reveal the differences between those values and the numerically computed values. It is heartening that at least the values provided by the two versions of the code are in close agreement with each other.

Although the calculated diffraction patterns do appear qualitatively correct (N intensity peaks in the y direction in the x=0 plane for a Fresnel number of N), it may be seen that indeed great quantitative accuracy has not always been achieved. It does not seem possible to ascribe these discrep-

TABLE II

COMPARISON OF TAP2 WITH "EXACT" RESULT FOR
$\bar{Y} = -0.8007815$ and $\bar{\alpha}^2 = 1.085736203$
FOR VARIOUS FRESNEL NUMBERS

N_F	Exact	TAP2
64	1.1388	1.234241
32	1.0059	0.9695197
21 1/3	1.3628	1.332852
16	1.3047	1.359248
12.8	1.2141	1.212875
10 2/3	1.2317	1.276262
9.1428	1.0337	1.067020
8	0.98616	1.068518
7.1111	0.98629	0.9425886
6.4	0.97958	1.013044

ancies to the small value of the initial field at the edge of the numerical grid, although that is a source of error. At lower Fresnel numbers, the fact that the numerical problem being solved is actually diffraction from an infinitely repeated array of apertures in the transverse plane ("aliasing") becomes visibly apparent. Calculations done at Fresnel numbers between 3.6 and 0.36 (to check the guess that since the Fresnel integral term in Eq. (83) seems to reach a maximum value around $N_F{}^o = 0.72$, the entire pattern should have a global maximum in the central intensity ratio near that point) rapidly degenerate into patent nonsense. Some attempts at filtering high transverse Fourier components by smoothing the initial field in the y direction ("soft aperturing") instead of suddenly truncating it to zero did not improve the numerical results. Notice that since the code operates on the electric field, a small error of x% in Table I corresponds to x/2% approximately in the actual numerical calculation.

Differences between TAP1 and TAP2 appear significant with respect to running time. Although these calculations do not provide a complete comparison, we note that TAP1 required 124 seconds of 7600 CPU time to calculate eight diffraction patterns, while TAP2 required 91 seconds to calculate ten patterns (including Fresnel numbers 7.111 and 6.4 in addition to those listed in Table I). TAP1 calculated only five patterns in the same time unless its detailed contour plots were eliminated.

In Appendix B the complete diffraction pattern resulting from the initial field of Eq. (75) is derived. In Table II a comparison of the "exact" and TAP2 values for the intensity ratio in the x=0 plane for a specific value of y is made. We have picked the value $y' = -0.1601563$ (Eq. (14) scaling) or $\bar{y} = -0.8007815$ (Eq. (76) scaling). The parameter $\bar{\alpha}^2$ (Eq. (B-2a)) is equal to 1.085736203 for this problem.

The numerical results demonstrated conservation of the quantities of Eqs. (11) and (26) to six significant figures in these calculations.

In conclusion, we have derived a number of exact conservation laws for the nonlinear parabolic wave equation. These relations appear to be known under the name "moment theory" and were first derived in Ref. 3. The precise finite Fourier transform method used by the code to solve the equation is made explicit. Some input parameters are cited in Appendix A. Comparison of numerically computed results for a pure diffraction problem reveals very good agreement between the two different versions of this code and fair (usually better than 10% in the intensity) agreement with the exact solution (derived in Appendix B) over a considerable range of Fresnel numbers.

REFERENCES

1. B. R. Suydam, "Self Focusing of Very Powerful Laser Beams II," IEEE J. of Q. El. QE-10, 837 (Nov. 1974).

2. M. Lax, W. H. Louisell, and W. B. McKnight, "From Maxwell to Paraxial Wave Optics," Phys. Rev. A 11, 1365 (Apr. 1975).

3. S. N. Vlasov, V. A. Petrishchev, and V. I. Talanov, "Usrednennoe opisanie volnovykh puchkov v lineinykh i neleinykh sredakh (Metod momentov)" (in Russian), Izv. Wyssh. Ucheb. Zaved. Radiofiz., 14, pp. 1353-1363 (1971).

4. T. Pearcey, "Table of the Fresnel Integrals to Six Decimal Places," Cambridge University Press, 1956; see also L. Levi, "Applied Optics," John Wiley and Sons, Inc. (New York, 1968), p. 523-524. For x > 5, the following asymptotic expressions were used from Levi:

$$\begin{matrix} C(x) \\ S(x) \end{matrix} = 0.5 \pm \left(.3183099 - \frac{.0968}{x^4}\right)\frac{1}{x}\begin{pmatrix} \sin\left(\frac{\pi}{2}x^2\right) \\ \cos\frac{\pi}{2}x^2 \end{pmatrix} - \left(.10132 - \frac{.154}{x^4}\right)\frac{1}{x^3}\begin{pmatrix} \cos\left(\frac{\pi}{2}x^2\right) \\ \sin\left(\frac{\pi}{2}x^2\right) \end{pmatrix} + E(x)$$

where $E(x) < 3 \times 10^{-7}$.

APPENDIX A
INPUT DATA

The following parameters are entered via FORTRAN Namelist input: ℓ is the length to which the transverse coordinates are scaled and $k = \frac{\omega n}{c}$ is the light wave vector in the medium of linear refractive index n.

1. ALFA = $\alpha = k\ell^2 \frac{g}{2}$; g = intensity gain ($\alpha < 0$) or loss ($\alpha > 0$) in cm^{-1}.

2. BETA = $\beta = \left(\frac{\omega}{c}\right)^2 \ell^2 n_2 \left(\frac{4\pi}{c} I_0\right)$; $I_0 = \frac{cn}{8\pi} |E_R|^2$ is some reference intensity and n_2 is the nonlinear refractive index. The code computes the scaled electric field $E'(x,y;z) = E(x,y,z)/|E_R|$ so that if $E'(0,0,0) = 1$, the scaling intensity is just the initial central intensity.

3. GAMA = $\gamma = \frac{8\pi}{cn} I_0 \gamma^*$, γ^* = unscaled nonlinear saturation parameter .

4. DZ = $\frac{\Delta z}{k\ell^2}$ dimensionless step size for physical step size Δz.

5. NZ = integer number of steps in longitudinal direction.

6. MX(MY): number of grid points in X(Y) direction is $2^{MX}(2^{MY})$; $1 \le MX(MY) \le 8$ for both versions of the code.

7. NPLOT: film plot every NPLOT longitudinal steps.

8. NP: printer plot every NP longitudinal steps.

9. IDRUN: optional identification number.

10. IFILM: movie if IFILM = 2; otherwise no movie.

The two versions of the code have somewhat different initial field options. Either one or several Gaussian beams (with or without initial curvature; propagating either along or at an angle to the z axis; with different initial amplitudes) can be chosen. The Gaussian structure is of the form:

$$E(x,y;0) = E_0 \, e^{-\frac{1}{2}\left[\left(\frac{x}{a_x}\right)^2 + \left(\frac{y}{a_y}\right)^2\right]}$$

with the code parameters GWX and GWY then given by

$$GWX(GWY) = \frac{a_x}{\ell}\left(\frac{a_y}{\ell}\right) .$$

The code parameters XO1(YO1), XO2(YO2), ... center the initial Gaussians at (XO1,YO1), (XO2,YO2), ... instead of (0,0). These Gaussians may be given different amplitudes AMP1, AMP2, ...,different initial focal lengths RO1,RO2, ..., and different propagation directions (NXO1,NYO1), (NXO2,NYO2), ...

Various other input quantities are available depending on which version of the code is used.

APPENDIX B

EVALUATION OF COMPLETE DIFFRACTION PATTERN OF TEST PROBLEM

The scaled form of the diffraction integral of Eq. (74), using the transverse coordinate scaling in Eq. (76) and the initial field in the aperture of Eq. (77), is given by Eq. (78), which we repeat here.

$$E(\bar{x},\bar{y};z) = \left(-\frac{ia}{\pi}\right)\left(\frac{L}{2}\right)^2 E_0 \cdot e^{-ia\left(\frac{L}{2}\right)^2\left(\bar{x}^2 + \bar{y}^2\right)} I_x(\bar{x})\, I_y(\bar{y}) \qquad \text{(B-1a)}$$

$$I_x(\bar{x}) = \int_{-\infty}^{+\infty} d\bar{x}' \, e^{-\frac{1}{2}\left(\frac{L/2}{w_x}\bar{x}'\right)^2} \cdot e^{-i(a-b)\left(\frac{L}{2}\right)^2 \bar{x}'^2 + 2ia\left(\frac{L}{2}\right)^2 \bar{x}\bar{x}'} \qquad \text{(B-1b)}$$

$$I_y(\bar{y}) = \int_{-1}^{+1} d\bar{y}' \, e^{-i(a-b)\left(\frac{L}{2}\right)^2 \bar{y}'^2 + 2ia\left(\frac{L}{2}\right)^2 \bar{y}\bar{y}'} . \qquad \text{(B-1c)}$$

$I_x(\bar{x})$ has already been evaluated. Defining:

$$\bar{\alpha} = \bar{\alpha}(0) = \frac{\sqrt{2}\, w_x}{(L/2)} \qquad \text{(B-2a)}$$

$$\bar{\alpha}(z) = \frac{1 + \bar{\alpha}^4 (a-b)^2\left(\frac{L}{2}\right)^4}{a^2\left(\frac{L}{2}\right)^4 \bar{\alpha}^2} = \bar{\alpha}^2\left\{\left(1 - \frac{z}{F}\right)^2 + \frac{1}{\left(\pi N_F^{o}\bar{\alpha}^2\right)^2}\right\} \qquad \text{(B-2b)}$$

$$N_F^{o} = \frac{(L/2)^2}{\lambda z} \qquad \text{(B-2c)}$$

we find that

$$I_x(\bar{x}) = \sqrt{\frac{\pi\bar{\alpha}}{\bar{\alpha}(z)\, a (L/2)^2}} \, e^{i\frac{\theta}{2}} \exp\left\{-\left[\frac{\bar{x}}{\bar{\alpha}(z)}\right]^2 + i\left(\frac{\bar{x}\,\bar{\alpha}}{\bar{\alpha}(z)}\left(\frac{L}{2}\right)\sqrt{a-b}\right)^2\right\} \qquad \text{(B-2d)}$$

$$\tan\theta = -(a-b)\left(\frac{L}{2}\right)^2 \bar{\alpha}^2 . \qquad \text{(B-2e)}$$

Turning to the other integral, let us define A and B as

$$A = (a - b)\left(\frac{L}{2}\right)^2 \qquad \text{(B-3a)}$$

$$B = 2a\left(\frac{L}{2}\right)^2 \bar{y} \quad . \qquad \text{(B-3b)}$$

Then we can transform I_y into

$$I_y(\bar{y}) = e^{i\frac{B^2}{4A}} \int_{\sqrt{\frac{2}{\pi}}\left(-\sqrt{A} - \frac{B}{2\sqrt{A}}\right)}^{\sqrt{\frac{2}{\pi}}\left(\sqrt{A} - \frac{B}{2\sqrt{A}}\right)} \frac{du}{\sqrt{A}} \sqrt{\frac{\pi}{2}}\, e^{-i\frac{\pi}{2}u^2} \quad .$$

Assume that a-b > 0 (z < F) so $\sqrt{A}$ is real. This becomes

$$I_y(\bar{y}) = e^{i\frac{B^2}{4A}} \sqrt{\frac{\pi}{2A}} \left\{ \int_{-\sqrt{\frac{2}{\pi}}\left(\sqrt{A} + \frac{B}{2\sqrt{A}}\right)}^{0} du\, e^{-i\frac{\pi}{2}u^2} + \int_{0}^{\sqrt{\frac{2}{\pi}}\left(\sqrt{A} - \frac{B}{2\sqrt{A}}\right)} du\, e^{-i\frac{\pi}{2}u^2} \right\}$$

$$= \sqrt{\frac{\pi}{2A}}\, e^{i\frac{B^2}{4A}} \left\{ C\left[\sqrt{\frac{2A}{\pi}}\left(1 - \frac{B}{2A}\right)\right] + C\left[\sqrt{\frac{2A}{\pi}}\left(1 + \frac{B}{2A}\right)\right] - i\left(S\left[\sqrt{\frac{2A}{\pi}}\left(1 - \frac{B}{2A}\right)\right] + S\left[\sqrt{\frac{2A}{\pi}}\left(1 + \frac{B}{2A}\right)\right]\right) \right\} \quad .$$

(B-4)

Thus, Eqs. (B-2), (B-3), and (B-4) give the complete diffracted field.

Recognizing that

$$A = \pi \frac{(L/2)^2}{\lambda z}\left(1 - \frac{z}{F}\right) = \pi N_F$$

and that

$$B = 2a\left(\frac{L}{2}\right)^2 \bar{y} = 2\pi N_F^{\,o} \bar{y} \quad ,$$

we can write the resulting intensity pattern as

$$I(\bar{x},\bar{y},z) = I_0\left(\frac{N_F^{\,o}}{2N_F}\right)\left(\frac{\bar{\alpha}}{\bar{\alpha}(z)}\right) e^{-2\left(\frac{\bar{x}}{\bar{\alpha}(z)}\right)^2} \cdot \left\{\left[C(\xi_+) + C(\xi_-)\right]^2 + \left[S(\xi_+) + S(\xi_-)\right]^2\right\} \qquad \text{(B-5)}$$

$$N_F^{\,o} = \frac{(L/2)^2}{\lambda z}$$

$$N_F = \frac{(L/2)^2}{\lambda z}\left(1 - \frac{z}{F}\right)$$

$$\bar{\alpha} = \sqrt{2}\,\frac{w_x}{(L/2)}$$

$$\bar{\alpha}(z) = \bar{\alpha}\sqrt{\left(1 - \frac{z}{F}\right)^2 + \frac{1}{\left(\pi N_F^{\,o}\bar{\alpha}^2\right)^2}}$$

$$\xi_+ = \sqrt{2N_F}\left(1 + \frac{N_F^{\,o}}{N_F}\bar{y}\right)$$

$$\xi_- = \sqrt{2N_F}\left(1 - \frac{N_F^{\,o}}{N_F}\bar{y}\right)$$

$$\bar{x}(\bar{y}) = \frac{x}{L/2}\left(\frac{y}{L/2}\right) \quad .$$

For an initially plane wave, $F \to +\infty$, $N_F \to N_F^{\,o}$ and $\xi_{\pm} \to \sqrt{2N_F^{\,o}}\,(1 \pm \bar{y})$, and the intensity pattern goes to

$$I_{F\to\infty}(\bar{x},\bar{y},z) = I_0\,\frac{1}{2}\left(\frac{\bar{x}}{\bar{\alpha}(z)}\right) \cdot e^{-2\left(\frac{\bar{x}}{\bar{\alpha}(z)}\right)^2}\left\{\left[C(\xi_+^{\,o})+C(\xi_-^{\,o})\right]^2 + \left[S(\xi_+^{\,o})+S(\xi_-^{\,o})\right]^2\right\} \qquad \text{(B-6a)}$$

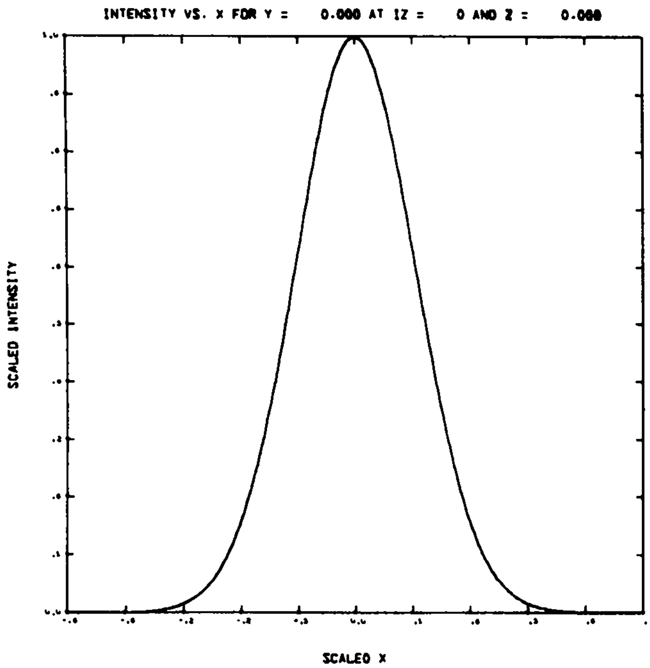
$$\xi^{o}_{\pm} = \sqrt{2N_F^{\,o}}\left(1 \pm \bar{y}\right) \quad . \qquad \text{(B-6b)}$$

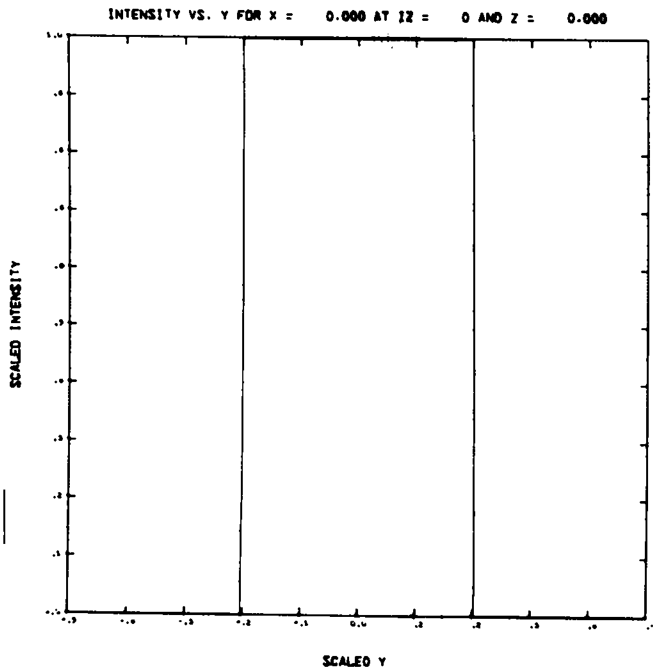
One can verify that this reduces to Eq. (83) (with $N_F \to N_F^o$) as $\bar{x},\bar{y} \to 0$. Finally, the intensity in the $\bar{x} = 0$ plane is, for an initial plane wave,

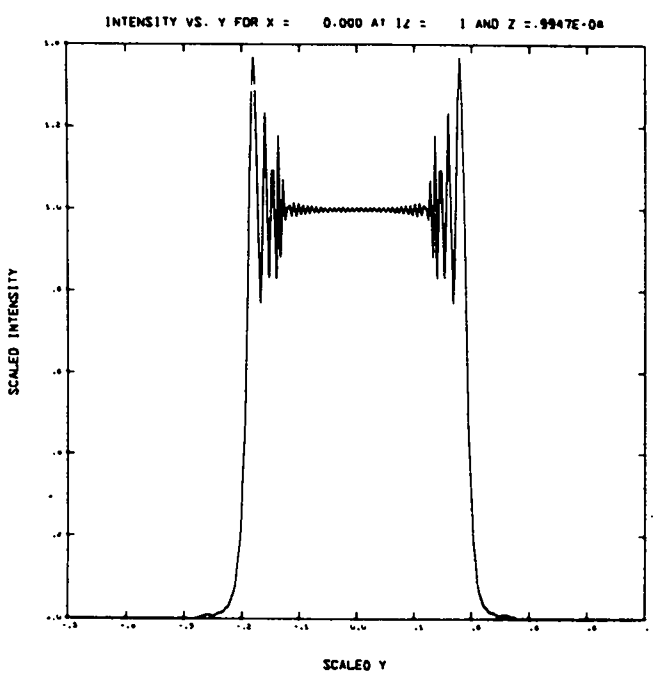
$$I_{F\to\infty}(\bar{x} = 0, \bar{y}; z) = \frac{I_0}{2} \frac{\pi N_F^o \bar{\alpha}^2}{\sqrt{1 + \left(\pi N_F^o \bar{\alpha}^2\right)^2}} \cdot \left\{ \left[C(\xi_+^o) + C(\xi_-^o)\right]^2 + \left[S(\xi_+^o) + S(\xi_-^o)\right]^2 \right\} . \tag{B-7}$$

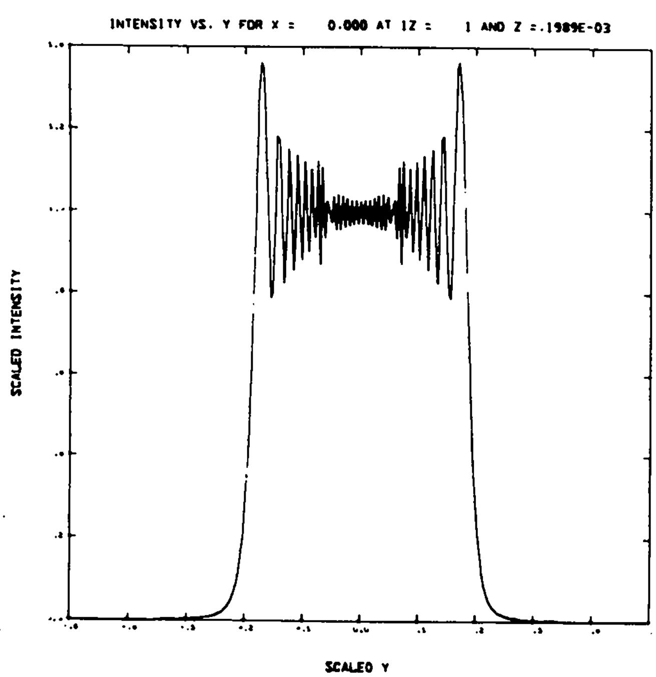
The following figures represent plane sections of the two-dimensional intensity distributions of Eq. (B-6) calculated using TAP2. Since the intensity in the y=0 plane is always Gaussian, it is shown only for the initial (z=0) distribution. The Fresnel number N_F^o (used in Tables I and II) corresponding to the indicated scaled longitudinal distance z from the aperture plane is given below.

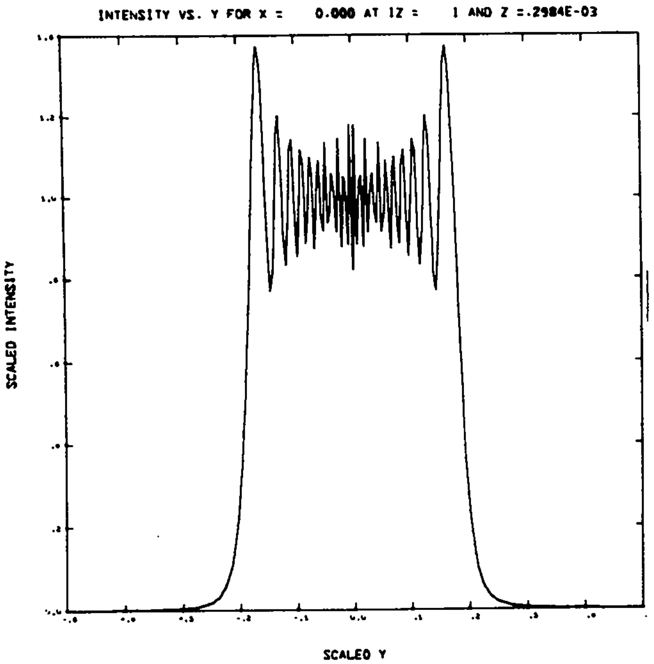
z	N_F^o
0.00	∞
0.9947E-04	64
0.1989E-03	32
0.2984E-03	21 1/3
0.3979E-03	16
0.4974E-03	12.8
0.5968E-03	10 2/3
0.6963E-03	9.1438
0.7958E-03	8
0.8952E-03	7.111
0.9947E-03	64

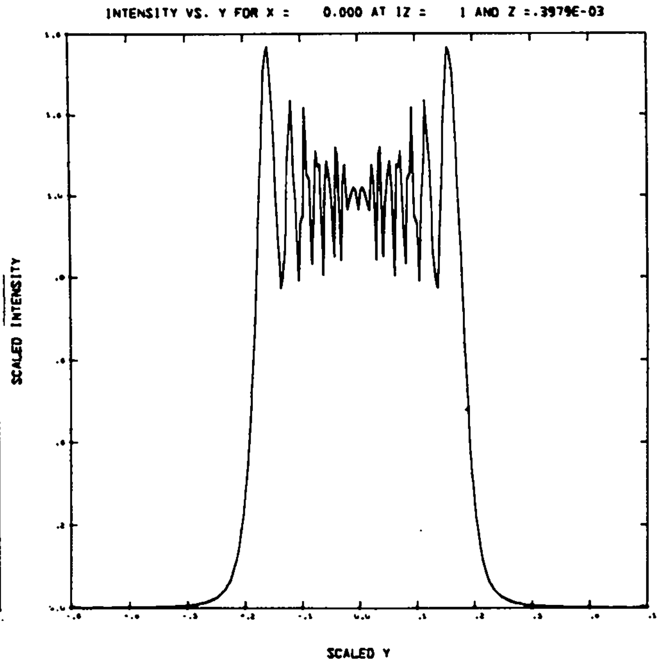

INTENSITY VS. X FOR Y = 0.000 AT IZ = 0 AND Z = 0.000
SCALED INTENSITY
SCALED X

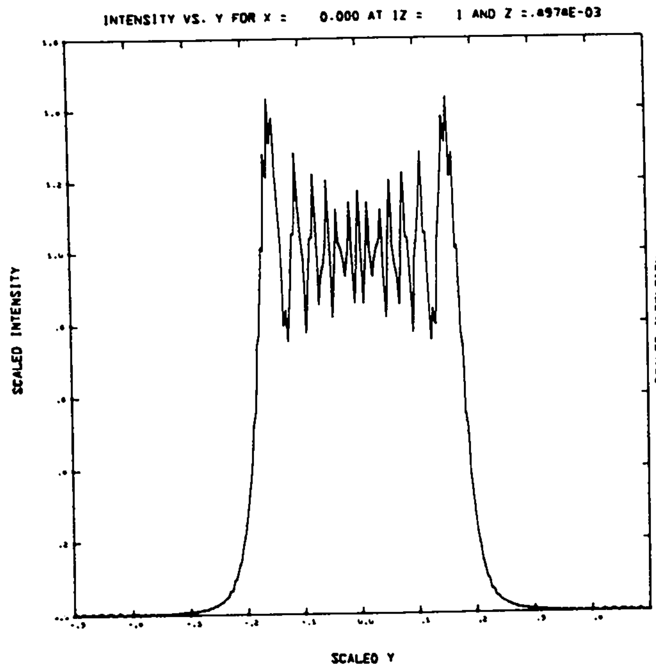

INTENSITY VS. Y FOR X = 0.000 AT IZ = 0 AND Z = 0.000
SCALED INTENSITY
SCALED Y

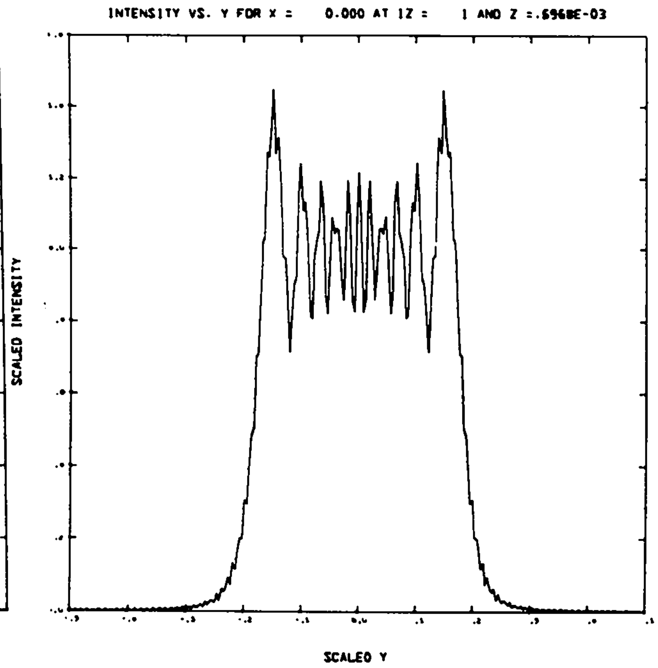

INTENSITY VS. Y FOR X = 0.000 AT IZ = 1 AND Z =.9947E-04
SCALED INTENSITY
SCALED Y

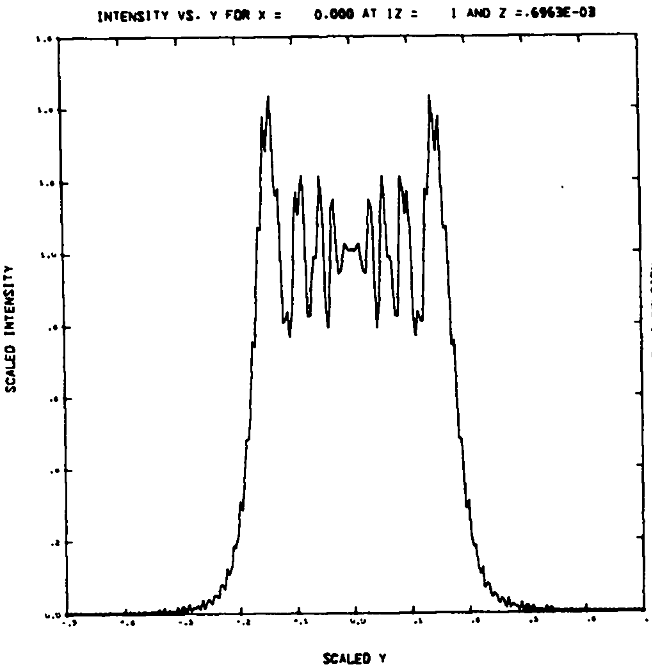

INTENSITY VS. Y FOR X = 0.000 AT IZ = 1 AND Z =.1989E-03
SCALED INTENSITY
SCALED Y


INTENSITY VS. Y FOR X = 0.000 AT IZ = 1 AND Z =.2984E-03
SCALED INTENSITY
SCALED Y

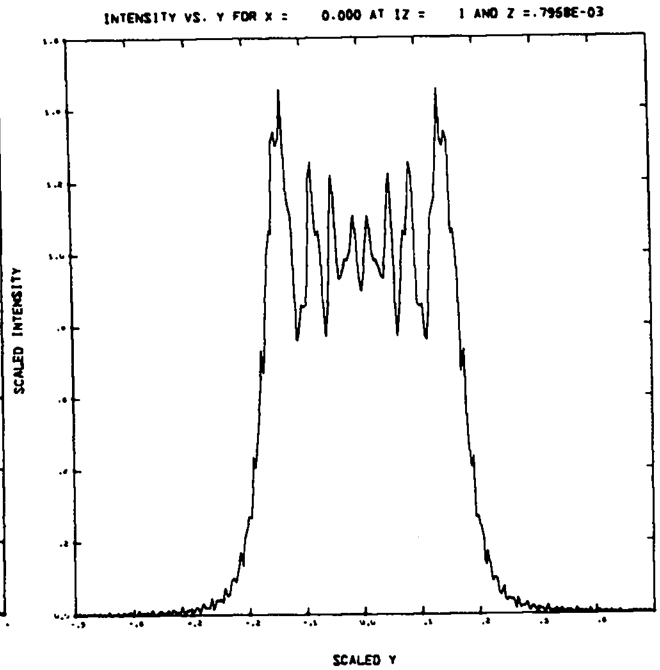

INTENSITY VS. Y FOR X = 0.000 AT IZ = 1 AND Z =.3979E-03
SCALED INTENSITY
SCALED Y


INTENSITY VS. Y FOR X = 0.000 AT IZ = 1 AND Z =.4974E-03
SCALED INTENSITY
SCALED Y

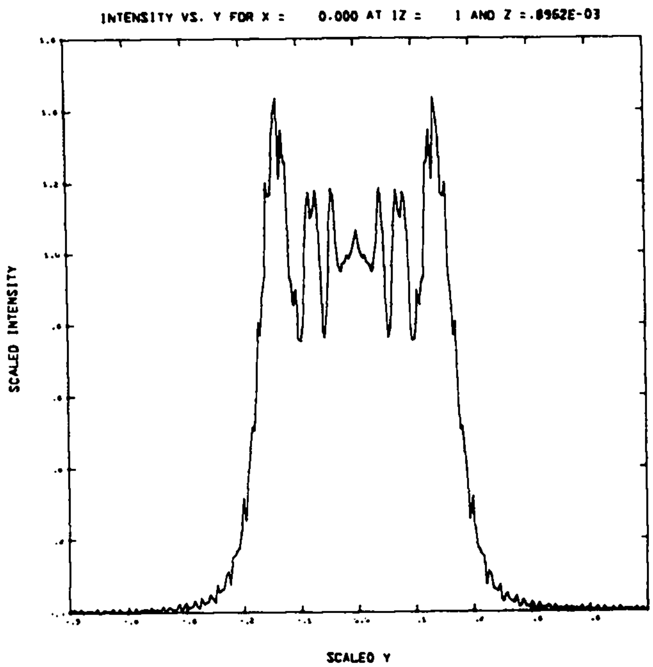

INTENSITY VS. Y FOR X = 0.000 AT IZ = 1 AND Z =.5968E-03
SCALED INTENSITY
SCALED Y



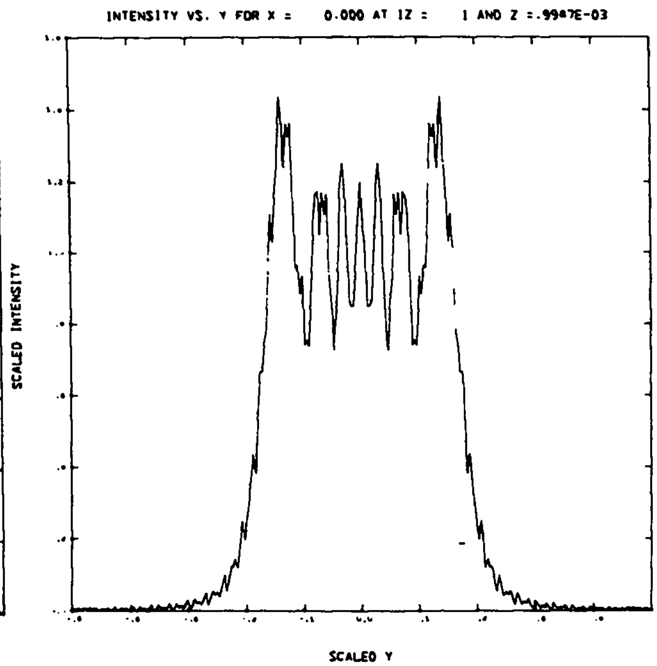
INTENSITY VS. Y FOR X = 0.000 AT IZ = 1 AND Z =.6963E-03
SCALED INTENSITY
SCALED Y



INTENSITY VS. Y FOR X = 0.000 AT IZ = 1 AND Z =.7958E-03
SCALED INTENSITY
SCALED Y



INTENSITY VS. Y FOR X = 0.000 AT IZ = 1 AND Z =.8952E-03
SCALED INTENSITY
SCALED Y



SCALED INTENSITY
SCALED Y